

Default Methodology for Analysis of Airborne
Exposure to Mixtures of Chemicals in Emergencies:

The User's Guide for the Chemical Mixture Methodology

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Compatible with PAC Revision 27

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FOREWORD

This document provides a user's guide for the Chemical Mixture Methodology (CMM) Workbook. It presents an introduction to the CMM, a description of the CMM Workbook and each of its worksheets, and instructions on how to use the CMM Workbook.

The CMM provides recommended default emergency exposure guidelines for mixtures of chemicals. The CMM makes extensive use of Health Code Numbers (HCNs) to examine the additive impact that each chemical component in a chemical mixture may have on specific target organs. The CMM is a more realistic predictor of potential human health impacts than can be obtained using the (1) nonconservative method of separately analyzing the consequences of each chemical component or the (2) overly conservative method of adding the exposures from each chemical together, regardless of the human organ targeted by the chemical.

The CMM is designed to support U.S. Department of Energy emergency planning hazards assessments (EPHAs), safety analyses, and assessments during emergency response situations. Development of the CMM and the preparation of this user's guide were sponsored by the U.S. Department of Energy Office of Emergency Management and Policy.

ACRONYMS AND ABBREVIATIONS

AEGL	Acute Exposure Guideline Level
AIHA	American Industrial Hygiene Association
CASRN	Chemical Abstracts Service Registry Number
CFR	Code of Federal Regulations
C_i	airborne concentration of chemical "i"
CMM	Chemical Mixture Methodology
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
EPHA	Emergency Planning Hazards Assessment
ERPG	Emergency Response Planning Guideline
HCN	Health Code Number
HI	Hazard Index
L_i	Concentration limit for chemical "i"
NA-41	DOE Office of Emergency Management and Policy
PAC	Protective Action Criteria
PEL	Permissible Exposure Limit
SCAPA	Subcommittee on Consequence Assessment and Protective Actions
TEEL	Temporary Emergency Exposure Limits
TWA	Time-Weighted Average

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SECTION 1. INTRODUCTION

The Chemical Mixture Methodology (CMM) Workbook is set up to automatically apply the U.S. Department of Energy (DOE) Subcommittee on Consequence Assessment and Protective Actions (SCAPA) recommended default methodology for a user-supplied mixture of chemicals. This methodology was originally published in *Applied Occupational and Environmental Hygiene* (Craig et al., 1999) and an updated description is provided in the *Journal of Applied Toxicology* (Yu et al., 2010). Both research articles are available at <http://orise.orau.gov/emi/scapa/chem-mixture-methodology/background.htm>.

The CMM provides recommended default emergency exposure guidelines for exposure to airborne mixtures of chemicals. Developed and maintained under the sponsorship of the DOE's Office of Emergency Management and Policy (NA-41), the CMM is recommended for use in Emergency Planning Hazards Assessments (EPHAs) (see [DOE O 151.1C](#), DOE, 2005), Documented Safety Analyses (see [10 CFR 830](#), DOE, 2001), and for consequence assessments supporting emergency response exercises or actual accident situations.

The CMM assesses mixtures of potentially hazardous chemicals that are separable into their component elements or compounds by pure physical processes. The individual chemicals may have been stored as a mixture prior to the event that initiated their atmospheric release, or they may have been stored separately and only mixed after their release to the atmosphere. The CMM does not account for any chemical reactions that may occur in the atmosphere as the mixture is transported away from its source. One of the assumptions of the CMM is that the health impacts from exposure to each chemical in mixture are additive – potential synergistic and antagonistic effects that might depart from this simple additive assumption are not considered¹ (Craig et al., 1999).

The first step performed by the CMM is to calculate the **hazard index (HI)** for each chemical species (i) at a receptor location, as shown in Eqn. 1:

$$HI_i = C_i / L_i \quad \text{Eqn. 1}$$

where C_i is the concentration of chemical "i" at the receptor and L_i is the selected concentration limit.

The DOE recommends using **Protective Action Criteria (PAC)** values as concentration limits, either [PAC-1, -2, or -3](#) for chemical "i" (i.e., $L_i = PAC_i$). The PAC values have been developed to assist in emergency planning of chemical release events and are

¹ The CMM does not consider reactions between the chemicals in the mixture that in some cases could generate new chemicals, alter the chemical mixture, or change the mixture's dispersion properties. This level of complexity is beyond the current scope of the CMM.

composed of Acute Exposure Guideline Levels (AEGLs) (Rusch et al., 2000; Rusch et al., 2002), Emergency Response Planning Guidelines (ERPGs) (Rusch, 1993), and Temporary Emergency Exposure Limits (TEELs) (Craig et al., 1995, Craig et al., 2000).² The PAC-1 limit is the lowest concentration associated with mild, transient health effects. The PAC-2 limit is the lowest concentration associated with irreversible or other serious health effects that could impair the ability to take protective action. The PAC-3 limit is the lowest concentration associated with life-threatening health effects. The PAC values are presented in a searchable database and as lists of tables and spreadsheets (see <http://www.atlant.com/DOE/teels/teel.html>).

If $HI_i \leq 1.0$, the concentration of a chemical “i” does not exceed its concentration limit. If PAC-2 is being used as the concentration limit, exposed individuals should not experience any health effect that would impair their ability to take effective protective actions. However, if $HI_i > 1.0$, the chemical concentration would exceed the PAC-2 concentration limit, and the exposed individual may experience health effects that could impair their ability to take effective protective actions.

For a chemical mixture, the HI_i for each chemical at a receptor point of interest can be summed, as in Eqn. 2:

$$\sum_{i=1}^n HI_i = HI_1 + HI_2 + \dots + HI_n \quad \text{Eqn. 2}$$

This cumulative HI is a “simple sum of the HIs” for all the chemicals in the mixture and this provides an initial indication of the potential health effects associated with exposure to the chemical mixture. However, this simple approach may provide an overly conservative estimate of health effects when the chemicals in the mixture impact different target organ systems.

To illustrate this, consider two chemical mixtures, each containing just two chemicals. In this example, the HI is calculated for each chemical in the two mixtures based on the airborne concentration of the chemical at the receptor point of interest and the PAC-2 concentration limit for the chemical. In the first mixture, assume both chemicals are acute respiratory toxins and an HI of 0.6 is calculated for each chemical. Summing the HIs for both chemicals in the mixture gives a cumulative HI of 1.2; this indicates that there is the potential for exposed individuals to suffer acute health effects that may impact their ability to take effective protection actions.

² The AEGLs are developed by the U.S. Environmental Protection Agency (EPA) National Advisory Committee and the National Research Council AEGL Subcommittee; ERPGs are produced by the American Industrial Hygiene Association (AIHA) Emergency Response Planning Committee; and TEELs are developed by DOE.

In the second mixture, assume the chemicals affect different target organ systems (i.e., there is no overlap in the target organs affected). Both chemicals have an HI of 0.6, but one chemical is an acute respiratory irritant and the other is an acute bladder toxin. Simply summing the HIs for these two chemicals will give the same cumulative HI of 1.2 as obtained for the first mixture.

Although these two mixtures generate the same cumulative HI values, the ability of exposed individuals to take effective protection actions should be considerably different for these two mixtures. For the first mixture, both chemicals have an accumulated effect on the respiratory system that could diminish the ability of some exposed individuals to take timely protective actions. For the second mixture, both the respiratory system and bladder are affected by exposure to the chemical, but neither organ system is challenged to the extent that an exposed individual's ability to take timely protective actions should be impaired. Exposure to the second mixture would likely be less deleterious to an individual's ability to protect oneself than exposure to the first mixture. However, the simple summing of the HIs to form a cumulative HI for the mixture does not make this distinction.

