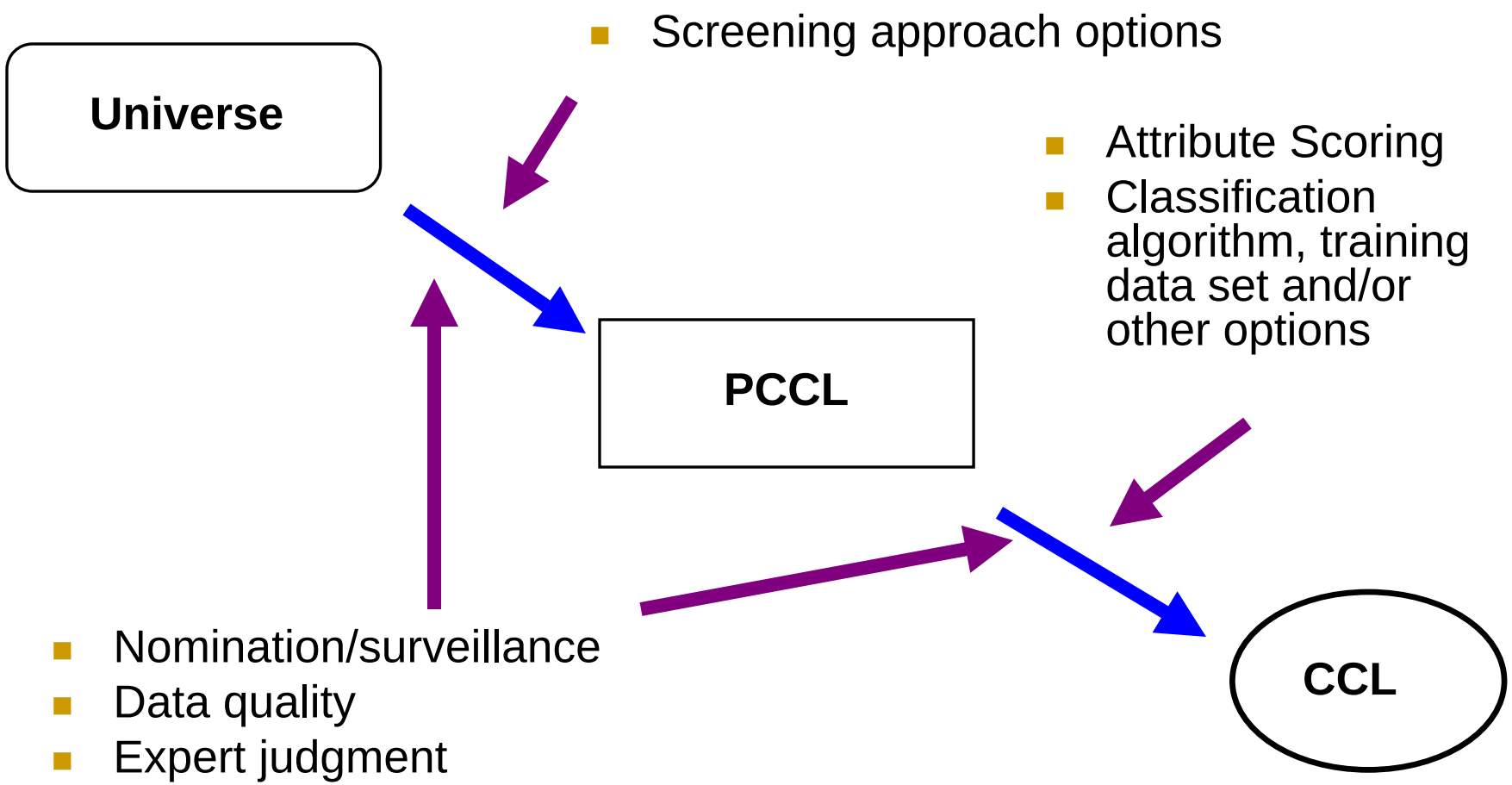
Screening the CCL Universe to the PCCL: Evaluation of Options for Screening Approaches

Report for the NDWAC CCL Work Group

Plenary Meeting

November 13 - 14, 2003

Critical path decisions



Key Issues for Universe to PCCL Screening

1. **What are the options for Screening Criteria for the Universe to the PCCL?**
2. What are the pros/cons, and implications of each type of approach?
3. Which elements should be used for screening?
4. Are there recommendations on how EPA should pursue this?

