

CMM Wizard Prototype

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PNNL

What is the CMM Wizard?

- An online version of the CMM that is accessible via the Internet (does not require Excel)
- Provides comparable functionality to the CMM Workbook
- Designed to be user friendly / easy-to-use
- Provides output that is easy to read and print
- Chemical data are stored in an up-to-date Access database
- Input files and output products can be saved and re-loaded back into the Wizard
- Can process up to six receptor distances at a time
- No limit on the number of chemicals in a mixture
- Allows rapid queries of chemical information.

Wizard Development Team

- All work done by DOE Science and Mathematics Teachers Applied Research (STAR) interns (funded by the NSF).
- Each intern spends 10 weeks at PNNL
 - Kim Schutte: 2010
 - Alex Booth: 2011
- Mentorship provided by Xiao-Ying Yu, Cliff Glantz, Jeremy Rishel, and Nino Zuljevic



CMM Wizard: 2012

CHEMICAL MIXTURE METHODOLOGY WIZARD

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What is CMM Wizard?

The CMM Wizard provides information that assists DOE planners to ensure that in emergency response situations the exposure of workers and the public to airborne mixtures of hazardous chemicals does not exceed protective thresholds. The CMM computes Hazard indices (HIs) for each chemical in the mixture (an HI is the ratio of the airborne concentration of the chemical at a receptor location to the appropriate protective action threshold concentration for that chemical). Health Code Numbers (HCNs) are then used to assess the additive health impact from all of the chemicals in a mixture based on the chemicals' specific modes of toxicity (e.g., acute systemic toxins, carcinogens, asphyxiants) and target organs (e.g., cardiovascular system toxin, gastrointestinal tract, brain). HI values that are less than "1" indicate that protective threshold are not exceeded for the chemical mixture.

How do I use the CMM Wizard?

Using the CMM Wizard is easy! Go to the next webpage, Step 1, and select the chemicals in the mixture you wish to study by searching the Wizard's database (chemicals can be added to a mixture by searching for their name or CASID). In Step 2, you have the option of entering the summary meteorological conditions that are representative of the atmospheric conditions present when the chemical mixture would be released. In Step 3, select the downwind receptor locations of concern. Up to six downwind distances can be selected. Provide the airborne concentration of each chemical at the designated receptor (concentration information is typically obtained using a standard chemical exposure model like EPICode or ALOHA). That's all the input the model needs! The last page in the Wizard is used to present CMM results. You can display results for different analysis products, receptor locations, and protective action criteria values. You can assign a name to your chemical mixture so that it can be saved for re-use in other test cases.

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Step 1: Select the Chemicals in the Mixture

In this step, select the chemicals to use in the mixture. You can load chemicals from a previously defined mixture (click the "Load" button above) or define a new mixture by quickly searching for chemicals in the CMM database. You can search by chemical name, CASRN, or SAX number.

Enter information (partial information is acceptable) and click Search. The first value on your search list will be displayed – click the list button (*) to see other items on your list. Highlight the item that matches your choice and click the Add button to add it to your list. If you have made a mistake, highlight the item on your list and click the Remove button.

Search: Search

Disodium dihydrogen silicate | z-0017 | N.I.S., etc. Add Remove

Trisodium arsenate | 13464-38-5 | N.I.S.
Butyl ether, n-, (Dibutyl ether) | 142-96-1 | BRH750
Chlorine | 7782-50-5 | CDV750
Butylcyclohexane, (1-Cyclohexylbutane) | 1678-93-9 | N.I.S.

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Step 2: Input Chemical Concentrations at User-Specified Receptors

In this step, you will do the following:

- enter a name for the chemical mixture (if not already specified)
- specify downwind receptor distances (up to 6 distances may be provided)
- provide airborne concentration data for each chemical at each downwind receptor distance. Concentration data are typically obtained by running a chemical dispersion model (e.g., ALOHA, EPICode).