An alternative to the simple summing of the HIs, and one that would distinguish between the two mixtures in the above example, is the **Health Code Number (HCN)** approach that is incorporated into the CMM. HCNs are similar to medical diagnostic codes in that they are code numbers that identify specific adverse health effects (e.g., acute respiratory toxins, acute skin irritation, chronic liver toxins, carcinogens). Currently, over 60 different HCNs are available for characterizing the potential health effects associated with exposure to a chemical (see **Table 1**). This includes separate HCNs for acute and chronic health effects. Acute effects are the most life-limiting factors in an emergency event. A threshold of seven days was chosen to align with the nature of chemical emergency events, because some could go for a few days but seldom beyond a week. In addition, the shorter duration for acute exposures indicated in Sax's Dangerous Properties of Industrial Materials (Lewis, 2004), lack of sub-acute HCNs, and the indication time (sometimes months) for chronic exposures led to this definition (Lewis, RA, 1998; Lewis, RJ, 2004; NIOSH, 2008). Acute and chronic health effects to the same target organ set are not considered additive because these impacts occur over different time scales.

For each chemical in the CMM data set, HCNs can be assigned. If more than ten HCNs are identified, the top ten highest ranking HCNs in terms of potential adverse health effects are used. **Table 2** provides the priority ranking list for HCNs based on an internal HCN development procedure written by Rocky Petrocchi.

Table 1. HCN Listing. The names of acute HCNs are displayed using a red font and chronic HCNs are displayed using a blue font.

HCN	HCN Name/Description	HCN	HCN Name/Description
1.00	OSHA carcinogen (29 CFR 1910.1000) — chronic effect	4.09	Kidney—acute effects
1.01	Bladder carcinogen — chronic effect	4.10	Liver—acute effects
1.02	Liver carcinogen — chronic effect	4.11	Skin—acute effects other than irritation
2.00	Suspect carcinogen or mutagen — chronic effect	4.12	Skin perforation—acute effects other than skin absorption
2.01	Kidney carcinogen — chronic effect	4.13	Bone—acute effects
2.02	Liver carcinogen — chronic effect	5.00	Reproductive toxin—acute effects
3.00	Systemic toxin—chronic effects	5.10	Reproductive toxin—chronic effects
3.01	Bladder—chronic effects	6.00	Cholinesterase toxin—acute effect
3.02	Hematological effects—chronic, unspecified	7.00	Nervous system toxin—acute effects
3.03	Bone—chronic effects	7.01	Central nervous system—acute effects
3.04	Bone marrow—chronic blood-forming system and other chronic effects	7.10	Nervous system toxin—chronic effects
3.05	Brain—chronic effects	7.11	Central nervous system—chronic effects
3.06	Eye—chronic ocular effects	8.00	Narcotic — acute effect
3.07	Gastrointestinal tract—chronic effects	9.00	Respiratory sensitizer — chronic effect
3.08	Heart, Cardiovascular system—chronic effects	10.00	Respiratory toxin — chronic effects
3.09	Kidney—chronic effects	11.00	Respiratory toxin — acute effects other than irritation
3.10	Liver—chronic effects	11.01	Respiratory irritant — acute severe or moderate but not mild irritant effects
3.11	Skin—chronic effects including dermatitis and sensitization	12.00	Blood toxin, anemia — chronic effect
3.12	Skin perforation—nasal septum perforation and other chronic effects other than skin absorption	13.00	Blood toxin, methemoglobinemia — acute effect
4.00	Systemic toxin—acute short-term high hazard effects	14.00	Severe irritant
4.01	Eye—acute, other than irritation	14.01	Eye irritant— severe
4.02	Nose—acute effects other than irritation	14.02	Skin irritant — severe
4.03	Bladder—acute effects	15.00	Moderate irritant
4.04	Bone marrow—acute blood-forming system and other acute effects	15.01	Eye irritant — moderate
4.05	Brain—acute effects	15.02	Skin irritant — moderate
4.06	Hematological effects—acute, unspecified	16.00	Mild irritant
4.07	Gastrointestinal tract—acute effects	16.01	Eye irritant — mild
4.08	Heart, Cardiovascular system—acute effects	16.02	Skin irritant — mild
		17.00	Asphyxiants, anoxiants — acute effect
		18.00	Explosive, flammable safety (no adverse effects with good housekeeping)
		19.00	Generally low risk health effects—nuisance particles, vapors or gases
		20.00	Generally low risk health effects—odor

Table 2. HCN's Listing by Health Effect Ranking. The names of acute HCNs are displayed using a red font and chronic HCNs are displayed using a blue font.

Rank	HCN	HCN Name/Descriptions	Rank	HCN	HCN Name/Descriptions
1	17.00	Asphyxiants, anoxiants — acute effect	31	1.02	Liver carcinogen — chronic effect
2	18.00	Explosive, flammable safety (no adverse effects with good housekeeping)	32	2.00	Suspect carcinogen or mutagen — chronic effect
3	13.00	Blood toxin, methemoglobinemia — acute effect	33	2.01	Kidney carcinogen — chronic effect
4	6.00	Cholinesterase toxin—acute effect	34	2.02	Liver carcinogen — chronic effect
5	14.01	Eye irritant— severe	35	3.05	Brain—chronic effects
6	14.00	Severe irritant	36	7.11	Central nervous system—chronic effects
7	15.01	Eye irritant — moderate	37	7.10	Nervous system toxin—chronic effects
8	15.00	Moderate irritant	38	10.00	Respiratory toxin — chronic effects
9	4.01	Eye—acute, other than irritation	39	9.00	Respiratory sensitizer — chronic effect
10	11.01	Respiratory irritant — acute severe or moderate but not mild irritant effects	40	3.09	Kidney—chronic effects
11	14.02	Skin irritant — severe	41	3.02	Hematological effects—chronic, unspecified
12	15.02	Skin irritant — moderate	42	3.04	Bone marrow—chronic blood-forming system and other chronic effects
13	4.00	Systemic toxin—acute short-term high hazard effects	43	3.10	Liver—chronic effects
14	4.08	Heart, Cardiovascular system— acute effects	44	3.07	Gastrointestinal tract—chronic effects
15	4.05	Brain—acute effects	45	3.01	Bladder—chronic effects
16	7.01	Central nervous system—acute effects	46	3.03	Bone—chronic effects
17	8.00	Narcotic — acute effect	47	3.06	Eye—chronic ocular effects
18	7.00	Nervous system toxin—acute effects	48	12.00	Blood toxin, anemia — chronic effect
19	11.00	Respiratory toxin — acute effects other than irritation	49	5.00	Reproductive toxin—acute effects
20	4.02	Nose—acute effects other than irritation	50	5.10	Reproductive toxin—chronic effects
21	4.09	Kidney—acute effects	51	4.11	Skin—acute effects other than irritation
22	4.06	Hematological effects—acute, unspecified	52	3.11	Skin—chronic effects including dermatitis and sensitization
23	4.04	Bone marrow—acute blood-forming system and other acute effects	53	4.12	Skin perforation—acute effects other than skin absorption
24	4.10	Liver—acute effects	54	3.12	Skin perforation—nasal septum perforation and other chronic effects other than skin absorption
25	4.07	Gastrointestinal tract—acute effects	55	3.00	Systemic toxin—chronic effects
26	4.03	Bladder—acute effects	56	16.01	Eye irritant — mild
27	4.13	Bone—acute effects	57	16.00	Mild irritant
28	3.08	Heart, Cardiovascular system— chronic effects	58	16.02	Skin irritant — mild
29	1.00	OSHA carcinogen (29 CFR 1910.1000) — chronic effect	59	19.00	Generally low risk health effects— nuisance particles, vapors or gases
30	1.01	Bladder carcinogen — chronic effect	60	20.00	Generally low risk health effects—odor

The HCN-based approach in the CMM assumes that the HIs from different chemicals are additive only if the chemicals have HCNs that have the same **target organ effects** or **modes of action**³. The target organ effect refers to the toxic effects on a specific organ or tissue (e.g., brain, blood, kidney, liver, heart). The mode of action is based on the major HCN categories. In some cases it is linked to an acute or chronic biological mechanism (e.g., asphyxiation, carcinogenic effects).