Options for Screening Criteria

1. Qualitative
   - Nature of information – available data is screen
   - Contaminants that line up to the Gates go through
2. Semi-quantitative
   - Pragmatic (i.e. using the number of or % of contaminants) or
   - Substantive (i.e. using technical criteria such as thresholds) screens
     - Binning of chemicals
     - Ranking of chemicals
     - Other simple evaluations
3. Quantitative
   - Quantitative comparison of chemicals with demonstrated water occurrence and demonstrated health effects

   (i.e. Gate 1)

Key Issues for Universe to PCCL Screening

1. What are the alternatives for Screening Criteria for the Universe to the PCCL?
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QUALITATIVE APPROACH

- Contaminants that line up to a Gate will pass through to the PCCL
- Example CCL Universe Data Set Analysis

Category or Criteria of Data/Information Available; Gate Screening Criteria	Number of Chemicals in Example Data Set Meeting the Criteria	Percentage of Chemicals in Example Data Set Meeting the Criteria
Health Effects DATA AND Occurrence DATA; **Gate 1**	211	1.89%
Health Effects Information AND Occurrence DATA; **Gate 2**	27	0.24%
Health Effects DATA AND Occurrence Information; **Gate 3**	714	6.42%
Health Effects Information AND Occurrence Information; **Gate 4**	789	7.09%
Subtotal of Candidates Through Gates 1-4:	**1,741**	**15.6%**

Qualitative Approach – Pros & Cons

PROs	Transparent – easy to describe data gathering process Inclusive – sends all contaminants with the health effects and occurrence data and/or information to the PCCL
CONs	May be too inclusive or not selective enough for the downstream processes.

Binning Approach

- Preliminary Analysis (results presented at the Sept. plenary)
  - Compared bins delimited by data set (pragmatic) vs. values (substantive)
  - Data Set: QSAR Data
  - Data Elements - Solubility and LOAEL
  - Found :
    - Binning approach is simple, but binning criteria affect results
    - Generally see similar results in bins, but get more contaminants using Substantive (value) criteria
    - Concerns were raised over: data elements used, and use of bins rather than ranking

- NDWAC members requested:
  - Add LD50, octanol water partition coefficient (log Kow), and Henry's Law Constant (HLC) as elements
  - Compare binning to ranking
  - Conduct a quantitative screening for Gate 1

Ranking Approach

- For each data element, chemicals were ranked in order by the magnitude of their values, from 1 (greatest concern) to 277 (least concern) (Chemicals having identical values were assigned the same rank).
- Ranks were normalized (put on the same scale from 0-1) for each element, then summed across elements. The sums were also ranked.
- Ranks across different combinations of elements were compared.

Ranking Data Element Correlation Analyses

- Low for health effect data elements (both absolute values and rankings) – was anticipated

Table 1 Health Effects	LD50 Normal Rank	LOAEL Normal Rank
LD50 Normal Rank	1	
LOAEL Normal Rank	0.45	1

- High for solubility and log K_{ow} (rankings)
- HLC not correlated to either solubility or log K_{ow}

Table 2 Occurrence elements	Log Kow Normal Rank	Solubility Normal Rank	HLC Normal Rank
Log Kow Normal Rank	1		
Solubility Normal Rank	0.86	1	
HLC Normal Rank	0.19	-0.01	1

Binning and Ranking Correlation Results

- Compared chemicals passing through binning using different combinations of elements (e.g. LOAEL & Kow vs. LOAEL &HLC)
  - Binning and ranking and yield similar results for screening, at least 60 percent agreement for data element combinations
- Compared the percentage of chemicals passing through binning by different combinations
  - Maximum overlap is 77%
- Identified the lowest ranking chemical in each bin combination
  - Got greater numbers of contaminants with ranking than binning

