Semiconductor DFE work at Berkeley: Environmental Value Systems Analysis (EnV-S) and Future Work

NSF/SRC Center for Environmentally Benign Semiconductor Manufacturing April 14, 2004



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Outline of presentation

- 1. Semiconductor DFE Research at Berkeley The Environmental Value Systems Analysis (EnV-S) Tool
- Case Study 1 Comparing Completed Systems (CVD Abatement)
- 3. Case Study 2 Informing Design of Equipment (Copper CMP Wastewater Treatment)
- 4. Conclusions

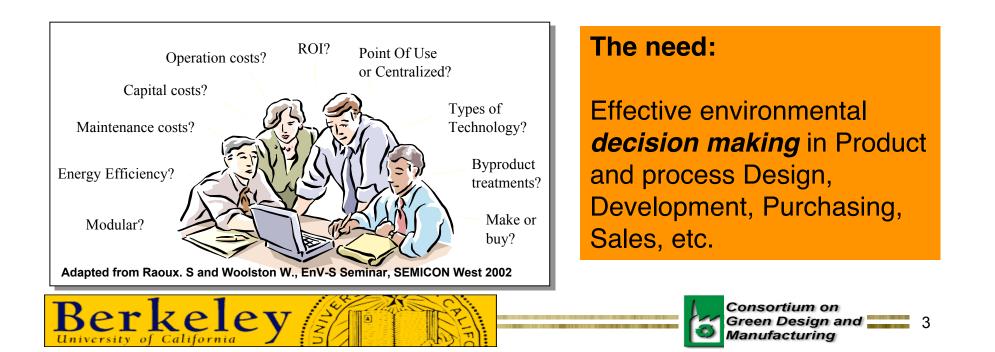


Why Improve environmental performance?

- Responsibility towards sustainable industrial development - Corporate Responsibility
- Growing public and customer awareness Image
- Preempt/inform future, regulations on waste generation, facilities operation - Avoid problems
- Increase revenues and emerge as market leaders through product differentiation - \$\$\$

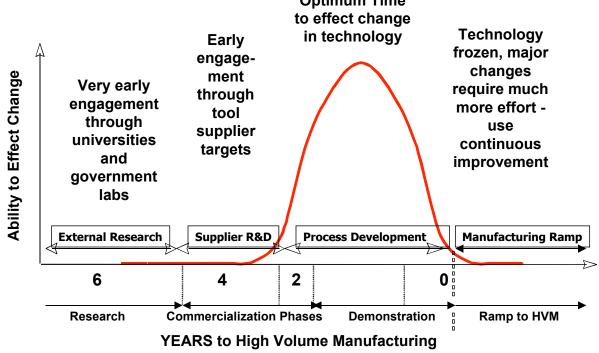
COST





Challenges - Rate of change

- Technology change every 18 months
- Equipment change every 3-4 years

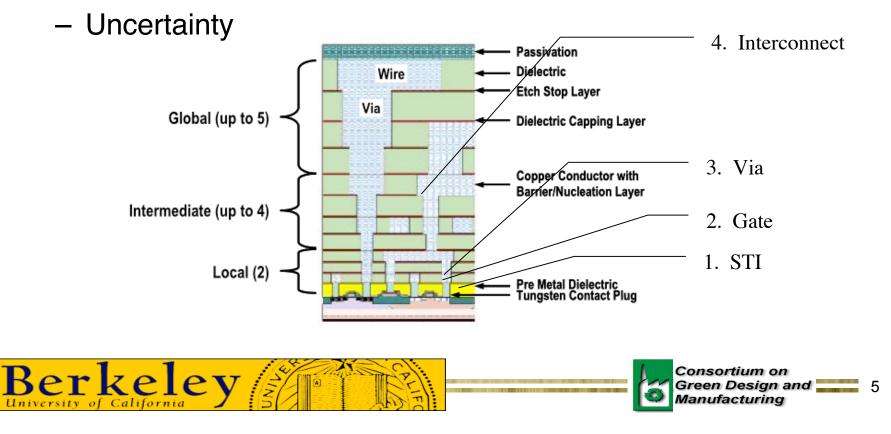


Adapted from McManus, T. J. 2002, "Integrating EHS into the Business, Delivering a Market/Business Advantage," Presentation at U C Berkeley, Sept. 27th.



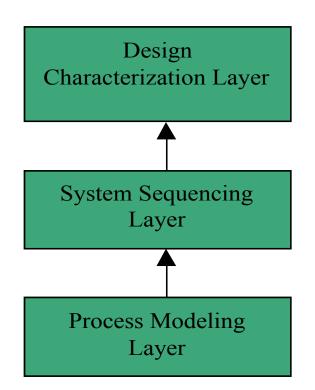
Challenges - chemical use and complexity

- Numerous process steps ~250
- Numerous chemicals used ~200 possible agents
 - New chemicals
 - Unavailable health data



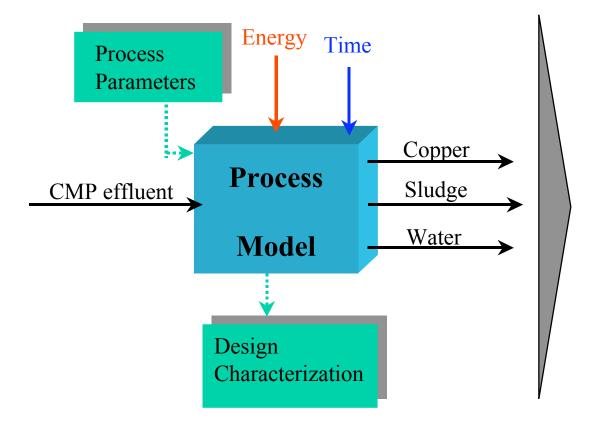
A "bottom-up" semiconductor DFE tool

- The Environmental Value Systems Analysis (EnV-S)
- Three layers





Process Modeling Layer: Unit process model approach



A set of analytical/empirical process models are used to describe the process.

Inputs include process parameters, mass/flow data, energy, unit costs, etc.