If warranted by initial screening results, the next step in the method involves using the toxicity classification provided by the HCNs. The CMM assumes that different target organ groups do not interact with each other to any significant degree. Therefore, exposures can be separated, and same or similar toxicity can be added within these target organ bins. This is illustrated in Eqn. 3.

$$\sum_{i=1}^n HI_{i(p)} = HI_{1(p)} + HI_{2(p)} + \dots + HI_{n(p)} \quad \text{Eqn. 3}$$

Note: “*p*” represents a specific target organ or mode of action.

Eqn. 3 is applied separately to acute and chronic effects because of the different time scales. The overall cumulative HCN-based HI for the chemical mixture is the greatest cumulative HI calculated for any of the target organ effects or modes of action. Because the HCN-based approach focuses on health effects involving specific modes of action and target organ effects, it has the potential to produce cumulative HI values for a chemical mixture that are less than the value obtained by simply summing all the HIs.

It should be noted that several radioactive chemicals are provided in the CMM data set. These chemicals are included only when their chemical toxicity is significant compared to their radiological health effects. Currently, this is limited to the following low-specific-activity radioactive isotopes:

- “Uranium of low enrichment in the form of compounds that are relatively soluble in body fluids (e.g., carbonates, nitrates, fluorides, sulfates). Depending on the exact proportions of the different uranium isotopes, the chemical toxicity concern becomes dominant as the nominal enrichment (²³⁵U weight percent) decreases through the range from about 16% to 5%” (DOE-HDBK-1046-2008, 2008).
- Thorium and some of its compounds.

³ Also called **modes of toxicity**

SECTION 2. THE CMM WORKBOOK

Two versions of the Microsoft Excel-based CMM Workbook are offered to meet user needs. The first version of the CMM Workbook is intended for most users and allows a maximum of 15 chemicals in a mixture. It is downloadable from the CMM webpage at <http://orise.orau.gov/emi/scapa/hcn.htm>. The second version allows a maximum of 30 chemicals in a mixture. A disadvantage in using the 30-chemical version is that in half of the workbook's worksheets, the additional rows reserved to display information for the extra set of 15 chemicals will drop the presentation of a key row of summary information out of the default display window (the user will need to manually scroll down to view this summary information). The 30-chemical version of the CMM Workbook can be obtained by sending an email request to the CMM development team at cmmdevelopment@listserv.orau.gov. Except for the minor differences associated with doubling the maximum number of chemicals permitted in a mixture, both versions of the CMM Workbook are identical.

The CMM workbook employs six worksheets:

1. *Input*
2. *Import*
3. *HIs by mode*
4. *HIs by target organ*
5. *Output*
6. *HCN-PAC*.

To use the CMM Workbook, the user enters information on a mixture of chemicals into the *Input* worksheet. This information includes the name of each chemical in the mixture, an identification number for each chemical, the specific PAC of concern, and the concentration of each chemical at a user-selected receptor location common to all chemicals in the mixture.

The *Input* worksheet has room for the entry of a maximum of either 15 or 30 chemicals in a given mixture, depending on the version of the CMM workbook that is being used.

To provide the user with ready access to the chemical-specific information required to complete the *Input* worksheet, reference information for each chemical is included in the *HCN-PAC* worksheet. This information includes the name of each chemical and its Chemical Abstracts Service Registry Number (CASRN), HCN values, and PAC values.

Figure 1 provides an overview of the steps followed to use the CMM Workbook.

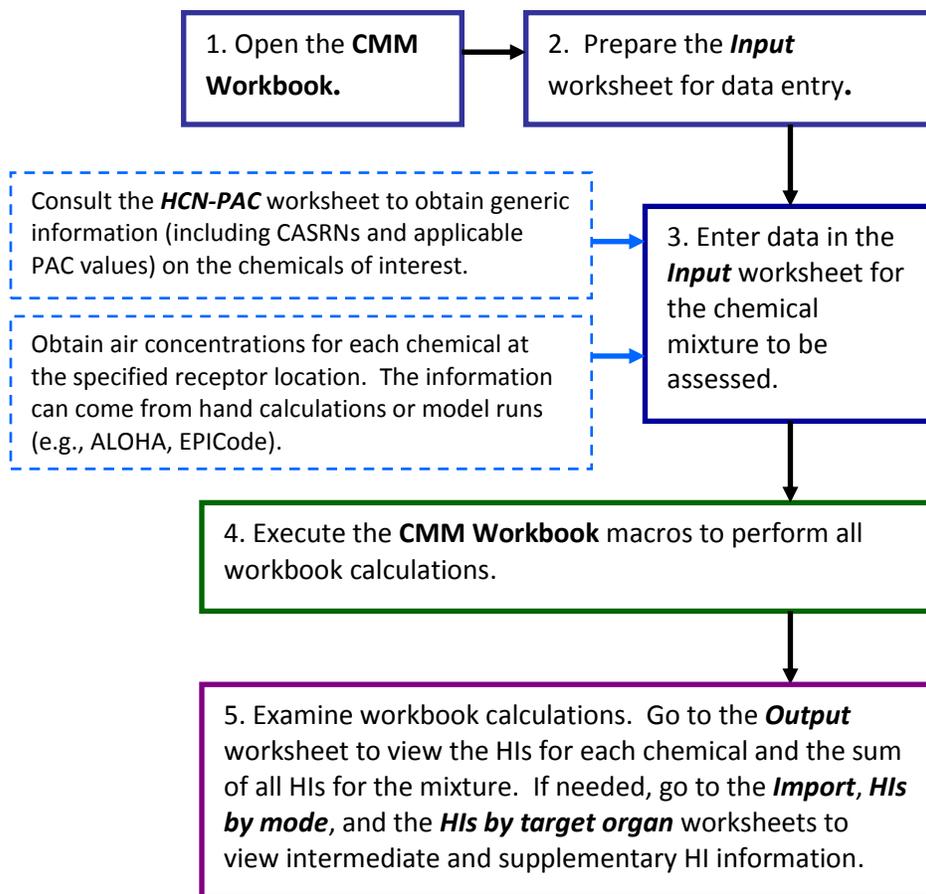


Figure 1. How to Use the CMM Workbook.

Information on the chemical concentrations at the user-specified receptor location, as required in the *Input* worksheet, must be provided by the user. This information typically is obtained from hand calculations or atmospheric dispersion modeling results (e.g., EPICode,⁴ ALOHA⁵).

⁴ EPICode is a software tool designed to aid emergency response personnel, emergency planners, and health and safety professionals in evaluating the atmospheric release of toxic substances. For information on EPICode, see <http://www.epicode.com/>.

⁵ ALOHA is an atmospheric dispersion model used for evaluating releases of hazardous chemical vapors. It is part of the CAMEO suite of tools. CAMEO is used to plan for and respond to chemical emergencies. For information on ALOHA, see <http://www.epa.gov/emergencies/content/cameo/what.htm>.

The CMM Workbook is designed to execute calculations automatically once data are entered or removed from the *Input* worksheet. However, in some cases it may be necessary to manually start the calculations. The user can click on the "Calculate" button to manually run the analysis. Alternatively, the option exists to execute the CMM worksheet calculations on a personal computer by simultaneously pressing **Ctrl** and = on the keyboard or simply pressing the **F9** key. On an Apple computer, simultaneously pressing **Apple** or **Command** and = on the keyboard does the same thing.