Binning/Ranking - Pros and Cons

Pragmatic Approach (Binning by %, ranking)	
PROs	Simple- requires only comparison to criteria Automatable- analysis can be structured to easily automate Transparent – can easily describe criteria Somewhat Selective - identifies most important contaminants, but perhaps not all.
CONs	Establishing criteria based on resources (e.g. want 1000 contaminants on PCCL/or Top 25%) may be difficult to agree upon Inclusivity may vary depending on available data

Binning and Ranking - Some Pros and Cons

Substantive (Binning by value; ranking)	
PROs	Simple- requires only comparison to criteria Automatable- analysis can be structured to easily automate Transparent - can easily describe criteria Inclusive - substantive criteria can be set to be inclusive but also can be exclusive Selective- criteria can be based on selectivity
CONs	Selected elements may not adequately capture key criteria May not be Inclusive if look only for a particular data element

Quantitative Approach (for Gate 1 Contaminants)

- For quantitative comparisons, health effects and occurrence data were compiled, and a ratio of Max Occ:Min HE was calculated for each set of available data elements.
- For 277 binning/ranking chemicals, 33 were in Gate 1, but most were Not Detected, so did not have Occurrence available in data set. Comparison was possible for 7 chemicals.
- Used different data set of 85 chemicals (from Example CCL Universe) for the Gate 1 quantitative analysis (no comparison to semi-quantitative)
- Results – Max Occurrence: Min Health Effects Ratios
  - 43% of the chemicals had ratios >1
  - 55.8% of the chemicals had ratios >0.1
  - 69.8% of the chemicals had ratios >0.01

Quantitative Approach - Pros & Cons

PROs	Inclusive - criteria can be set to be inclusive (or not!) Selective- criteria can be based on selectivity
CONs	Requires identifying many types of data and information Require significant documentation

Options for Universe to PCCL Screening

- Qualitative
- Semi-quantitative
  - Pragmatic/substantive
    - Binning
    - Ranking
    - Other simple prioritization
- Quantitative - Combination of Screening Approaches
    - Gate 1 Quantitative
    - Gate 2,3 Semi-quantitative
    - Gate 4 Semi-quantitative (higher/lower criteria)

Proposed Principles for Universe to PCCL Screening Approach and Criteria

- **Simple** - approach should not be overly complex or require significant analysis
- **Automatable** - approach should be designed to require a relatively low level of effort
- **Transparent** - approach and criteria should be clear
- **Inclusive** - approach should strive to include rather than exclude contaminants; criteria should be broad enough to be inclusive; elements used should allow inclusivity
- **Substantive** - approach should strive to identify contaminants that may be important for future CCLs

Discussion Questions for Universe to PCCL Screening

- Do you have recommendations for principles to consider when selecting a screening option?
- Do you agree that the options described are the correct set of screening options to consider? Are there others?
- What do you see as the advantages and disadvantages of these options?
- What do you recommend or what criteria should be used for how to choose a cutoff for entry to the PCCL in binning or ranking approaches?
- Do you agree with the five data elements proposed for the option that is based on use of a limited number of data elements? Should there be others or fewer?
- Which screening approach options do you lean toward? Are any unacceptable?
- Are any additional technical analyses needed to prepare you to make a final recommendation in January?

Appendix

- Data Sources for Binning/Ranking Analyses
- Binning Results for Data Elements
- Quantitative Analyses Results
- Summary of Contaminants with Available Data Elements from the Example Dataset

Data and Sources Binning/Ranking Analysis

- Data Set of 277 chemicals with all five data elements
- Sources of LOAELs/LD_{50}s
  - Measured: Registry of Toxic Effects of Chemical Substances (RTECS) (cumulative dose/duration)
  - Modeled: TOPKAT QSAR model - LOAEL and LD_{50} modules
- Sources of Solubility/Log K_{ow}/HLC
  - Measured: SRC CHEMFATE and PHYSPROP databases; HSDB; NTP; MacKay et al., (1999); IPCS
  - Modeled: WSKOWWIN, KOWWIN, and HENRYWIN (QSAR models from EPI Suite)

Binning by Substantive Criteria

Ranges for bins were obtained from authoritative sources (e.g. Hodge and Sterner 1956, Lyman *et al*.)