Output parameters include energy utilization, waste, generated, environmental and health impacts, cost



Equipment model library

- Build a library of platform based models
 - Key platform models

Process Platform	Broad Function
Rapid Thermal Processing	Film growth/annealing
Chemical Vapor Deposition	Film growth
Epitaxial/Polysilicon deposition	Film/layer growth
Physical Vapor Deposition	Film growth
Ion Implantation	Charge
Lithography	Patterning
Plasma Etching	Contacts/vias
Chemical Mechanical Planarization (CMP)	Local/global planarity
Electrochemical Plating (ECP)	Copper plating
Wet Cleaning	Cleaning at various stages

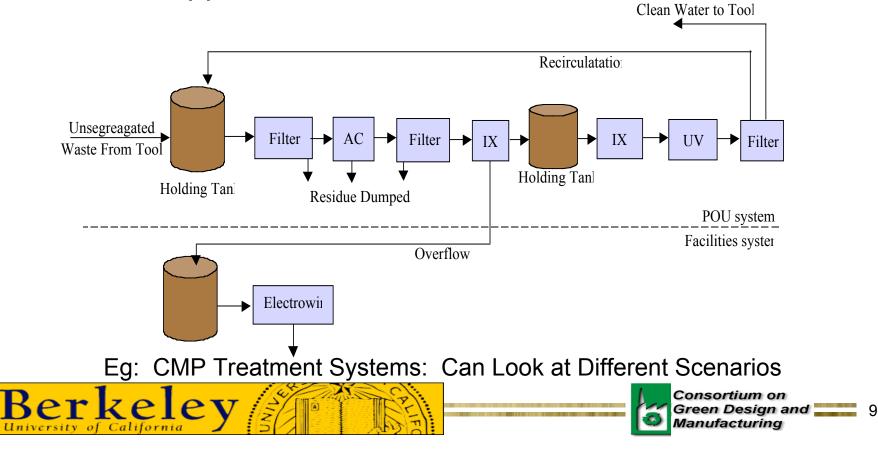
Broad function		
Electricity delivery		
UPW generation and distribution		
Cooling process equipment		
Cool HVAC and PCW		
Back to UPW front end/elsewhere		
HAPS removal		
VOC removal		
Meet discharge specifications		
Miscellaneous		





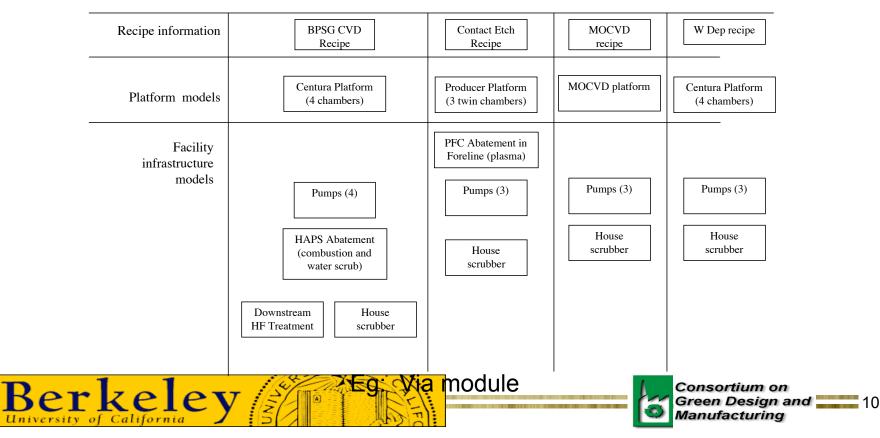
System Sequencing Layer

- To sets the boundary of the analysis
- Track primary and secondary flows
- Modular Approach: Can mix and match the models

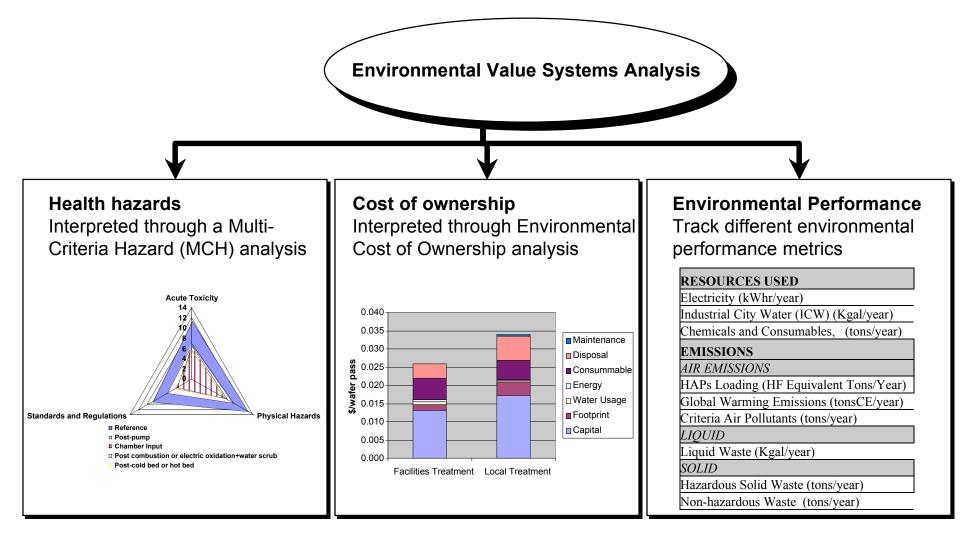


Sequencing (contd.)

- Hierarchical organization of databases
 - Keep pace with technology change
 - Proprietary, public and shared information
- Can assemble different manufacturing sequences



Design Characterization Layer







Three Applications for the EnV-S

- 1. Comparing alternative equipment
 - Case Example: CVD Abatement
- 2. Design of equipment
 - Case Example: Copper CMP abatement
- 3. Examining industry-wide environmental ramifications of equipment/processes
 - PFC emissions issues





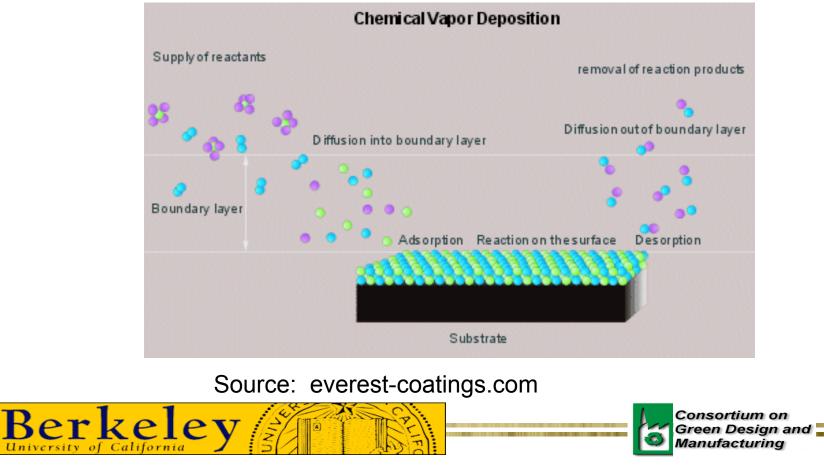
2. Case study 1: Comparing Alternative Equipment

- Eg: in purchasing decisions
- Compare dielectric chemical vapor deposition (DCVD) emissions abatement technologies



Application

- Deposit a dielectric film using Chemical Vapor Deposition (CVD)
- Material Deposited: Undoped Silicate Glass (USG)



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Application (contd.)