After the calculations are executed, HI information for each chemical in the input mixture and the sum of all HIs for the entire mixture will be provided in the *Output* worksheet. In addition, intermediate and supplementary information are provided in three other worksheets: *Import*, *HIs by mode*, and *HIs by target organ*.

Note that only the *Input* worksheet is used to enter information. The *HCN-PAC* worksheet can also be modified by the user (e.g., to add new chemicals or updated HCN or user defined concentration limit values), but the other four worksheets are password-protected to maintain the integrity of the CMM software.

SECTION 3. USING THE CMM WORKBOOK

In this section, the steps that are followed when using the Microsoft Excel-based CMM Workbook are presented. A number of different versions of Microsoft Excel are currently in common use, including Excel 2010, 2007, and 2003. Basic instructions and the figures presented in this section are tailored to the Office 2010 version of Excel. Where different procedures need to be followed for Excel 2007, additional instructions are also provided.

Step 1. Open the Workbook.

When opening the CMM Workbook, macros must be enabled. The CMM Workbook uses macros to perform all of its data lookups and calculations. To guard against macros that may have a malicious function, Excel 2010 offers its users four levels of security (Very High, High, Medium, and Low) for workbooks that use macros. If your version of Excel 2010 has its macro security level set to Very High or High, your computer likely will block execution of the CMM Workbook macros. To enable the macros in the CMM Workbook, the Excel security level should be set no higher than Medium as in earlier versions of Microsoft Excel. If set security level is set at a higher level, a Security Warning banner will appear (see Figure 2) and the user will have the option to enable the macros. In Microsoft Excel 2010, this is done by clicking on “**Enable Content**” button on the displayed security warning banner.

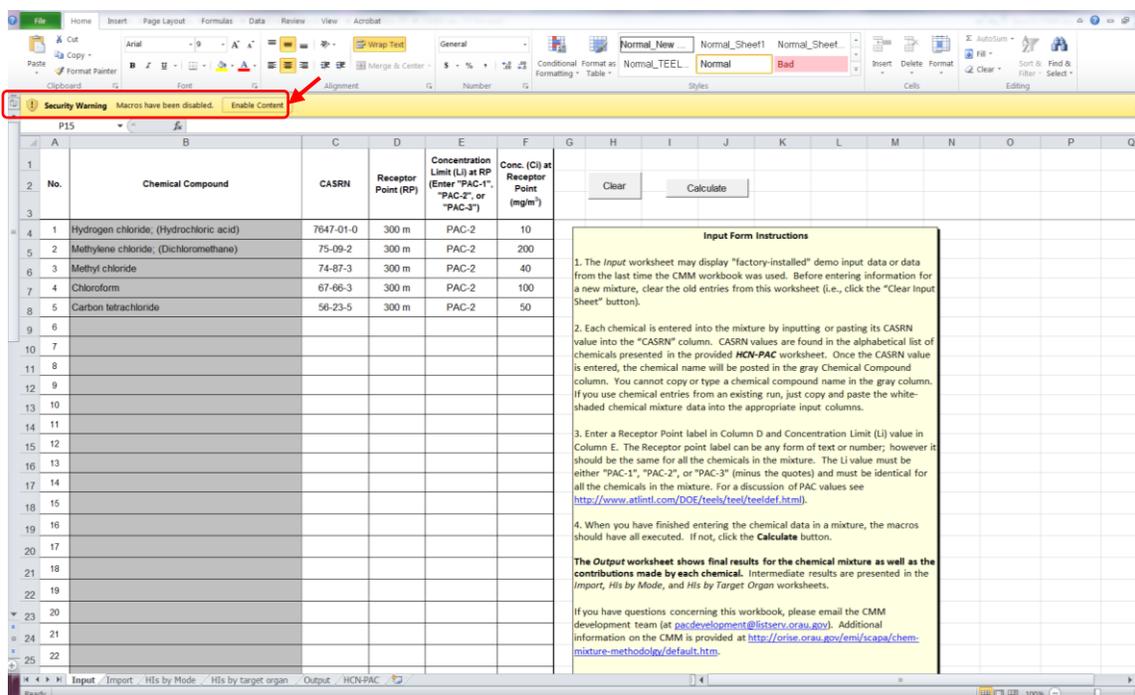


Figure 2. Setting the Security Level for Macros. Shown for Microsoft Excel 2010.

For users running Excel 2007, the macro security settings can be changed in the Trust Center to enable the workbook's macros to run. *Note: in some organizations, only a*

system administrator may be empowered to make these changes. To access the Trust

Center, click the **Microsoft Office Button**  and then click **Excel Options**. Next, click the **Trust Center** option on the left side of the pop-up Excel Options window, then click the **Trust Center Settings** button on the right side of the window to open the Trust Center window. Click the **Macro Settings** category on the left side of the **Trust Center** window, select either the **Disable all macros with notification** or **Enable all macros** option, then click the **OK** button on both the **Trust Center** and **Excel Options** windows to lock-in this change.

If **Disable all macros with notification** is enabled, a Security Warning ribbon will be displayed above the worksheet each time the CMM Workbook is opened. Click the **Options** button on this ribbon. In the **Security Options** pop-up window (with a heading of "Security Alert – Macro"), select the **Enable this content** option, then click the **OK** button. The workbook macros will now be operational.

Step 2. Prepare the Input Worksheet for Data Entry.

When the *Input* worksheet is accessed, information for a sample mixture of chemicals is likely to be displayed. This mixture may be the scenario example that came preloaded with the workbook, or it may be input data from the last time the workbook was saved. If editing or adding to the displayed mixture, the current material in the Input worksheet does not need to be cleared. However, the displayed mixture should be cleared from the worksheet before a new chemical mixture is entered. To do so, simply click on the "Clear" button (as shown in Figure 3).

No.	Chemical Compound	CASRN	Receptor Point (RP)	Concentration Limit (Li) at RP (Enter "PAC-1", "PAC-2", or "PAC-3")	Conc. (Ci) at Receptor Point (mg/m ³)
1	Hydrogen chloride; (Hydrochloric acid)	7647-01-0	300 m	PAC-2	10
2	Methylene chloride; (Dichloromethane)	75-09-2	300 m	PAC-2	200
3	Methyl chloride	74-87-3	300 m	PAC-2	40
4	Chloroform	67-66-3	300 m	PAC-2	100
5	Carbon tetrachloride	56-23-5	300 m	PAC-2	50
6	Carbon tetrachloride	56-23-5			
7					
8					
9					
10					
11					
12					
13					
14					
15					

Clear

Calculate

Input Form Instructions

- The *Input* worksheet may display "factory-installed" demo input data or data from the last time the CMM workbook was used. Before entering information for a new mixture, clear the old entries from this worksheet (i.e., click the "Clear Input Sheet" button).
- Each chemical is entered into the mixture by inputting or pasting its CASRN value into the "CASRN" column. CASRN values are found in the alphabetical list of chemicals presented in the provided *HCN-PAC* worksheet. Once the CASRN value is entered, the chemical name will be posted in the gray Chemical Compound column. You cannot copy or type a chemical compound name in the gray column. If you use chemical entries from an existing run, just copy and paste the white-shaded chemical mixture data into the appropriate input columns.
- Enter a Receptor Point label in Column D and Concentration Limit (Li) value in Column E. The Receptor point label can be any form of text or number; however it should be the same for all the chemicals in the mixture. The Li value must be either "PAC-1", "PAC-2", or "PAC-3" (minus the quotes) and must be identical for all the chemicals in the mixture. For a discussion of PAC values see <http://www.atlintl.com/DOE/teels/teel/teeldef.html>.
- When you have finished entering the chemical data in a mixture, the macros should have all executed. If not, click the **Calculate** button.

