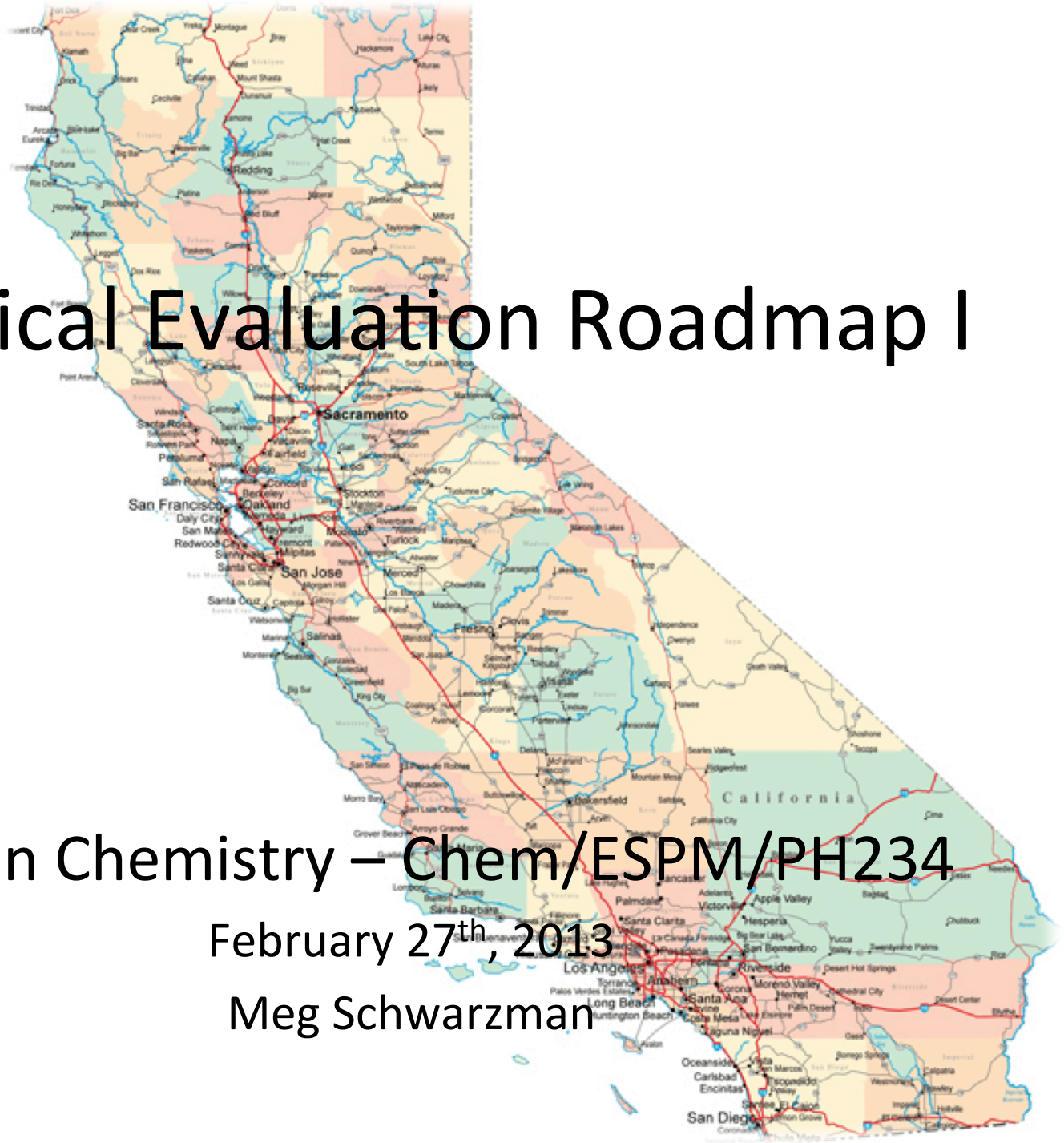
Chemical Evaluation Roadmap I



Green Chemistry – Chem/ESPM/PH234

February 27th, 2013

Meg Schwarzman

Technical Performance & Impacts Module Overview

Date	Topic	Details	Instructor
Wed Feb20	Unit operations	Define the bounds of your biomass to energy technology.	Mulvihill
Mon Feb 25	Energy density + emissions	Address efficiency of conversion processes; define inputs/outputs of each process	Mulvihill
Wed Feb 27	Chem eval roadmap I	Intro to hazard traits (all) and process for completing charts. Start phys/chem and acute toxicity in class	Schwarzman
Mon Mar 4	Chem eval roadmap II	Human Health Hazard traits – data sources & interpretation	Schwarzman
Wed Mar 6	Chem eval roadmap III	Ecotox hazard traits – data sources & interpretation	Vulpe
Mon Mar 11	Synthesis	Work with all three hazard traits tables, digging deeper into the data and developing conclusions.	Vulpe + all
Wed Mar 13	Environmental fate + exposure	Understanding environmental fate and exposure potential for chemicals associated with your biomass- energy process	McKone
Mon Mar 18	Maximizing performance	Prepare a 5 minute overview for the technical performance of your biomass-energy process for presenting in class	Mulvihill +all