- Equipment Utilized
 - Three CVD chambers



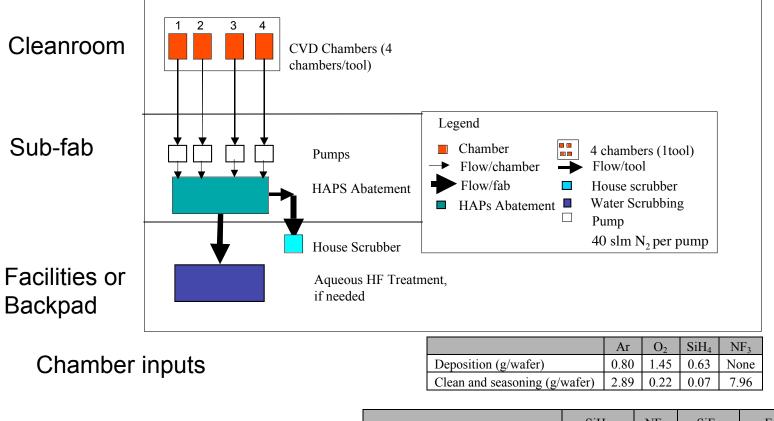


Source: http://appliedmaterials.com





Analysis scope



Post pump emissions

	SiH ₄	NF ₃	SiF ₄	F ₂	HF
Deposition (g/wafer)	<5.71E-3	None	None	None	None
Clean and seasoning (g/wafer)	None	0.06	0.46	5.89	0.05





Environmental Issues and Abatement

- Emissions include F_{2.}
 - Transporting F_2 is problematic
 - Could lead to release of HF (HAPs)
- Other potentially hazardous, toxic and flammable emissions (SiF₄, SiH₄, etc.)

Abatement Technologies	SiF ₄	F ₂	SiH ₄	HF	NF ₃	Selected for Analysis?
Catalytic and Water Scrub	Y	Y	Ν	Y	Y	Ν
Burn and Water Scrub	Y	Y	Y	Y	Y	Y
Burn and Dry Scrub (Hot or Cold	Y	Y	Y	Y	Y	N^1
bed)						
Plasma	N^2	Y	N^2	Y	Y	Ν
Cold Bed	Y	Y ³	Y	Y	Y	Y
Hot Bed	Y	Y^3	Y	Y	Y	Y
Electric Oxidation and Water	Y	Y	Y	Y	Y	Y
Scrub						
Note:						

Note:

¹Not considered, because a dry scrubber could abate F_2 directly, without the need for a burner

²Can abate, but form solids that cause production problems and may require other technologies to remove.

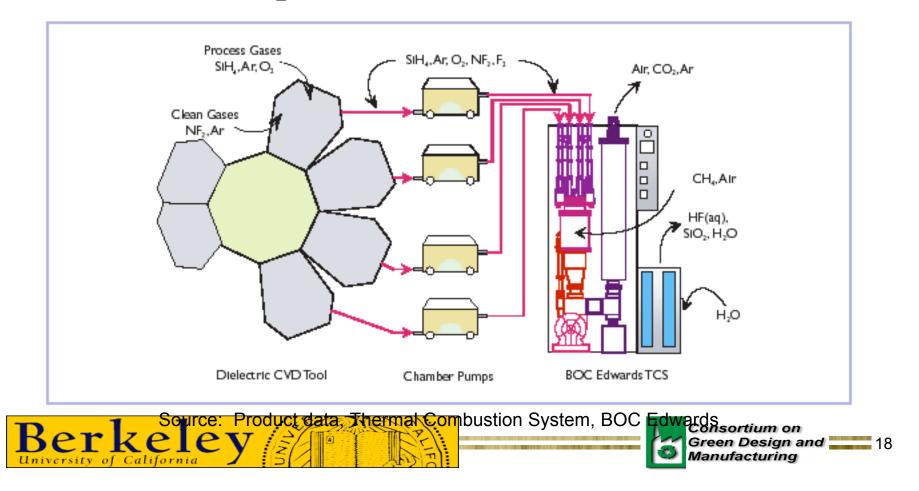
 3 = low capacity





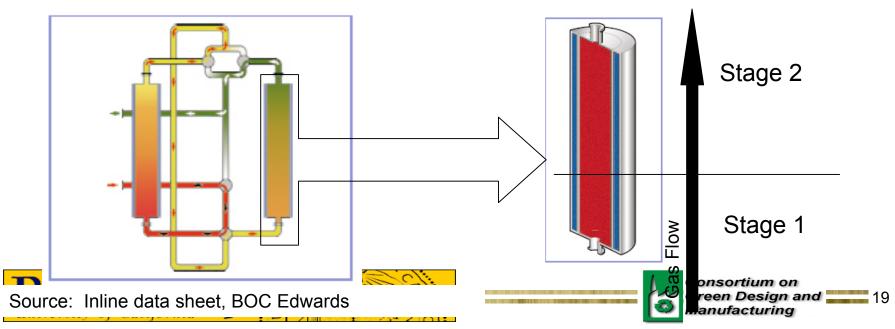
Abatement Technologies Considered

- Option 1. Combustion and Water Scrubbing
 - Use methane, or other fuel to burn flammable emissions and break down F_2 into HF



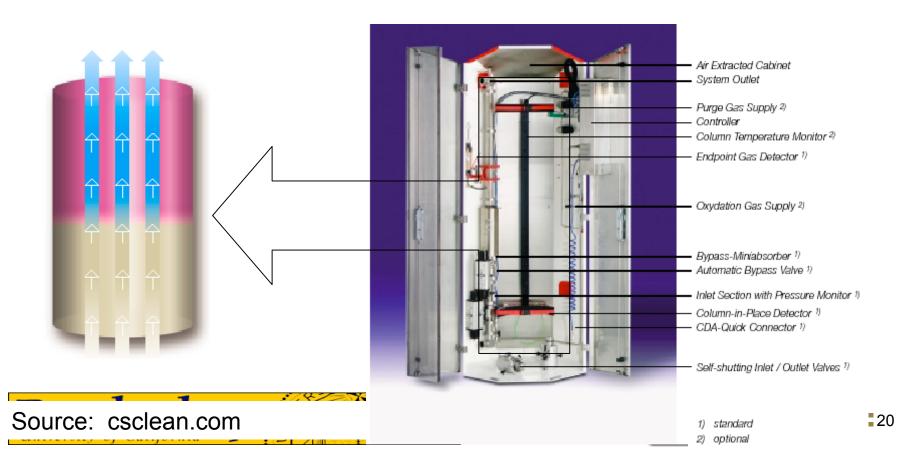
Abatement Technologies Contd.