The Output worksheet shows final results for the chemical mixture as well as the contributions made by each chemical. Intermediate results are presented in the *Import*, *His by Mode*, and *His by Target Organ* worksheets.

If you have more than 15 chemicals in a mixture, please email the CMM development team (at pacdevelopment@listserv.orau.gov) to request a version of the workbook that can accommodate up to 30 chemicals in a mixture. You may use this email address or directly contact a CMM team member with other requests or questions (contact info for the team is provided at <http://orise.orau.gov/emi/scapa/contacts.htm#cmm>).

Figure 3. Clearing Old Data from the *Input* Worksheet in Excel.

If using Excel 2007, on the **Home** tab, in the **Editing** group, click the arrow next to the **Clear** button , then click **Clear Contents**.

Note: As chemical names and other information are entered into the *Input* worksheet, this input is shared and displayed in the other worksheets.

Step 3. Enter Data in the Input Worksheet.

Before entering data in the *Input* worksheet, users should check the *HCN-PAC* worksheet lookup table to ensure that each chemical in the subject mixture is listed in the *HCN-PAC* worksheet. The chemical names, CASRNs, HCNs, and PAC values for all chemicals supported in the workbook are provided in the *HCN-PAC* worksheet. The workbook will not execute any calculations for chemicals not listed in the *HCN-PAC* worksheet.

- 3.1 In the *Input* worksheet, insert in Column C (using the paste function or manually enter using the keyboard) the CASRN of each chemical in the mixture. CASRNs are generally obtained by looking up each chemical in the *HCN-PAC* worksheet and noting or copying the CASRN number listed in Column C for each chemical. In cases where a chemical listed in the *HCN-PAC* worksheet does not have an official CASRN, a substitute or alternative CASRN (e.g., z-0001) has been provided. The workbook will accept this alternative CASRN in the *Input* worksheet. A CMM-accepted CASRN must be entered in the *Input* worksheet for a given chemical for an HI to be calculated for that chemical. Once a CASRN has been entered in the *Input* worksheet, the name of the corresponding chemical will automatically be displayed in Column B.
- 3.2 Enter location information for the receptor point of interest (e.g., “*offsite at 600 m*”, “*onsite at 300 m*”, “*fenceline*”) in Column D. This information is **not** used in workbook calculations but is helpful for quality control and reporting purposes. **All the chemicals in the mixture must use concentration data for the same receptor point of interest.**
- 3.3 Determine the governing concentration limit at the receptor point and enter this information in Column E. The governing concentration limit is the applicable PAC. Acceptable inputs for the concentration limit are “PAC-1”, “PAC-2”, or “PAC-3”. Values can be selected from the drop-down menu that appears when you click on a cell in Column E. Alternatively, the user can manually enter the name of the PAC limit; however, the input must follow the appropriate five-character format; all other formats or options will be rejected. A difference between the CMM Workbook Rev. 27 and previous revisions of the CMM is that “TEEL-0” is no longer accepted as a concentration limit or provided in the *HCN-PAC* worksheet. This is because TEEL-0 values are no longer being published in the PAC data set (effective with the release of

PAC Rev 27 in February, 2012). **All the chemicals in a mixture must use the same type of PAC value to determine the HI values for the mixture.**

- 3.4 If the chemical entered in the *Input* worksheet is listed in the *HCN-PAC* worksheet, the workbook uses the PAC-n (where n = 1, 2, or 3) entry in Column E to obtain the actual concentration *limit* value from the appropriate PAC column (i.e., Columns P, Q, or R) in the *HCN-PAC* worksheet. The value obtained is automatically inserted as the concentration limit (in units of milligrams per cubic meter [mg/m^3]) in Column D of the *Import* worksheet.
- 3.5 Calculate or otherwise obtain the airborne concentration (C_i) of each chemical “i” at the receptor point (as specified in Column D of the *Input* worksheet) and enter this value in Column F of the *Input* worksheet. This concentration must be in units of mg/m^3 . Concentrations may be obtained using values from existing data tables, manual calculations of atmospheric dispersion, or output from atmospheric dispersion models (e.g., ALOHA, EPICode).
- 3.6 Once the CASRN, concentration limit, and concentration data are entered for a given chemical in Columns C, E, and F, respectively, the workbook should automatically perform its calculations and update output data in the other worksheets. The user can also manually execute the workbook calculations. On a personal computer, this is done by simultaneously pressing **Ctrl** and = on your keyboard or by pressing the **F9** key. On an Apple computer, simultaneously press **Apple** or **Command** and = on your keyboard.

Step 4. Workbook Performs Calculations.

The following describes the process used by the workbook's macros in performing chemical mixture methodology calculations.

- 4.1 The HI_i for each chemical (see Eqn. 1) at the receptor point of interest is reported in the *Import* worksheet in Column E and also in the *Output* worksheet in Column D.
- 4.2 Initially, the workbook sums all the HI_i values (see Eqn. 2) to determine acceptability of the scenario being evaluated and whether protective actions or administrative controls should be applied. The sum of the HI_i values is provided in the *Import* worksheet in the last row of Column E and also in the *Output* worksheet in Column E. If the sum of the HI_i values is less than or equal to 1.0 *the designated emergency preparedness limit is not exceeded at the receptor location. As a result, further assessment may not be needed.* If the sum of the HI_i values is greater than 1.0, then the HCN-approach needs to be employed to provide a more realistic, although still

somewhat conservative, assessment of the hazard. To do this, the workbook continues with the following calculations.

4.3 The workbook determines the toxicological classification of each chemical (i.e., its HCNs) from the values provided in the *HCN-PAC* worksheet (Columns E through N). Up to 10 HCN values may be entered for each chemical. The workbook copies the HCN data for each chemical entered in the *Input* worksheet into the *Import* worksheet (Columns F through O). The category of each chemical is provided in the *HCN-PAC* worksheet in Column O and is copied into Column P of the *Import* worksheet. The chemical category provides the concentration-limit classification used to determine whether the toxicological consequences of exposure to a chemical are concentration-dependent, dose-dependent, or both (Craig et al., 1999, See **Table 3**). The chemical category is not used directly in the CMM calculations. However, it has an indirect impact because it is used to set the exposure period for atmospheric dispersion modeling (Column F in the *Input* worksheet).

Table 3. Information on Chemical Category, Concentration-Limit Classification, and Exposure Duration Treatment.

Category	Concentration-Limit Classification ^A	Exposure Duration Treatment ^B
1A	Ceiling/STEL standard	Concentration-dependent ^D
1B	Irritants	Concentration-dependent ^D
1C	Technologic feasibility ^C	Concentration-dependent ^D
2	Acute toxicants	Dose-dependent (exposure limits for 8 hours/day) ^E
3	Cumulative toxicants	Dose-dependent (exposure limits for 40 hours/wk) ^E
4	Both acute and cumulative	Dose-dependent (exposure limits for 8 hours/day and/or 40 hours/week) ^E

Notes:

A These categories are taken directly from Table 6.7 in *Patty's Industrial Hygiene and Toxicology* (Cralley and Cralley, 1985).

B For release durations less than 15 minutes, concentrations may be calculated over a shorter time period but for not less than 1 minute if the chemical is known to exert immediate toxic effects.

C Permissible exposure limits (PELs) for substances in this category have been set (by the U.S. Department of Labor Occupational Safety and Health Administration) either by technological feasibility or good hygiene practices. No adjustments should be made based on the length of exposure; that is, these PELs are treated as ceiling limits (see reference in Note A).

D For concentration-dependent chemicals, the concentration at the receptor point of interest is calculated as the peak 15-minute time-weighted average (TWA) concentration.

E For dose-dependent chemicals, the concentration at the receptor point of interest may be calculated as the peak 60-minute TWA concentration.