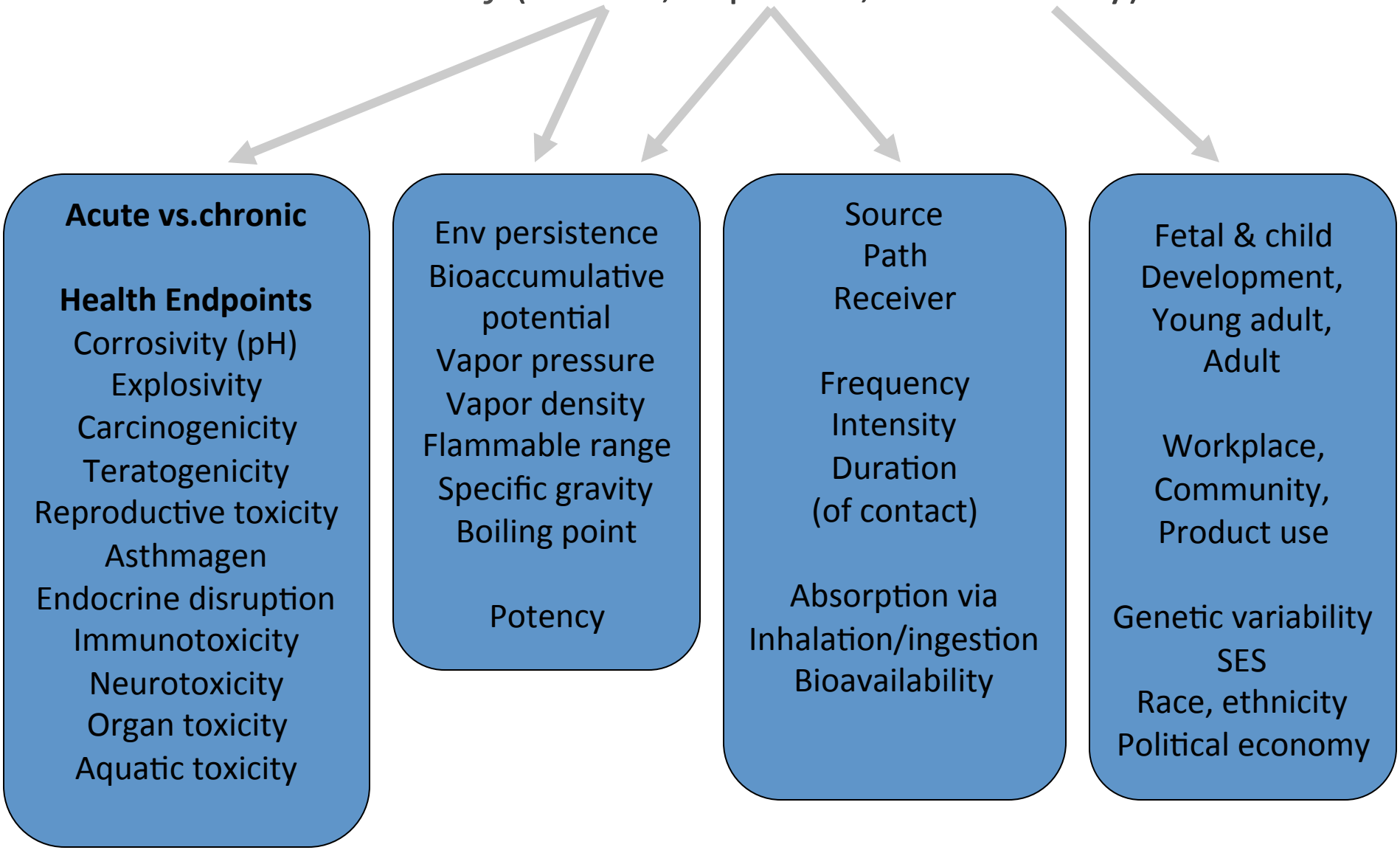
4 step process

1. Identify compounds of interest
2. Search for hazard information based on authoritative sources
3. Search for additional information, and note data gaps.
4. Identify preliminary conclusions and places where more finer distinctions are needed. *What differentiates your chosen technology (for better or worse)?*

Hazard trait tables

Endpoints Associated with Determinants of Risk

Risk = *f* (Hazard, Exposure, Vulnerability)



The Wide Range of Potency

Agent	LD_{50}, mg/kg
Ethyl alcohol	10,000
Sodium chloride	4,000
Ferrous sulfate	1,500
Morphine sulfate	900
Phenobarbital sodium	150
Picrotoxin	5
Strychnine sulfate	2
Nicotine	1
d-Tubocurarine	0.5
Hemicholinium-3	0.2
Tetrodotoxin	0.1
Dioxin (TCDD)	0.001
Botulinum toxin	0.00001

Table: Klaassen c. Casarett and Doull's Toxicology: The Basic Science of Poisons. 6th Ed. 2001. p. 8.

Brainstorming about your chemicals
5 minutes

What do you already know about each of the substances?

1. Name (s)
2. Most relevant form
3. Use/function
4. Hazard traits

Physical Chemical Properties Basics

Boiling point	
Vapor pressure	
Vapor density	
Flash point	
Flammable range	

Physical Chemical Properties Basics

Boiling point	Low BP = vaporization at lower temps
Vapor pressure	High VP = more vaporization
Vapor density	Substances with VD > 1 will sink in air
Flash point	Temp at which liquid produces enough vapor to ignite. Low FP = more vaporization, and easier ignition
Flammable range	% chemical in air required for combustion in presence of an ignition source. LEL = lower explosive limit UEL = upper explosive limit

P-chem question 1

Which of these has the highest ignition risk?

LEL (% fuel in air)	UEL (% fuel in air)	
2.2	9.6	(Propane)
1.4	7.6	(Gasoline)
5.0	17	(Methane)
2.5	100	(Acetylene)
4.0	75	(Hydrogen)

P-chem question 2

Which of these is most likely to produce the greatest exposure via inhalation?