- Option 2. Hot Bed Technologies
 - Stage 1:
 - A mixture of metals for thermal decomposition (SiH₄) and heat transfer.
 - Strong oxidizing agents to form metal halides
 - Stage 2
 - CaO for removal of acid gases and metal halides. Form salts



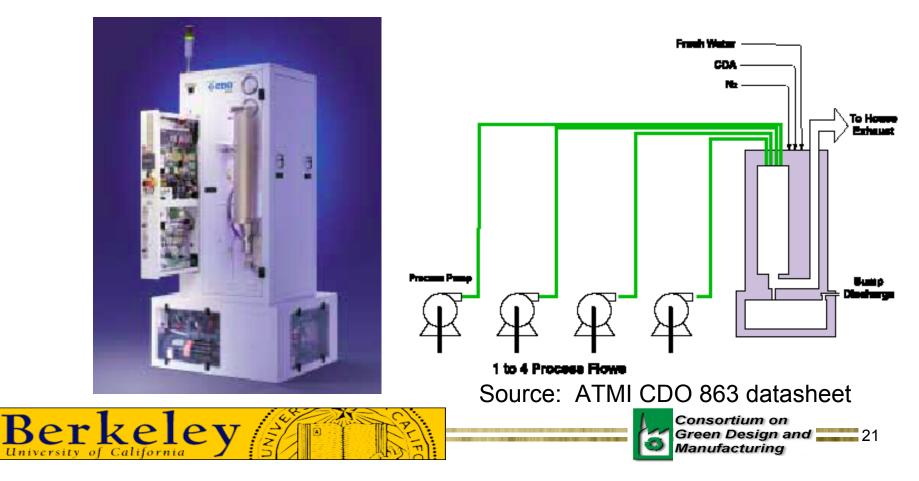
Abatement Technologies Contd.

- Option 3. Cold Bed Technologies
- Dry-bed chemisorption using metal oxides
- Passive operation at ambient temperature



Abatement Technologies Contd.

- Option 4. Electric Oxidation and Water scrubbing
 - Use electric heating
 - Addition of H_2 to reduce large F_2 flows into HF



Sample Data Used

Analysis <u>Units</u>	Combustion and Water Scrubbing	Hot Bed	Cold Bed	Fluoride Treatment	Oxid. and Water Scrubbing
Fixed Costs	~ \$90,000, 200 slm flow rate	~\$59,000 for ~9000 1 HF capacity	~\$78,000 for ~39,000 1 HF capacity	\$2,000,000 for a 100 gpm system	74,000, 200 slm flow rate
Electricity	~1.2 kW	~3 kW	~0.07 kW	13 kW (100 gpm system)	~5.6 kW
Water	City water use calculated based on $\sim 0.2\%$ F- concentration in drain; cooling water at 6 gpm	Cooling water at 6gpm, nominal fuel flow, same as combustion unit	No water use	No water use	City water use calculated based on ~0.2% F- concentration in drain; cooling water at 5 gpm
Consumab les	Spares ~ \$4000/year; fuel use ~37 slm CH ₄	Cartridge capacity is ~9000 1 HF, ~\$1,800	Cartridge capacity is ~39000 1 HF, ~\$4,000	Average incoming HF at 290 ppm; 50 % excess CaCl ₂ and ~400 lb of NaOH/day	Spares ~ \$4000/year, hydrogen use is 1 to 1.5 times expected stoichiometric requirements for avg. fluorine loading (1.3 slm)



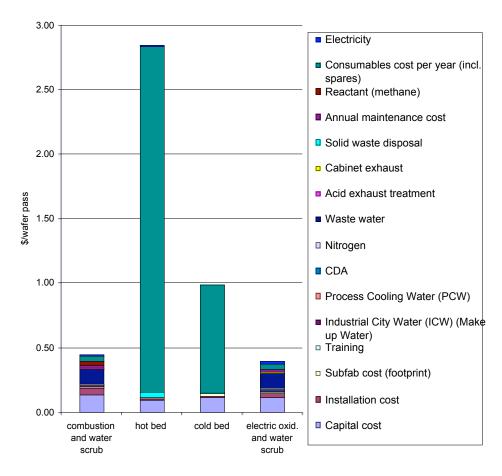


Process Data and Models Used (contd.)

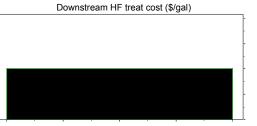
	Analysis <u>Units</u>	Combustion and Water Scrubbing	Hot Bed	Cold Bed	Fluoride Treatment	Oxid. and Water Scrubbing
	Disposal	Disposal costs relate to fluoride treatment models Exhaust costs calculated assuming complete combustion XCH_4 +Y(O ₂ +3.76N ₂) + $ZN_2 = XCO_2 +$ $2XH_2O+$ (3.76Y+Z)N ₂ + (Y- $2X)O_2$ X and Z are known inputs	Spent cartridges are usually a mixture of lime and metal oxides, and are non- hazardous Disposal costs are based on ~30 min changeout time Disposal weight is based on ~4g/l HF capacity Exhaust flow volumes assumed similar to input volumes (largely N ₂)	Spent cartridges are a mixture of silica and metal (usually iron) oxides, and are non- hazardous. Disposal costs are based on ~30 min changeout time Disposal weight is based on actual volume of ~200 l, and bulk density of iron oxides ~1.2g/cc Exhaust flows volumes assumed similar to input volumes (largely N ₂)	16 ppm of HF in discharge; removed fluorine goes to CaF ₂ sludge and pressed to 20% solids	Disposal costs relate to fluoride treatment models
Berk University of C	xele	y s				Consortium on Green Design an Manufacturing

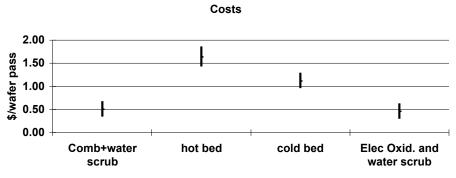


Results - CoO



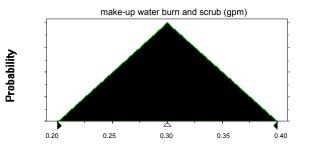
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Oxidation and Water Scrub Systems are the most cost-effective



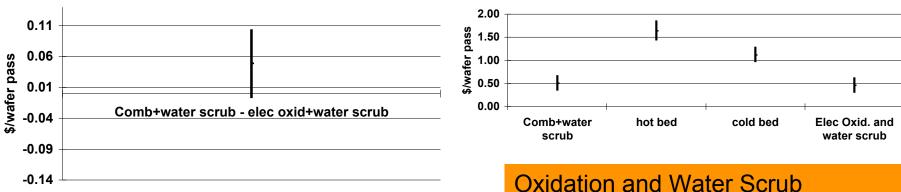






Results - CoO

Cost differences



Target Fore	ecast: co	st- Co	omb+w	s-elec oxi	d+ws	
Installation Cost (\$) - Elec Oxid. ws	28					
capital cost comb+water scrub (\$)	.19					
Capital Cost (\$) - Electric Oxid. ws	12					
methane burn and scrub (lpm)	.09					
installation comb+water scrub	.08					
CH4 costs (\$/1000 cf)	.05					
cooling water burn and scrub	.03			i - 1		
Electricity Use (KW) - Elec Ox. ws	02					
Cooling Water (gpm) - elec oxid. ws	02					
electricity costs (\$/KWhr)	02			i i		
CDA cost (\$/100 scf/yr)	02					
ind water disp cost (\$/gal)	01			1		
Cooling water (gpm) - hot bed	01					
	-1		-0.5	0	0.5	