	Bin 1 (Highest Concern)			Bin 2 (Moderate Concern)			Bin 3 (Lowest Concern)		
Data Elements	Range	# Chem	% Chem	Range	# Chem	% Chem	Range	# Chem	% Chem
LD50	< 50 mg/kg	24	8.66	50 - 500 mg/kg	72	26	> 500 mg/kg	181	65.3
LOAEL	< 0.1 mg/kg-day	12	4.33	0.1 - 100 mg/kg-day	223	80.5	> 100 mg/kg-day	42	15.2
Solubility	> 1,000 mg/L	99	35.7	1 - 1,000 mg/L	123	44.4	< 1 mg/L	55	19.9
Log Kow	< 1	67	24.2	1 - 4	126	45.5	> 4	84	30.3
Henry's Law Constant	< 1 X 10-5	191	69	1 X 10-5 - 1 X 10-3	61	22	> 1 X 10-3	25	9.03
	atm-m3/mol			atm-m3/mol			atm-m3/mol		

Quantitative Results – Gate 1

HE Data Element	Number of Chemicals	Occ:HE Values > 1	Percent of Total	Occ:HE Values > 0.1	Percent of Total	Occ:HE Values > 0.01	Percent of Total
All Data Elements	85	37	43.0%	48	55.8%	60	69.8%
ADI	1	0	0.0%	0	0.0%	1	100.0%
Lifetime Risk Level	17	6	35.3%	11	64.7%	13	76.5%
LOAEL	3	0	0.0%	0	0.0%	0	0.0%
MCL	3	1	33.3%	1	33.3%	3	100.0%
Minimum Risk Level	3	2	66.7%	2	66.7%	3	100.0%
Preliminary Remediation Goal	17	8	47.1%	12	70.6%	16	94.1%
RBC	13	9	69.2%	9	69.2%	11	84.6%
RfD	15	9	60.0%	11	73.3%	11	73.3%
Risk Threshold	2	2	100.0%	2	100.0%	2	100.0%
Slope Factor	1	0	0.0%	0	0.0%	0	0.0%
TD50	9	0	0.0%	0	0.0%	0	0.0%
TDLo - Lowest published toxic dose	1	0	0.0%	0	0.0%	0	0.0%

Finding: A+ C Quantitative Approach for derived (adjusted) Health Effect values

Occurrence Data Elements in CCL Universe Example Data Set	
Analyses	449
Max	251
Percent Detects	203
Median	159
Mean	151
Min	151
Detects	148
Percent PWS Detects	76
90th Percentile (Detects)	41
99th Percentile (Detects)	41
Max of Max Concentration	16
Number of States	16
Non-Detects	10
Non-Detects (Sites)	10
Percent Location Detects	10
Detects (Sites)	9
Threshold Exceedence	3
Wastewater Concentration	2
Concentrations	1

CCL Universe Example Data Set (~11,000)

Data Elements	Data Set	Total Number of Chemicals
LOAEL	IRIS	5
	RTECs	14
	LOAELs collected for Binning	190
	QSAR TOPKAT	387
LD50	CPH (All Tables)	579
	LD50s for Binning	361
	QSAR TOPKAT	68
Kow	RAI_Chemical_Factors	661
	QSAR (of 695)	664
HLC	RAI_Chemical_Factors	633
	PRG_VOC_Phys_Chem_data	180
	QSAR (of 695)	647
Solubility	RAI_Chemical_Factors	664
	PRG_VOC_Phys_Chem_data	90
	QSAR (of 695)	695

Health Effects Data Elements in CCL Universe Example Data Set	
TD50	1351
LD50	824
RfD	573
Preliminary Remediation Goal (MCLG?)	567
RBC	434
Lifetime Risk Level	422
Slope Factor	316
ADI	239
LOAEL	214
MCL	178
HA (DWEL, 1 day, 1o day)	168
CSFo	134
Lifetime Cancer Risk	125
Minimum Risk Level	123
MCLG	87
CSFi	76
TDLo - Lowest published toxic dose	18
LDLo - Lowest published lethal dose	10
TD05	7