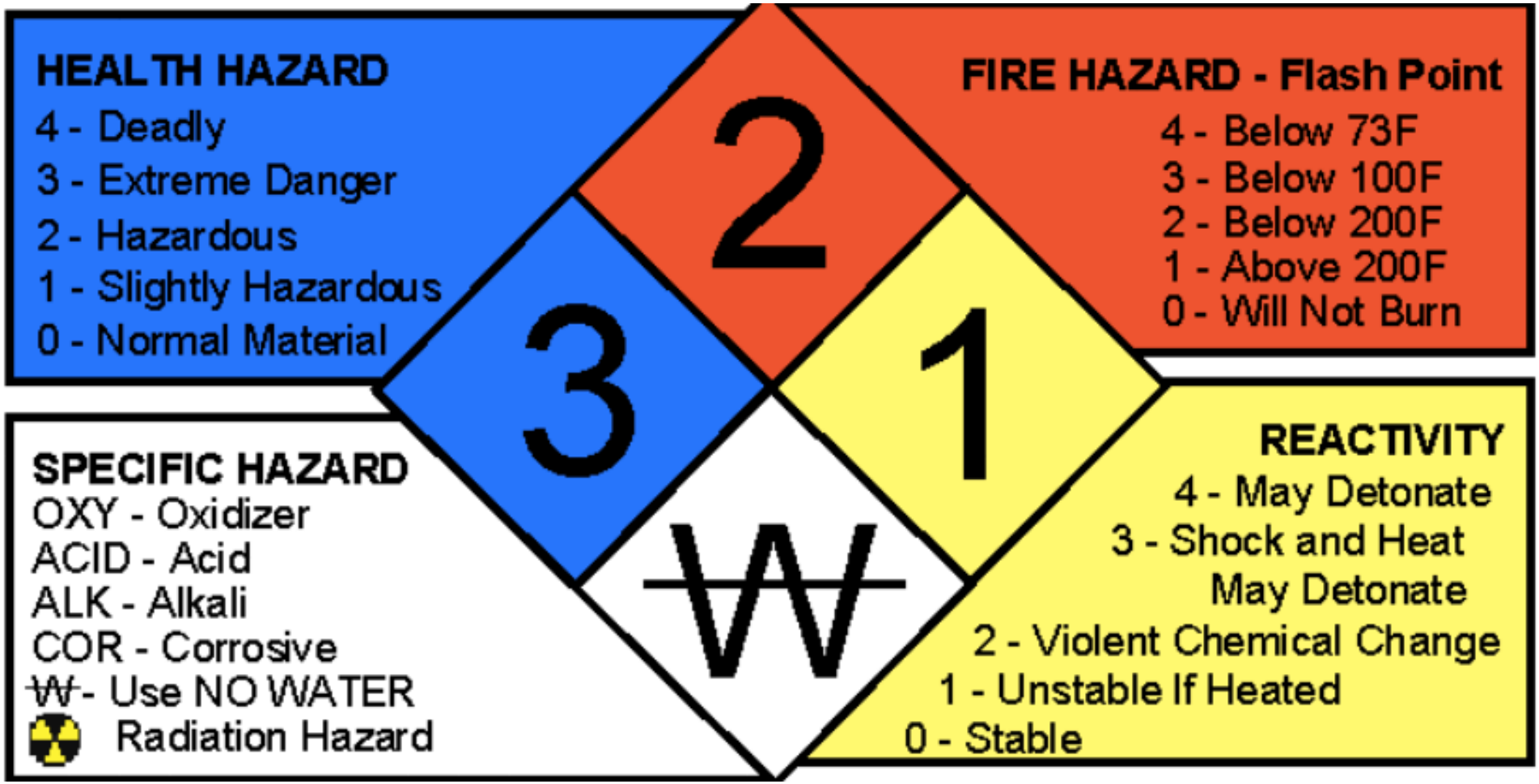
1) BP = 232^{o} F and VP = 20 mmHg (Toluene)
2) BP = 176^{o} F and VP = 75 mmHg (Benzene)
3) BP = 292^{o} F and VP = 9 mmHg (Xylene)

Interpreting P-Chem Properties

Property	High hazard	Moderate hazard	Low hazard
Flash Point	<100 deg F (Flammable)	100 – 200 deg F (Combustible)	>200 deg F (Combustible)
Flammable range*	>12 (Vapors extremely explosive)	2-12	<2
Boiling point	<100 deg F (Very volatile)	100-400 deg F	>400 deg F
Vapor pressure	>10 mmHg (Highly volatile)	1-10 mmHg	<1 mmHg
pH	1-4 Acid 10-14 Base	5-6 Acid 8-9 Base	7 Neutral

* Flammable Range is the difference between the Lower Explosive Limit (LEL) and Upper Explosive Limit (UEL), which are given in % in the NIOSH Pocket Guide and on the MSDS.

Material Safety Data Sheet



Step 1: Chemical Identification

Chemical name

CASRN

Sources

- Material Safety Data Sheets
- ChemIDplus http://chem.sis.nlm.nih.gov/chemidplus/
- Chem spider http://www.chemspider.com
- PubChem http://pubchem.ncbi.nlm.nih.gov

Step 2: P-chem Properties & Acute Tox

Physical-Chemical Properties

- NIOSH pocket guide on chemical hazards http://www.cdc.gov/niosh/npg/
- ChemIDplus http://chem.sis.nlm.nih.gov/chemidplus/

LD50 and Skin sensitization

- Material Safety Data Sheets
- ChemIDplus http://chem.sis.nlm.nih.gov/chemidplus/

For Monday, March 4th

- Complete P-Chem and Acute tox table
- Refer to the information sources document as needed (see slides from Wednesday and the link on the hazard traits tables)
- Make sure you've read the summary assignment document on bspace
- Look through the hazard trait documents on b-space (listed as readings for today). Also see explanation of the Green Screen here: http://www.cleanproduction.org/Greenscreen.v1-2.php
- Register for a free trial of Pharos http://www.pharosproject.net (use your berkeley.edu address)