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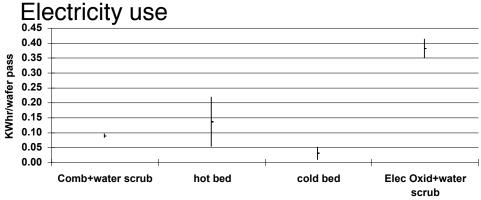
Oxidation and Water Scrub Systems are the most cost-effective

Need to examine capital and installation costs in more detail

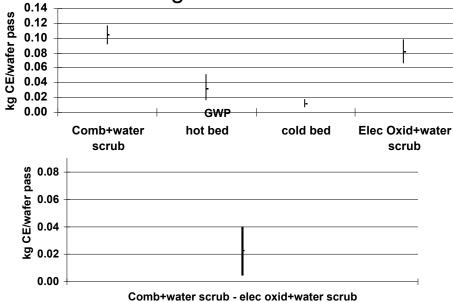
Costs



Environmental impacts



Global warming emissions



•Electric Oxidation systems use the most electricity -

•Carbon intensity of electricity could influence decisions between

•combustion and electric oxidation and water scrubbing systems





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Facility-Wide Environmental Impacts

- Water and Liquid Waste are higher for oxidation systems
- Solid Waste higher for bed systems

GENERAL FACILITY PARAMETERS	
Size of Wafer (inches)	12
Number of Wafer Starts per Week	5000
Number of USG Layers Considered	1

				Electric Oxidation and
	Combustion And			Water
RESOURCES USED	Water scrubbing	Hot bed	Cold bed	Scrubbing
Total Electricity (kWhr/year)	16,168	36,809	859	98,836
Industrial City Water (ICW)				315
(Kgal/year)	316	0	0	
Chemicals and Consumables,				4
(tons/year)	32	9	12	
EMISSIONS				
AIR EMISSIONS				
HAPs Loading, No Abatement (HF				2
Equivalent Tons/Year)	2	2	2	
Global Warming Emissions				22
(tonsCE/year)	26	9	2	
Criteria Air Pollutants (tons/year)	1.27E-01	0	0	1.14E-01
LIQUID				
HF Discharged as Liquid (From POU				0.02
Device) (tons/year)	0.02	0	0	
Final Liquid Waste (Kgal/year)	315	0	0	315
SOLID				
Hazardous Solid Waste (tons/year)	N/A	N/A	N/A	N/A
Non-hazardous Waste (tons/year)	6 ¹	9	12	6 ¹
¹ Mainly CaF ₂ After Fluoride Treatment				





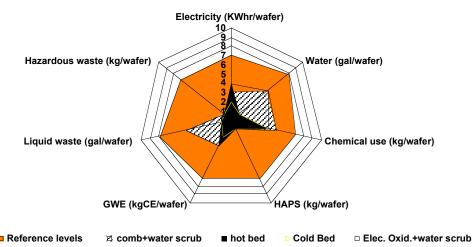
Facility-Wide Environmental Impacts

- Graphical Representation on a logarithmic scale of 1-10
- Can compare to facility reference levels

•Largest profiles for oxidation and water scrub systems —But they have the smallest COO

GENERAL FACILITY PARAMETERS	
Size of Wafer (inches)	12
Number of Wafer Starts per Week	5000
Number of USG Layers Considered	1

Impacts/USG layer



Score	Electricity	Water	Chemicals Used	HAPs
1	<10 Whr/wafer	<1 mgal/wafer	<0.1 g/wafer	<1 mg/wafer
2	1-10 Whr/wafer	1-10 mgal/wafer	0.1-1 g/wafer	1-10 mg/wafer
3	0.01-0.1 kWhr/wafer	0.01-0.1 gal/wafer	1-10 g/wafer	0.01-0.1 g/wafer
4	0.1-1 kWhr/wafer	0.1-1 gal/wafer	10-100 g/wafer	0.1-1 g/wafer
5	1-10 kWhr/wafer	1-10 gal/wafer	0.1-1 kg/wafer	1-10 g/wafer
6	10-100 kWhr/wafer	10-100 gal/wafer	1-10 kg/wafer	10-100 g/wafer
7	100-1000 kWhr/wafer	100-1000 gal/wafer	10-100 kg/wafer	0.1-1 kg/wafer
8	1000-10000 kWhr/wafer	1000-10000 gal/wafer	100-1000 kg/wafer	1-10 kg/wafer
9	10-100 mWhr/wafer	10-100 Kgal/wafer	1-10 tonnes/wafer	10-100 kg/wafer
10	>100 mWhr/wafer	>100 Kgal/wafer	>10 tonnes/wafer	>100-kg/wafer

University of California

Score	GWP (CE)	Liquid Waste	Hazardous Waste
1	<1 g/wafer	<1 mgal/wafer	<0.1 g/wafer
2	1-10 g/wafer	1-10 mgal/wafer	0.1-1 g/wafer
3	0.01-0.1 kg/wafer	0.01-0.1 gal/wafer	1-10 g/wafer
4	0.1-1 kg/wafer	0.1-1 gal/wafer	10-100 g/wafer
5	1-10 kg/wafer	1-10 gal/wafer	0.1-1 kg/wafer
6	10-100 kg/wafer	10-100 gal/wafer	1-10 kg/wafer
7	100-1000 kg/wafer	100-1000 gal/wafer	10-100 kg/wafer
8	1-10 tonnes/wafer	1000-10000 gal/wafer	100-1000 kg/wafer
9	10-100 tonnes/wafer	10-100 Kgal/wafer	1-10 tonnes/wafer
10	>100 tonnes/wafer	>100 Kgal/wafer	>10 tonnes/wafer
		Green Des Manufactu	ign and 28

Health impacts

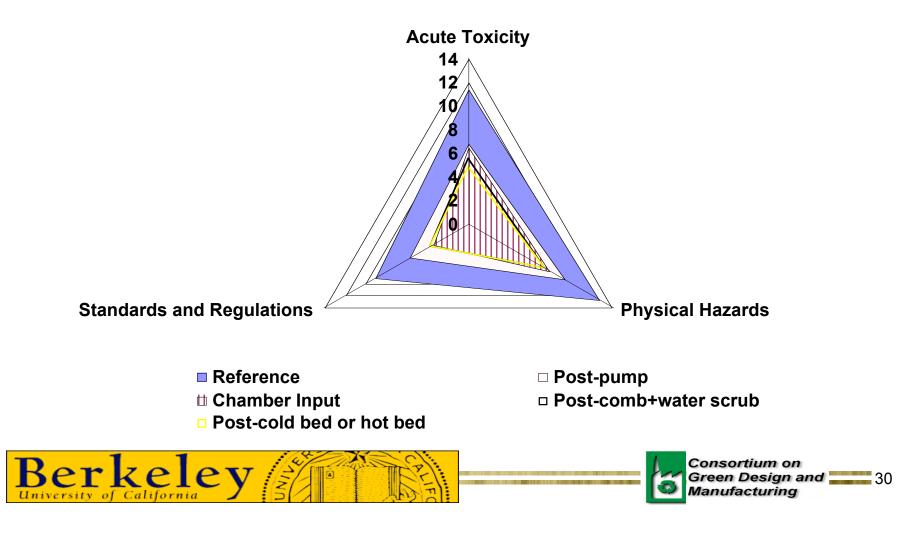
- Three categories
 - Acute toxicity,
 Physical Hazards,
 Standards and
 Regulations
- Compare chemical hazards to "worstcase" Reference chemical