4.4 The workbook sums the HIs of all chemicals having the same category grouping of HCNs. For example, the HIs for those chemicals that are in the “carcinogens” category (HCNs 1 and 2) are summed; the chronic, systemic toxins (HCN = 3.00, 3.01–3.12) are summed; and the acute systemic toxins (HCN = 4.00, 4.01–4.12) are summed. These summations are done automatically by the workbook. Results for each major HCN grouping are presented in Columns D through S in the *HI by mode* worksheet and in Columns D through AN of the *HIs by target organ* worksheet. The results of the *HIs by mode* and *HIs by target organ* worksheets are summarized in Columns G through J of the *Output* worksheet. The sum of the HIs for each HCN category grouping must be less than or equal to 1.0 for the exposure to be within prescribed limits. For the user's convenience in analyzing workbook data, all summed HIs greater than or equal to 0.5 are presented in bolded red font.

4.5 In performing summations, irritants are a special case. Irritants may be denoted as severe (HCN = 14.00), moderate (HCN = 15.00), or mild (HCN = 16.00). These are added together and weighted by severity (i.e., multiplied by 1.0 for severe, 0.5 for moderate, 0.25 for mild). Irritants that affect only one target organ also can be considered separately. For example, irritants affecting only the eyes are indicated by HCN = 14.01, 15.01, and 16.01; and irritants affecting only the skin are indicated by HCN = 14.02, 15.02; and 16.02. The CMM Workbook carries out computations for all chemicals that have HCN and PAC values listed in the *HCN-PAC* worksheet. If a chemical is not listed in the *HCN-PAC* worksheet, it may be added in the row after the last chemical on the list. The user will have to supply applicable HCNs and PACs for such chemicals.

Step 5. Examine Workbook Calculations.

The *Output* worksheet presents summary information on the HIs computed by the workbook. This information includes the following:

- the Individual HIs for each chemical in the mixture
- the Sum of all HIs for all the chemicals in the mixture
- the Sum of the Mode of Action (also called the “Toxic Mode” or “Endpoint”) HIs (i.e., summation for all the chemicals in the mixture of the HIs for each broad HCN category)
- the Sum of Target Organ Effect HIs category (i.e., summation for all the chemicals in the mixture of the HIs for each target organ category).

If the sum of all HIs is less than or equal to 1.0, the exposure to the chemical mixture is within established emergency preparedness limits. If the sum of all HIs is greater than 1.0, the cumulative HCN-based HIs should be examined. If the greatest of the HIs from all of

the Mode of Action or Target Organ Effect categories is less than or equal to 1.0, the exposure to the chemical mixture is within established limits.

The *Import*, *HI*s by mode, and the *HI*s by target organ worksheets provide supplementary information beyond what is summarized in the *Output* worksheet. The *Import* worksheet provides a convenient summary of key input information, HCN data, and HI results. The *HI*s by mode worksheet provides detailed HI results for each chemical and 16 HCN categories. The *HI*s by target organ worksheet provides detailed HI results for each chemical and up to 37 target organ or endpoint HCN categories.

The display of the CMM Workbook has been optimized for PCs at a zoom setting of 100%. Typical of the Excel workbook software, if a column is too narrow to display a cell's contents, the symbol ##### will appear in that cell. To remedy this problem on worksheets that have not been password-protected, the column width can be manually expanded to display the worksheet contents. On password-protected worksheets, the column width cannot be adjusted; however, increasing the zoom percentage (e.g., from 75% to 100%) should allow the worksheet contents to be displayed. If the problem persists or if the printout also shows ##### for some or all of the data, please send an email stating the problem to the CMM development team at cmmdevelopment@listserv.ornl.gov.

SECTION 4. CMM WORKSHEET DESCRIPTIONS

In this section, summary descriptions are provided of each of the CMM Workbook worksheets and for each worksheet column.

Worksheet 1 – *Input* (requires user input)
Chemical Compounds, Receptor Point, Concentration Limit, and Concentrations of Chemicals in the Mixture

Column	Heading	Information in the Column
A	No.	Sequential numbering of the chemicals in the mixture
B	Chemical Compound	Names of the chemicals in the mixture. The names in this gray column are automatically displayed and are based on the CASRN information entered in the next column.
C	CASRN	CASRNs of the chemicals in the mixture. Includes alternative Z number IDs for chemicals that do not have CASRNs. <i>Note:</i> It is suggested that the user copy the CASRN for each chemical from the <i>HCN-PAC</i> worksheet and paste them into the <i>Input</i> worksheet to avoid entry errors.
D	Receptor Point (RP)	Receptor Point
E	Concentration Limit (Li) at RP (Enter "PAC-1", "PAC-2", or "PAC-3")	Concentration Limit at Receptor Point. This is the applicable PAC, provided in the form of a "PAC-n" (minus the quotation marks); where n is 1, 2, or 3.
F	Conc. (C _i) at Receptor Point (mg/m ³)	Concentration at Receptor Point (in units of mg/m ³)

Note: The chemicals that initially appear in the *Input* worksheet are for illustrative purposes only. These data should be replaced with the user's chemicals.

Worksheet 2 – Import (calculations performed automatically)
HI Calculation and HCNs for Chemicals in Mixture

Column	Heading	Information in the Column
A	No.	Sequential numbering of the chemicals in the mixture
B	Chemical Compound	Names of the chemicals in the mixture. If the full name of a chemical is not visible, the vertical extent of the associated row can be increased to display additional information that may be hidden from view.
C	CASRN	CASRNs of the chemicals in the mixture. Includes alternative Z number IDs for chemicals that do not have CASRNs.
D	Conc. Limit PAC-n (mg/m ³)	Concentration Limit – a PAC (mg/m ³). This is the actual concentration limit value for the “PAC-n” specified in the <i>Input</i> worksheet, Column E. The concentration limit value, in units of mg/m ³ , is obtained from the <i>HCN-PAC</i> worksheet, Columns P, Q, or R for PAC-1, PAC-2, or PAC-3, respectively.
E	Hazard Index (HI)	Hazard Index (HI), <i>Input</i> Column F divided by <i>Import</i> Column D
Health Code Numbers (HCNs)		
F	HCN-1	Column E from <i>HCN-PAC</i> worksheet – 1 st listed HCN for the indicated chemical
G	HCN-2	Column F from <i>HCN-PAC</i> worksheet – 2 nd listed HCN for the indicated chemical
H	HCN-3	Column G from <i>HCN-PAC</i> worksheet – 3 rd listed HCN for the indicated chemical
I	HCN-4	Column H from <i>HCN-PAC</i> worksheet – 4 th listed HCN for the indicated chemical
J	HCN-5	Column I from <i>HCN-PAC</i> worksheet – 5 th listed HCN for the indicated chemical
K	HCN-6	Column J from <i>HCN-PAC</i> worksheet – 6 th listed HCN for the indicated chemical
L	HCN-7	Column K from <i>HCN-PAC</i> worksheet – 7 th listed HCN for the indicated chemical
M	HCN-8	Column L from <i>HCN-PAC</i> worksheet – 8 th listed HCN for the indicated chemical
N	HCN-9	Column M from <i>HCN-PAC</i> worksheet – 9 th listed HCN for the indicated chemical
O	HCN-10	Column N from <i>HCN-PAC</i> worksheet – 10 th listed HCN for the indicated chemical
P	Category	Column O from <i>HCN-PAC</i> worksheet -- the concentration-limit classification used to determine whether the toxicological consequences of exposure to a chemical are concentration-dependent or dose-dependent. Other information is provided as well; see Table 1 for details.

Check to see if all of the HI values in Column E are less than or equal to 1.0. If the sum is less than or equal to 1.0, then the exposure is within established limits. Row 34 presents the Sum of the HIs for all chemicals in the mixture.