Enter a unique file name for the chemical mixture (if not already listed):

Enter a name (e.g., "Fenceline") or distance with units (e.g., "100 m") for each receptor. Enter concentration data (in units of mg/m³) for each chemical at each selected receptor location. Use the colored buttons below to add additional receptor distances (up to 6), delete checked receptors, or clear existing concentration data.

Receptor 1	Receptor 2	Receptor 3	Receptor 4	Receptor 5	Receptor 6
200m	300m	400m	Fence	Highway	School
Chemicals in Mixture					
Name: Acetylene CASRN: 74-86-2 SAX: AC1750	10	8	6	4	2
Name: Butylcyclohexane, (1-Cyclohexylbutane) CASRN: 1678-93-9 SAX: N.I.S.	20	16	12	8	4
Name: Chlorine CASRN: 7782-50-5 SAX: CDV750	5	4	3	2	1
Name: Butyl ether, n- (Dibutyl ether) CASRN: 142-96-1 SAX: BRH750	5	4	3	2	1
Name: Trisodium arsenate CASRN: 13464-38-5 SAX: N.I.S.	0.25	0.2	0.15	0.1	0.05

Add Receptor Delete Checked Clear Checked

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Name: Receptor: PAC

Chemicals	Concentration	Concentration	Concentration	Concentration	Concentration	Concentration
	at 200 m	at 300 m	at 400 m	at Fence	at Highway	at School
Name: Acetylene CASRN: 74-86-2 SAX: AC1750	12 mg/m ³	9 mg/m ³	6 mg/m ³	4 mg/m ³	2 mg/m ³	1 mg/m ³
Name: Butylcyclohexane, (1-Cyclohexylbutane) CASRN: 1678-93-9 SAX: N.I.S.	20 mg/m ³	16 mg/m ³	12 mg/m ³	8 mg/m ³	4 mg/m ³	2 mg/m ³
Name: Chlorine CASRN: 7782-50-5 SAX: CDV750	5 mg/m ³	4 mg/m ³	3 mg/m ³	2 mg/m ³	1 mg/m ³	0.5 mg/m ³
Name: Butyl ether, n- (Dibutyl ether) CASRN: 142-96-1 SAX: BRH750	5 mg/m ³	4 mg/m ³	3 mg/m ³	2 mg/m ³	1 mg/m ³	0.5 mg/m ³
Name: Trisodium arsenate CASRN: 13464-38-5 SAX: N.I.S.	0.25 mg/m ³	0.2 mg/m ³	0.15 mg/m ³	0.1 mg/m ³	0.05 mg/m ³	0.025 mg/m ³

Hazard Index (HI) Summary:

	HI at 200 m for PAC-2	HI at 300 m for PAC-2	HI at 400 m for PAC-2	HI at Fence for PAC-2	HI at Highway for PAC-2	HI at School for PAC-2
Name: Acetylene CASRN: 74-86-2 SAX: AC1750	0.00	0.00	0.00	0.00	0.00	0.00
Name: Butylcyclohexane, (1-Cyclohexylbutane) CASRN: 1678-93-9 SAX: N.I.S.	0.50	0.40	0.30	0.20	0.10	0.05
Name: Chlorine CASRN: 7782-50-5 SAX: CDV750	2.50	2.00	1.50	1.00	0.50	0.25
Name: Butyl ether, n- (Dibutyl ether) CASRN: 142-96-1 SAX: BRH750	0.25	0.20	0.15	0.10	0.05	0.03
Name: Trisodium arsenate CASRN: 13464-38-5 SAX: N.I.S.	1.50	1.44	1.08	0.72	0.36	0.18

Hazard Index (HI) by Mode:

	HI at 200 m for PAC-2	HI at 300 m for PAC-2	HI at 400 m for PAC-2	HI at Fence for PAC-2	HI at Highway for PAC-2	HI at School for PAC-2
Asphyxiants:	0.00	0.00	0.00	0.00	0.00	0.00
Explosive, flammable safety:	0.00	0.00	0.00	0.00	0.00	0.00
Acute System Toxins:	5.95	4.84	3.63	2.42	1.21	0.61
Chronic System Toxins:	4.55	3.64	2.73	1.82	0.91	0.46
Narcotics:	0.25	0.20	0.15	0.10	0.05	0.03
Acute Respiratory Toxins:	2.75	2.20	1.65	1.10	0.55	0.28
Chronic System Toxins:	2.55	2.04	1.53	1.02	0.51	0.25
Irritants:	2.75	2.20	1.65	1.10	0.55	0.28

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Step 1: Select the Chemicals in the Mixture

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Search

Disodium dihydrogen silicate | z-0017 | N.I.S., etc. ▼

Add

Trisodium arsenate | 13464-38-5 | N.I.S.
Butyl ether, n-; (Dibutyl ether) | 142-96-1 | BRH750
Chlorine | 7782-50-5 | CDV750
Butylcyclohexane; (1-Cyclohexylbutane) | 1678-93-9 | N.I.S. ▲ ▼

Remove

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Step 2: Input Chemical Concentrations at User-Specified Receptors

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Enter a unique file name for the chemical mixture (if not already listed):

Enter a name (e.g., "Fenceline") or distance with units (e.g., "100 m") for each receptor. Enter concentration data (in units of mg/m³) for each chemical at each selected receptor location. Use the colored buttons below to add additional receptor distances (up to 6), delete checked receptors, or clear existing concentration data.

	Receptor 1 <input type="checkbox"/>	Receptor 2 <input type="checkbox"/>	Receptor 3 <input type="checkbox"/>	Receptor 4 <input type="checkbox"/>	Receptor 5 <input type="checkbox"/>	Receptor 6 <input type="checkbox"/>
Receptor Names/Distances:	<input type="text" value="200 m"/>	<input type="text" value="300m"/>	<input type="text" value="400m"/>	<input type="text" value="Fence"/>	<input type="text" value="Highway"/>	<input type="text" value="School"/>
Chemicals in Mixture	Concentration (mg/m³)					
Name: Acetylene CASRN: 74-86-2 SAX: ACI750	<input type="text" value="10"/>	<input type="text" value="8"/>	<input type="text" value="6"/>	<input type="text" value="4"/>	<input type="text" value="2"/>	<input type="text" value="1"/>
Name: Butylcyclohexane; (1-Cyclohexylbutane) CASRN: 1678-93-9 SAX: N.I.S.	<input type="text" value="20"/>	<input type="text" value="16"/>	<input type="text" value="12"/>	<input type="text" value="8"/>	<input type="text" value="4"/>	<input type="text" value="2"/>
Name: Chlorine CASRN: 7782-50-5 SAX: CDV750	<input type="text" value="5"/>	<input type="text" value="4"/>	<input type="text" value="3"/>	<input type="text" value="2"/>	<input type="text" value="1"/>	<input type="text" value="0.5"/>
Name: Butyl ether, n-; (Dibutyl ether) CASRN: 142-96-1 SAX: BRH750	<input type="text" value="5"/>	<input type="text" value="4"/>	<input type="text" value="3"/>	<input type="text" value="2"/>	<input type="text" value="1"/>	<input type="text" value="0.5"/>
Name: Trisodium arsenate CASRN: 13464-38-5 SAX: N.I.S.	<input type="text" value="0.25"/>	<input type="text" value="0.2"/>	<input type="text" value="0.15"/>	<input type="text" value="0.1"/>	<input type="text" value="0.05"/>	<input type="text" value="0.025"/>



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Name: **Display Style** **@ Receptor** **@ PAC**

Summary 100 m PAC-2

Stability Class:

D-Neutral

Wind Speed:

5 m/s

Wind Direction:

From the west

Chemicals:

Concentration at 100 m

Name: Acetylene
CASRN: 74-86-2
SAX: ACI750

200 mg/m3

Name: Isobutyl chloride; (1-Chloro-2-methylpropane)
CASRN: 513-36-0
SAX: CIU500

10 mg/m3

Name: Methylene fluoride;
(Difluoromethane; HFC-32)
CASRN: 75-10-5
SAX: MJQ300

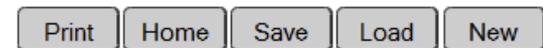
7.5 mg/m3

Hazard Index(HI) Summary:

HI at 100 m for PAC-2

Name: Acetylene
CASRN: 74-86-2
SAX: ACI750

0.08





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Step 3:
Input Met Data

Name:	Display Style	@ Receptor	@ PAC
	Summary	100 m	PAC-2
Stability Class:	Wind Speed:	Wind Direction:	
D-Neutral	5 m/s	From the west	
Chemicals:	Concentration at 100 m		
Name: Acetylene CASRN: 74-86-2 SAX: ACI750	200 mg/m3		
Name: Isobutyl chloride; (1-Chloro- 2-methylpropane) CASRN: 513-36-0 SAX: CIU500	10 mg/m3		
Name: Methylene fluoride; (Difluoromethane; HFC-32) CASRN: 75-10-5 SAX: MJQ300	7.5 mg/m3		

Hazard Index(HI) Summary:	HI at 100 m for PAC-2
Name: Acetylene CASRN: 74-86-2 SAX: ACI750	0.08
Name: Isobutyl chloride; (1-Chloro- 2-methylpropane) CASRN: 513-36-0 SAX: CIU500	1.33
Name: Methylene fluoride; (Difluoromethane; HFC-32) CASRN: 75-10-5 SAX: MJQ300	0.00
Sum of HIs:	1.41



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PAC-2

Hazard Index(HI) Summary:	HI at 100 m for PAC-2	HI at Fenceline for PAC-2
Name: Acetylene	0.08	0.00
CASRN: 74-86-2		
SAX: AC1750		
Name: Isobutyl chloride; (1-Chloro-2-methylpropane)	1.33	0.01
CASRN: 513-36-0		
SAX: CIU500		
Name: Methylene fluoride; (Difluoromethane; HFC-32)	0.00	0.00
CASRN: 75-10-5		
SAX: MJQ300		
Sum of HIs:	1.41	0.01
Hazard Index(HI) by Mode:	HI at 100 m for PAC-2	HI at Fenceline for PAC-2
Asphyxiants:	0.08	0.00
Explosive, flammable safety:	0.08	0.00
Acute System Toxins:	1.41	0.01
Nervous System Toxins:	0.08	0.00
Narcotics:	0.08	0.00
Acute Respiratory Toxin:	0.08	0.00
Chronic System Toxins:	1.33	0.01
Reproductive Toxins:	0.00	0.00
Chronic Respiratory Toxin:	0.00	0.00
Hazard Index(HI) by Target Organ:	HI at 100 m for PAC-2	HI at Fenceline for PAC-2
Blood toxin, methemo-globinemia and asphyxiants (A):	1.41	0.01
Brain toxin (A):	1.41	0.01
Nervous system, including CNS, narcosis and cholinesterase toxin (A):	1.41	0.01
Respiratory system toxin, including severe and moderate irritation (A):	1.41	0.01
Hematological system, unspecified effects (A):	1.41	0.01
Gastrointestinal tract toxin (A):	1.41	0.01
Skin toxin, other than irritation (A):	1.41	0.01
Bladder toxin (A):	1.33	0.01
Bone toxin (A):	1.33	0.01
Bone marrow toxin (A):	1.33	0.01
Eye toxin (acute, other than irritation) (A):	1.33	0.01
Heart, Cardiovascular system toxin (A):	1.33	0.01
Kidney toxin (A):	1.33	0.01
Liver toxin (A):	1.33	0.01
Skin perforation (A):	1.33	0.01
Nose toxin, other than irritation (A):	1.33	0.01
Reproductive system toxin (A):	1.33	0.01
Stomach toxin (A):	1.33	0.01

Discussion, Questions, Comments?



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