Berkeley

Endpoints	Actual Value	Scaled Score	Reference Chemical	
Category 1: Acute Toxicity			Chemical	
Lethal Dose, 50% of Population (LD50) or	15 ug/m3	9	Sarin	
Lethal Dose (LD)	15 ug/m5	,	Salin	
Lethal Concentration, 50% of population	5 mg/m3	8	Sarin	
(LC50) or Lethal Concentration (LC)	5 mg/m5	0	Saliii	
Threshold Dose Level (TDL)	2 ug/m3	9	Sarin	
Threshold Concentration Level (TCL)	10 mg/m3	10	Lead	
Irritation Dose in Eye (ID (eye))	50 ug	8		
		5	Mercury chloride	
Irritation Dose on Skin (ID (skin)): OVERALL SCORE CATEGORY 1	500 mg		Mercury chloride	
	-	8.17		
Category 2: Physical Hazards	10.00	10		
Flash Point (FP)	-49 °C	10	Pentane	
Lower Explosive Limit (LEL)	1.5%	9	Aniline	
Explosive Limit Range (EL Range)	22%	8	Aniline	
Corrosivity (pH)		1	Hydrochloric acid	
National Fire Protection Agency Flammability (NFPA FR)	4	10	Pentane	
National Fire Protection Agency Reactivity (NFPA RR)	4	10	Nitroglycerine	
National Fire Protection Agency Health (NFPA HR)	4	10	Hydrogen cyanide	
Hazard Management Information System Flammability (HMIS FH)	4	10	Hydrogen cyanide	
Hazard Management Information System Reactivity (HMIS RH)	4	10	Pentane	
Hazard Management Information System Health (HMIS HH)	4	10	Nitroglycerine	
Hazard Management Information System Personal Protective Equipment (HMIS PP)	4	10	Hydrogen cyanide	
OVERALL SCORE CATEGORY 2		9.92		
Standards And Regulations		5.52		
OSHA Permissible Exposure Limit (OSHA PEL)	0.1 mg/m3	6	Mercury chloride	
NIOSH Time Weighted Average (NIOSH TWA)	0.1 mg/m3	5	Mercury chloride	
ACGIH Threshold Limit Value (TLV)	25 ug/m3	4	Mercury chloride	
OSHA/ACGIH Short Term Emission Limit (STEL)	5 mg/m3	5	Hydrogen cyanide	
National Ambient Air Quality Standard (NAAOS)	1.5 ug/m3	7	Lead	
Maximum Contaminant Level (MCL)	10 ug/l	4	Antimony	
Secondary Max Contaminant Level (SMCL)	0.2 mg/l	2	Hydrogen Cyanid	
Reportable Quantity (RQ)	1 lb	9	Cyclophosphamid	
OVERALL SCORE CATEGORY 3		8.10		

Health Hazards

- Three categories
 - Acute toxicity, Physical Hazards, Standards and Regulations



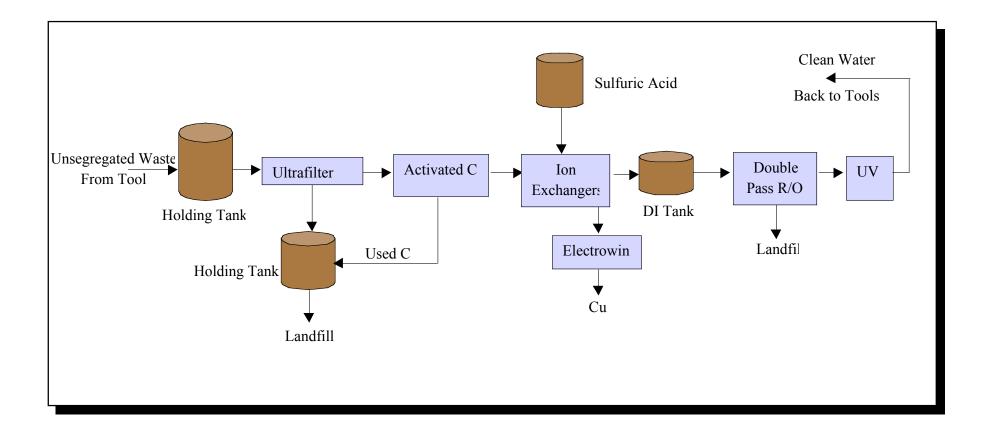
3. Case Study 2 - Informing Design of Equipment

- Copper CMP Waste Treatment
- Focus on how local regulatory and economic factors affect system design
- Examine Two Facility Waste Treatment Systems
 - Treat and Recycle
 - Treat and Discharge