Worksheet 3 - HIs by mode (calculation performed automatically)
Summation of HIs by Mode of Action for Chemicals in Mixture

Column	Heading	Information in the Column
A	No.	Sequential numbering of the chemicals in the mixture
B	Chemical Compound	Names of the chemicals in the mixture. If the full name of a chemical is not visible, the vertical extent of the associated row can be increased to display additional information that may be hidden from view.
C	CASRN	CASRNs of the chemicals in the mixture. Includes alternative Z numbers for chemicals without CASRNs.
Hazard Indices (HIs) for Chemicals		
D	HCN = 1 or 2 Carcinogens	Cumulative HI for Carcinogens
E	HCN = 14, 15, or 16 Irritants	Computed HI for Irritants
F	HCN = 3 Chronic Systemic Toxins	Cumulative HI for Chronic Systemic Toxins
G	HCN = 4 Acute Systemic Toxins	Cumulative HI for Acute Systemic Toxins
H	HCN = 5 Reproductive Toxins	Cumulative HI for Reproductive Toxins
I	HCN = 6 Cholinesterase Toxins	Cumulative HI for Cholinesterase Toxins
J	HCN = 7 Nervous System Toxins	Cumulative HI for Nervous System Toxins
K	HCN = 8 Narcotics	Cumulative HI for Narcotics
L	HCN = 9 Respiratory Sensitizers	Cumulative HI for Respiratory Sensitizers
M	HCN = 10 Chronic Respiratory Toxins	Cumulative HI for Chronic Respiratory Toxins
N	HCN = 11 Acute Respiratory Toxins	Cumulative HI for Acute Respiratory Toxins
O	HCN = 12 Blood Toxins - Anemia	Cumulative HI for Blood Toxins - Anemia
P	HCN = 13 Blood Toxins - Methemoglobinemia	Cumulative HI for Blood Toxins - Methemoglobinemia
Q	HCN = 17 Asphyxiants	Cumulative HI for Asphyxiants
R	HCN = 18 Explosive, flammable safety	Cumulative HI for Explosive, flammable safety
S	HCN = 19, 20 Other & nuisance	Cumulative HI for Other & nuisance

All Sums of the Mode of Action (“Toxic Mode or Endpoint-specific”) HIs are provided at the bottom of the worksheet (e.g., Row 34, Columns D through S). The sum of HIs for each Mode of Action category must be equal to or less than 1.0 to be within established limits. If not, chemical-specific HIs can be examined to pinpoint the chemicals in the mixture that are significant contributors to the sum(s).

Worksheet 4 – HIs by target organ (calculation performed automatically)**Summation of Hazard Indices by Target Organ for Chemicals in Mixture****Note: (C) = Chronic, (A) = Acute**

Column	Heading	Information in the Column
A	No.	Sequential numbering of the chemicals in the mixture
B	Chemical Compound	Names of the chemicals in the mixture. If the full name of a chemical is not visible, the vertical extent of the associated row can be increased to display additional information that may be hidden from view.
C	CASRN	CASRNs of the chemicals in the mixture. Includes alternative Z numbers for chemicals without CASRNs.
Hazard Indices for Chemicals By Target Organ		
D	Carcinogens unspecified target organ (C)	Cumulative HI for HCN = 1.00, 2.00
E	Bladder cancer (C)	Cumulative HI for HCN = 1.01, 1.00, 2.00
F	Kidney cancer (C)	Cumulative HI for HCN = 2.01, 1.00, 2.00
G	Liver cancer (C)	Cumulative HI for HCN = 1.02, 2.02, 1.00, 2.00
H	Bladder toxin (C)	Cumulative HI for HCN = 3.01, 3.00
I	Bladder toxin (A)	Cumulative HI for HCN = 4.03, 4.00
J	Hematological system unspecified effects (C)	Cumulative HI for HCN = 3.02, 3.00
K	Hematological system unspecified effects (A)	Cumulative HI for HCN = 4.06, 4.00
L	Bone toxin (C)	Cumulative HI for HCN = 3.03, 3.00
M	Bone toxin (A)	Cumulative HI for HCN = 4.13, 4.00
N	Bone marrow toxin (C)	Cumulative HI for HCN = 3.04, 3.00
O	Bone marrow toxin (A)	Cumulative HI for HCN = 4.04, 4.00
P	Brain toxin (C)	Cumulative HI for HCN = 3.05, 3.00
Q	Brain toxin (A)	Cumulative HI for HCN = 4.05, 4.00
R	Eye toxin (chronic ocular effects) (C)	Cumulative HI for HCN = 3.06, 3.00
S	Eye toxin (acute, other than irritation) (A)	Cumulative HI for HCN = 4.01, 4.00
T	Gastrointestinal tract toxin (C)	Cumulative HI for HCN = 3.07, 3.00
U	Gastrointestinal tract toxin (A)	Cumulative HI for HCN = 4.07, 4.00
V	Heart, Cardiovascular system toxin (C)	Cumulative HI for HCN = 3.08, 3.00
W	Heart, Cardiovascular system toxin (A)	Cumulative HI for HCN = 4.08, 4.00

Column	Heading	Information in the Column
X	Kidney toxin (C)	Cumulative HI for HCN = 3.09, 3.00
Y	Kidney toxin (A)	Cumulative HI for HCN = 4.09, 4.00
Z	Liver toxin (C)	Sum of HIs for HCN = 3.10 and 3.00
AA	Liver toxin (A)	Cumulative HI for HCN = 4.10, 4.00
AB	Skin toxin, incl. dermatitis & sensitization (C)	Cumulative HI for HCN = 3.11, 3.00
AC	Skin toxin, other than irritation (A)	Cumulative HI for HCN = 4.11, 4.00
AD	Skin perforation (C)	Cumulative HI for HCN = 3.12, 3.00
AE	Skin perforation (A)	Cumulative HI for HCN = 4.12, 4.00
AF	Nose toxin, other than irritation (A)	Cumulative HI for HCN = 4.02, 4.00
AG	Reproductive system toxin (C)	Cumulative HI for HCN = 5.10, 3.00
AH	Reproductive system toxin (A)	Cumulative HI for HCN = 5.00, 4.00
AI	Nervous system, including CNS, narcosis, cholinesterase toxin (A)	Cumulative HI for HCN = 7.00, 7.01, 8.00, 6.00, 4.00
AJ	Nervous system, including CNS (C)	Cumulative HI for HCN = 7.10, 7.11, 3.00
AK	Respiratory system toxin, including sensitizers (C)	Cumulative HI for HCN = 9.00, 10.00, 3.00
AL	Respiratory system toxin, including severe & moderate irritation (A)	Cumulative HI for HCN = 11.00, 11.01, 4.00
AM	Blood toxin, anemia (C)	Cumulative HI for HCN = 12.00, 3.02, 3.00
AN	Blood toxin, Methemoglobinemia and asphyxiants (A)	Cumulative HI for HCN = 13.00, 17.00, 4.06, 4.00

All Sums of Target Organ Effect HIs are provided at the bottom of the worksheet (e.g., Row 34, Columns D through AN). The sum of HIs for each Target Organ effect category must be less than or equal to 1.0 to be within established limits. If not, chemical-specific HIs can be examined to pinpoint the chemicals in the mixture that are significant contributors to the sum(s).