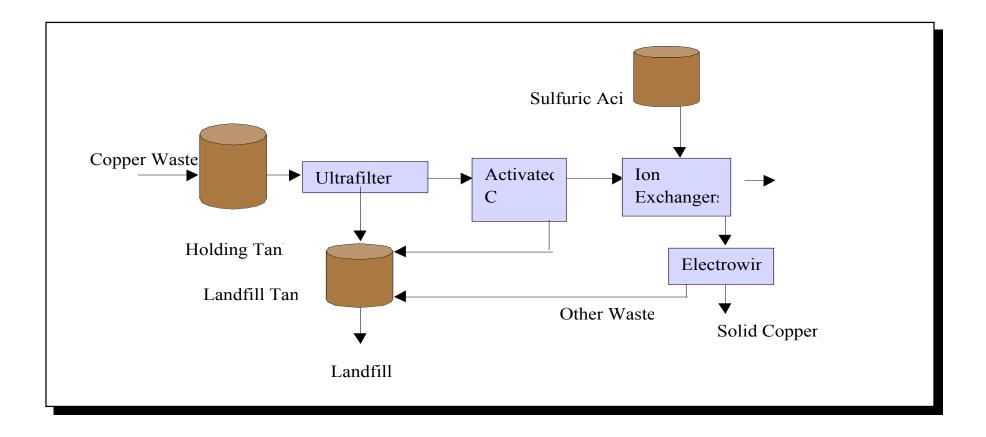


Facilities system: Treat and recycle



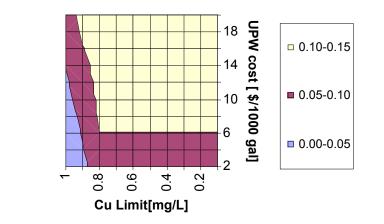


Facilities system: Treat and Discharge

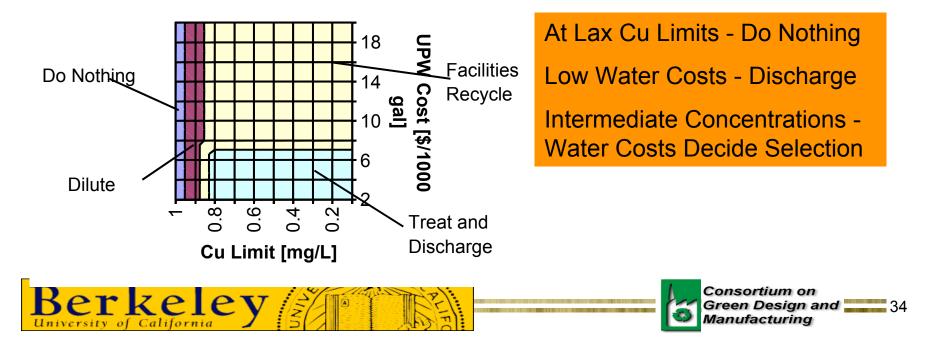




Overall Decision Map



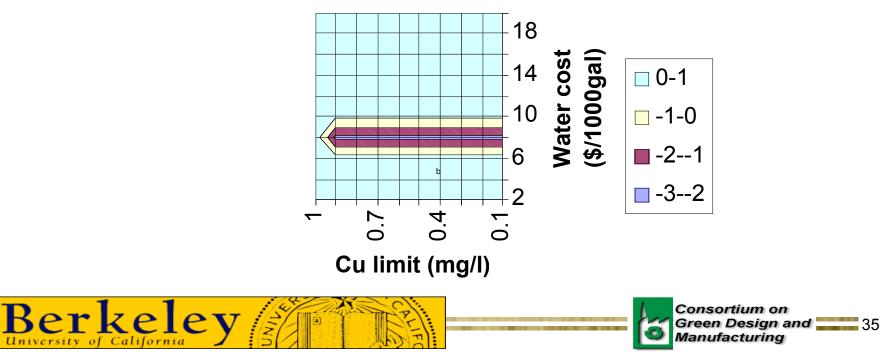
Incremental Cost over 'minimum' requirements (replacement of DIW+AWN discharge costs)



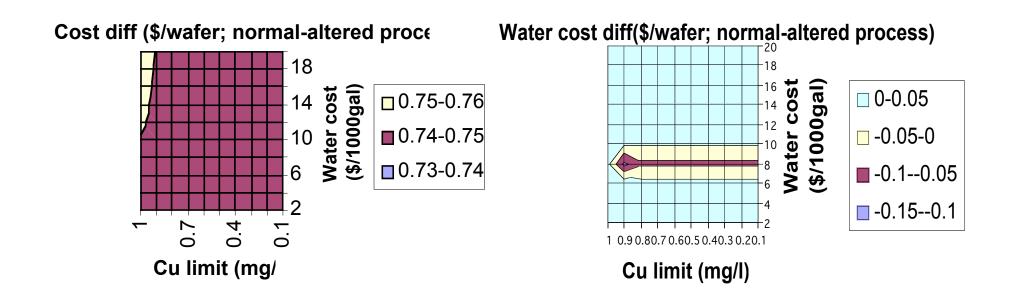
Copper CMP process alterations

- Scenario 1: Identify high water use steps
 - Decrease rinse times on platens (decreased water use) by decreasing unbalanced MRR.
 - Increased polish time, but decreased CoO
 - Increased water use with new process at \$8/1000gal
 - owing to increased selection of T&D as most cost effective option

Water diff (gpm; normal-altered processes)



CMP process alterations: Scenario 1





4. Conclusions

- Expand the library of models and data to cover all the fab operations (costs, resource use, emissions)
 - Use the hierarchical data structure
- Run more detailed case studies
- Combine fab-level analysis to upstream and downstream life cycle cost and environmental data - hybrid approaches
 Collaborate with MIT, U of A, NCSU
- Other directions QSAR, chemical screening, etc.



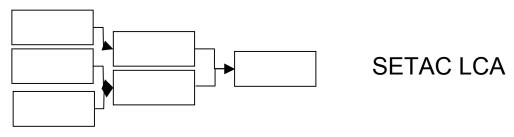
Additional Slides



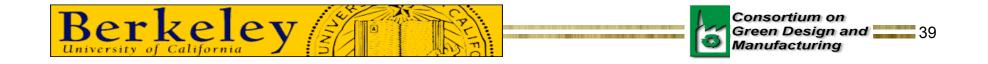
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Upstream life cycle impacts

- Main LCA obstacles
 - Effort and time for detailed SETAC life cycle inventory analyses
 - several months of data collection efforts
 - Boundary problems remain
 - Studies revisited with changes in equipment/processes and chemical sets,
 - Track comprehensive environmental impact data throughout the supply chain.



• Therefore, use a hybrid LCA approach



Economic Input Output LCA

What is the EIOLCA approach?

Developed by Carnegie Mellon University

- Sectoral approach using Leontief Matrices
- Basis of matrix unit economic output of one sector links to economic outputs of many other sectors.
- The Department of Commerce's 485x485 commodity input-output model of the US economy serves as basis.
- Potentially more inclusive than typical SETAC based LCA methods.
- Dollar values are translated to environmental impacts using several different available databases.

Output from sectors	Input to sectors				Intermediate output O	Final demand	Total output	
	1	2	3	n		F	X	
1	X ₁₁	X ₁₂	X ₁₃	X _{1n}	<i>O</i> ₁	F ₁	X ₁	
2	X ₂₁	X ₂₂	X ₂₃	X _{2n}	02	F ₂	X ₂	
3	X ₃₁	X ₃₂	X ₃₃	X _{3n}	<i>O</i> ₃	F ₃	X ₃	
n	X _{n1}	X _{n2}	X _{n3}	X _{nn}	0 _n	F _n	X _n	
Intermediate input /	<i>I</i> 1	<i>I</i> ₂	<i>I</i> ₃	I _n	!	!	!	
Value added V	<i>V</i> ₁	V ₂	V ₃	V _n	!	GDP	!	
Total input X	<i>X</i> ₁	X ₂	X ₃	X _n	!	!	!	

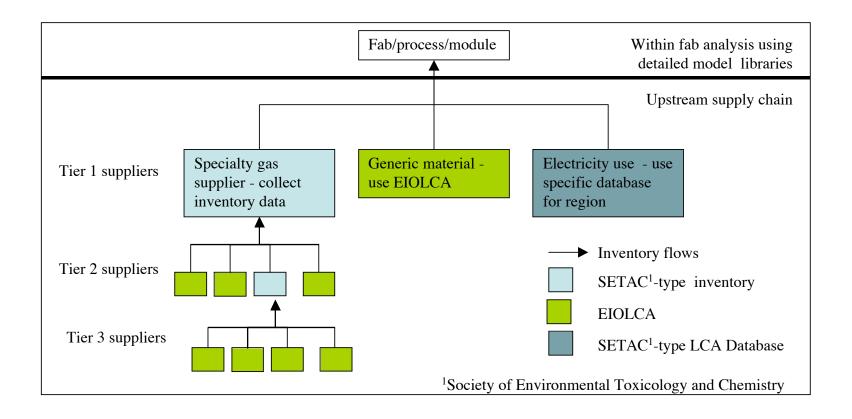
Source: www.eiolca.net





Upstream life cycle impacts (contd.)

• So - adopt a hybrid approach





Hazard Scaling

Category 1: Acute Toxicity										
	Endpoints									
Scaled Score	LD ₅₀ or LD	LC ₅₀ or LC	TDL	TCL	ID (eye)	ID (skin)				
1	>1 kg/kg	>10 kg/m ³	>100 g/kg	>1 kg/m ³	>100 ml, 100 g	>1 L, 1 kg				
2	<1 kg/kg	<10 kg/m ³	<100 g/kg	$<1 \text{ kg/m}^3$	<100 ml, 100 g	<1L, 1 kg				
3	<100 g/kg	<1 kg/m ³	<10 g/kg	<100 g/m ³	<10 ml, 10 g	<100 ml, 100 g				
4	<10 g/kg	<100 g/m ³	<1 g/kg	<10 g/m ³	<1 ml, 1 g	<10 ml, 10 g				
5	<1 g/kg	$<10 \text{ g/m}^{3}$	<100 mg/kg	$<1 \text{ g/m}^{3}$	<100 µL, 100 mg	<1 ml, 1 g				
6	<100 mg/kg	$<1 \text{ g/m}^{3}$	< 10 mg/kg	<100 mg/m ³	<10 µL, 10 mg	<100 µL, 100 mg				
7	< 10 mg/kg	<100 mg/m ³	<1 mg/kg	$< 10 \text{ mg/m}^{3}$	<1 µl, 1 mg	<10 µL, 10 mg				
8	<1 mg/kg	$< 10 \text{ mg/m}^{3}$	<100 µg/kg	<1 mg/m ³	<100 nl, 100 µg	<1 µL, 1 mg				
9	<100 µg/kg	$<1 \text{ mg/m}^3$	<10 µg/kg	$<100 \ \mu g/m^{3}$	<10 nl, 10 µg	<100 nL, 100 µg				
10	<10 µg/kg	<100 ug/m ³	<1 µg/kg	$<10 \ \mu g/m^{3}$	<1 nL, 1 µg	<10 nL, 10 µg				

Catego	ry 3: Standards an	d Regulations						
	Endpoints							
Scaled	STEL	OSHA PEL (8	NIOSH			RQ	MCL/MC	
Score	(OSHA/ACGIH)	hr)	TWA (8 hr)	TLV (8 hr)	NAAQS	(lbs)	LG	SMCL
1	>10 g/m ³	>1 g/m ³	>1 g/m ³	>10 mg/m ³	>1 g/m ³	!	>1 g/L	>1 g/L
2	<10 g/m ³	$<1 \text{ g/m}^{3}$	$<1 \text{ g/m}^{3}$	< 10 mg/m ³	<1 g/m ³	!	<1 g/L	<1 g/L
			<100				<100	<100
3	<1 g/m ³	<100 mg/m ³	mg/m ³	<1 mg/m ³	<100 mg/m ³	!	$\mu g/L$	μg/L
								<10
4	<100 mg/m ³	< 10 mg/m ³	$< 10 \text{ mg/m}^{3}$	<100 µg/m ³			<10 µg/L	µg/L
5	< 10 mg/m ³	$<1 \text{ mg/m}^3$	$<1 \text{ mg/m}^3$	$<10 \ \mu g/m^{3}$	<1 mg/m ³	<5000	<1 µg/L	<1 µg/L
					<100			<100
6	<1 mg/m ³	<100 µg/m ³	$<100 \ \mu g/m^{3}$	$<1 \ \mu g/m^{3}$	ug/m ³	<1000	<100 ng/L	ng/L
								<10
7	$<100 \ \mu g/m^{3}$	$<10 \ \mu g/m^{3}$	$<10 \ \mu g/m^{3}$	<100ng/m ³	<10 ug/m ³	<100	<10 ng/L	ng/L
8	$<10 \ \mu g/m^{3}$	$<1 \ \mu g/m^3$	<1 μ g/m ³	<10 ng/m ³	<1 ug/m ³	<10	<1 ng/L	<1 ng/L
								<100
9	$<1 \mu g/m^{3}$	<100ng/m ³	<100ng/m ³	<1 ng/m ³	<100ng/m ³	1	<100 pg/L	pg/L
								<10
10	<100ng/m ³	<10 ng/m ³	<10 ng/m3	<100 pg/m ³	<10 ng/m ³	<1	<10 pg/L	pg/L

Category 2: Physical Hazards												
Endpoints												
Scaled Score	FP (C)	LEL	EL Range	рН	HMIS HH	HMIS FH	HMIS RH	HMIS PP	NFPA FR	NFPA RR	NFPA HR	
1	> 121							A,B			!	
2	<121		!	pH<6,>8.5		!	!	С	!		!	
3	!	!	!	!	1	1	1	D	1	1	1	
4	<87.8	!	<5%	pH<5,>9.5	!	!	!	E	!	!	!	
5	!	>5%	>5%		2	2	2	F	2		2	
6	<60	<5%	>10%	pH<4,>10.5				G		2	!	
7	!	<4%	>20%	!	!	!	!	Н	!	!	!	
8	<37.8	<3%	>30%	pH<3,>11.5	3	3	3	Ι	3	3	3	
9	!	<2%	>40%		!	!	!	J	!	!	!	
10	<22.8	<1%	>50%	pH<2,>12.5	4	4	4	К	4	4	4	





Hazard Equations

Category Score, j, of a chemical i:

 $C_{i,j} = \sum_{k=1}^{m} \frac{X_{i,j,k}}{m}$ With m endpoints with scores X

Process Score, I, for category j

$$PC_{i,j} = \log M_p + \log \sum_{i=1}^{L} (m_i \cdot \log^{-1} C_{i,j})$$

m_i is the mass fraction of chemical i

Reference calculation, for category j

 $PC_{\text{Ref},j} = \log M_{\text{Ref}} + C_{\text{Ref},j}$ M_{Ref} is the largest process mass compared