Worksheet 5 – Output (calculations performed automatically)
Mixture Methodology Output Summary

Column	Heading	Information in the Column
A	No.	Sequential numbering of the chemicals in the mixture
B	Chemicals in mixture	Names of the chemicals in the mixture, if the full name of a chemical is not visible, the vertical extent of the associated row can be increased to display additional information that may be hidden from view.
C	Chemical CASRN	CASRNs of the chemicals in the mixture. Includes alternative Z numbers for chemicals without CASRNs.
D	Individual Hazard Index (HI)	Summation of HIs for each chemical in the mixture
E	Sum of all HIs	Summation of all HIs for all chemicals
F	--	(Blank column)
Sum of Toxic Mode or Endpoint HIs		
G	Mode or Endpoint	Key Mode of Action and Target Organ Effect categories for which HI sums are ≥ 0.25
H	HI sum ≥ 0.25	HI sums that are ≥ 0.25 are shown. Information is not provided for those categories of HCNs with HI sums < 0.25 . Values ≥ 0.5 are displayed using a bolded red font.
Sum of Target-Organ HIs		
I	Target Organ	Target Organ categories for which HI sums are ≥ 0.25
J	HI sum ≥ 0.25	HI sums that are ≥ 0.25 are shown. Information is not provided for those Target Organ categories with HI sums < 0.25 . Values ≥ 0.5 are displayed using a bolded red font.

This worksheet summarizes information in worksheets 2, 3, and 4. If the Sum of all HIs is less than or equal to 1.0 (Column E), the exposure to the chemical mixture at the receptor location of interest is within emergency preparedness exposure limits. If the Sum of all HIs is greater than 1.0 (Column E), then the Mode of Action (Columns G and H) and Target Organ Effect (Columns I and J) results should be examined. If the greatest of the cumulative HI values for any Mode of Action (Column H) or Target Organ Effect (Column J) category is less than or equal to 1.0, then the exposure is within established limits.

Columns H and J present HI sums equal to or greater than 0.25. This value was chosen because it captures HI sums that are approaching levels of significance. Values equal to or greater than 0.5 are further highlighted in a **bold red** font because the 0.5 value may be a generally accepted action level because it is within a factor of two of exceeding the exposure limit.

Worksheet 6 – HCN-PAC⁶ (used by the workbook as a look-up table only)
HCNs and PACs (mg/m³)

Column	Heading	Information in the Column
A	No.	Sequential numbering of chemicals
B	Chemical Compound	Names of the chemicals. For a given chemical, if any of the PAC values are AEGLs, then the name is in 12 point font and bolded . Similarly, if any of the PAC values are ERPGs, then the name is in 10 point font and bolded . And finally, if any of the PAC values are TEELs, then the name is in 10 point font and non-bolded.
C	CAS Registry Number (CAS RN)	CASRN for each chemical. Includes alternative Z numbers for chemicals without CASRNs. For a given chemical, if any of the PAC values are AEGLs, then the CASRN is in 12 point font and bolded . Similarly, if any of the PAC values are ERPGs, then the CASRN is in 10 point font and bolded . And finally, if any of the PAC values are TEELs, then the CASRN is in 10 point font and non-bolded.
D	Sax Number (Lewis Sr., 2004)	SAX number for each chemical
Health Code Numbers (HCNs) for PAC Rev. 27 Chemicals		
E	HCN-1	1 st listed HCN for the indicated chemical
F	HCN-2	2 nd listed HCN for the indicated chemical
G	HCN-3	3 rd listed HCN for the indicated chemical
H	HCN-4	4 th listed HCN for the indicated chemical
I	HCN-5	5 th listed HCN for the indicated chemical
J	HCN-6	6 th listed HCN for the indicated chemical
K	HCN-7	7 th listed HCN for the indicated chemical
L	HCN-8	8 th listed HCN for the indicated chemical
M	HCN-9	9 th listed HCN for the indicated chemical
N	HCN-10	10 th listed HCN for the indicated chemical
O	Category	This gives the concentration-limit classification used to determine whether the toxicological consequences of exposure to a chemical are concentration-dependent or dose-dependent. Other information is provided as well; see Table 2 for details.

⁶ The HCN-PAC worksheet was called the HCN-TEEL worksheet in all versions of the workbook released prior to October 2007.

Column	Heading	Information in the Column
PAC Rev 26 values based on AEGLs, ERPGs, and TEELs (mg/m³)		
P	PAC-1	Values are provided for each of the three PAC categories based on the data provided in Rev 27 of the PAC data set. If a PAC value is an AEGL, then it is in 12 point font and bolded . If a PAC value is an ERPG, then it is in 10 point font and bolded . PACs are in 10 point font, regular non-bolded.
Q	PAC-2	
R	PAC-3	

All PAC and TEEL values are given in units of milligrams per cubic meter. Some of these values were expressed originally in parts per million and were converted to milligrams per cubic meter.

Data in this worksheet are copied from other sources of information. The *HCN-PAC* worksheet is not intended to be printed as part of the mixture methodology results printout.

This worksheet will be updated periodically as PACs and HCNs are developed for new chemicals or as PACs are otherwise changed or HCNs updated (see <http://orise.orau.gov/emi/scapa/teels.htm> for more information).

SECTION 5. REFERENCES

- Cralley LJ and Cralley LV. 1985. Theory and rationale of industrial hygiene practice. Patty's industrial hygiene and toxicology. 2nd ed. New York, Chichester, Brisbane, Toronto, Singapore: John Wiley & Sons. p 150-185.
- Craig DK, Baskett RL, Davis JS, Dukes L, Hansen DJ, Petrocchi AJ, Powell TJ, Sutherland PJ, Tuccinardi J, TE. 1999. Recommended default methodology for analysis of airborne exposures to mixtures of chemicals in emergencies. *Applied Occupational and Environmental Hygiene* **14**(9):609-617.
- Craig DK, Davis JS, DeVore R, Hansen DJ, Petrocchi AJ, Powell TJ. 1995. Alternative guideline limits for chemicals without environmental response planning guidelines. *Am. Ind. Hyg. Assoc. J.* **56**:919-925.
- Craig DK, Davis JS, Hansen DJ, Petrocchi AJ, Powell TJ, Tuccinardi J, T. E. 2000. Derivation of temporary emergency exposure limits (TEELs). *Journal of Applied Toxicology* **20**:11-20.
- DOE (U.S. Department of Energy). 2001. Nuclear Safety Management. *Federal Register*. Code of Federal Regulations, Part 830. 10 CFR Part 830. 66(7): 1810Washington, DC. p 1810-1824.
- DOE (US Department of Energy). 2005. DOE O 151.1C. Comprehensive emergency management system November 2, 2005 ed. p 90.
<https://www.directives.doe.gov/directives/current-directives/151.1-BOrder-c/view>
- DOE (U.S. Department of Energy). 2008. DOE-HDBK-1046-2008. Temporary emergency exposure limits for chemicals: Methods and practice. August 2008. Washington, DC. p 52.
- Lewis, RA. 1998. Lewis Dictionary of Toxicology. 1st Edition. Informa Healthcare.
- Lewis, RJ. Sr. 2004. Sax's Dangerous Properties of Industrial Materials. 11th Edition, Volumes 1 -3. John Wiley & Sons.
- NIOSH (National Institute for Occupational Safety and Health). 2008. Registry of Toxic Effects of Chemical Substances (RTECS), Comprehensive Guide to the RTECS.
- Rusch GM, Garrett R, Tobin P, Falke E, Lu PY. 2000. The development of acute exposure guideline levels for hazardous substances. *Process Saf. Prog.* **19**(2):98-102.
- Rusch GM, Garrett R, Tobin P, Falke E, Lu PY. 2002. The development of acute exposure guideline levels for hazardous substances. *Drug Chem. Toxicol.* **25**(4):339-348.
- Rusch GM. 1993. The history and development of emergency response planning guidelines. *Journal of Hazardous Materials* **33**(2):193-202.
- Yu X-Y, Petrocchi AJ, Craig DK, Glantz CS, Trott DM, Ciolek J, Lu P-Y, Bond J-A, Tuccinardi J, TE. 2010. Development and applications of the chemical mixture methodology. *J. Applied Toxicology* **30**: 513-524.