Additivity and Apportionment Refresher

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Additive Effects of Chemicals

- Concept is simple
  - When exposed to more than one chemical, their effects may combine
- Several possibilities for cumulative effects
  - Interact to produce greater toxicity than expected
  - Interact to produce less toxicity than expected
  - Not interact -- effects are simply additive
- Evaluation of cumulative effects of chemicals is not new in risk assessment
  - Basic approaches date back at least to EPA RAGS guidance in 1989

Changes with Ch. 62-780 FAC

- Two approaches are available for site assessment:
  - Simple: Compare concentrations with cleanup targets in look-up tables.
  - More complicated: Use basic risk assessment steps in setting cleanup targets and determining whether they have been met.

Changes with Ch. 62-780 FAC

- Key risk assessment aspects
  - Using a 95% UCL as the EPC (with a few exceptions)
  - Ability to use site-specific exposure scenarios
  - Factoring potential additive effects of chemicals in determining cleanup targets
  - “Package deal” -- all are incorporated together

Cherry Picking

- If only conservative factors are modified/refined, overall conservatism of criteria is diminished.
- If the goal is to produce a more refined, accurate, site-specific assessment, should take a balanced approach of assessing inherently conservative and unconservative factors.
- Under Ch. 62-780, this means that if you use 95% UCL and/or alternative exposure assumptions, you have to also address the issue of potential additive effects of chemicals.

Key Misconception

- "Incorporation of more site-specific information always leads to a less expensive cleanup."
- Stems from assumption that all aspects of the derivation of default criteria are conservative.
  - Many of the models and assumptions are in fact conservative, but not all
  - Some assumptions are neutral
  - Some models/assumptions are un-conservative
  - Overall balance is conservative, which is important for regulatory purposes

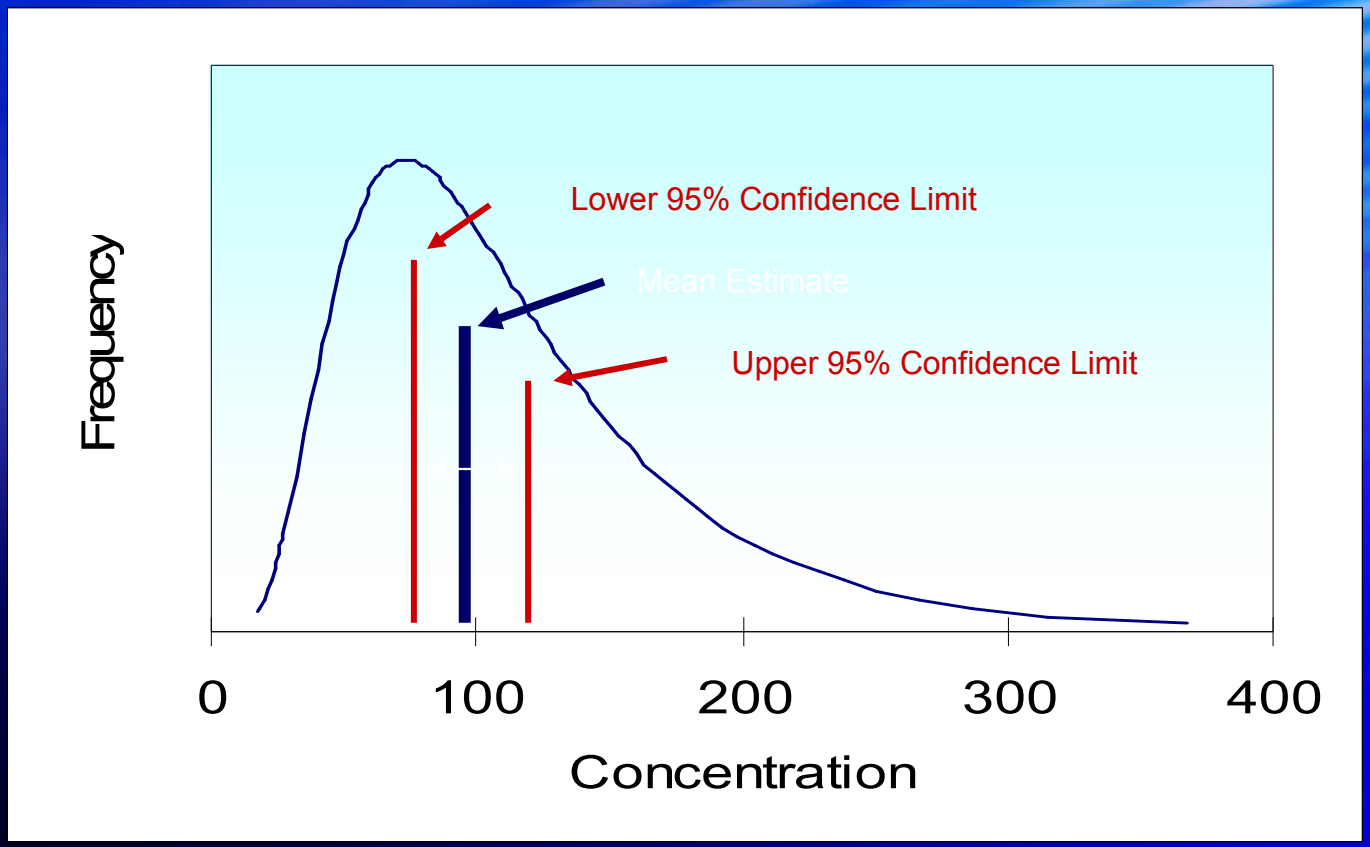
95% UCL

- Rationale as an EPC is that it represents a reasonable exposure concentration *within an exposure unit* over a *prolonged period of time*.
  - Exposure unit - Must identify areas over which individuals will have equal and random contact.
  - Applicable for chronic, but not necessarily acute exposure.

95% UCL

- Several ways to calculate a 95% UCL
  - Best method for a given data set depends upon the number of samples, variability, skewness, and percent non-detects.
  - FLUCL and ProUCL 3 both calculate a 95% UCL; only FLUCL is tested to work with more than 15% ND's. [Note: ProUCL 4 will reportedly handle censored data better than ProUCL 3)

95% UCL


Lower 95% Confidence Limit
Mean Estimate
Upper 95% Confidence Limit
Frequency
0
100
200
300
400
Concentration

How many samples?

- A reliable 95% UCL calculation requires enough samples to determine the shape of the distribution.
  - We require at least 7 detects (ND's don't help); at least 10 total samples
- Highly censored data sets (>70% ND) are a problem.

Bounding Method

- A 95% UCL can be calculated with as few as 3 detects using the Bounding Method.
- FLUCL reverts to the Bounding Method automatically if there are less than 7, but 3 or more detects.
- The Bounding Method calculates a "worst case" 95% UCL from the censored data set, not an actual 95% UCL

cPAHs, PCDDs and PCDFs

- Each is a class of closely related chemicals. Chemicals within each class are thought to produce toxicity through the same mode of action. When combined, they are thought to produce effects through dose addition.
- Concentrations of members of the class are converted to toxicologically-equivalent concentrations of an index chemical.
  - For cPAHs, the index chemical is benzo(a)pyrene
  - For dioxins and furans, the index chemical is 2,3,7,8-TCDD

Toxic Equivalents

- Toxic equivalents (TEQs) are calculated by multiplying the concentration by the Toxic Equivalency Factor (TEF) for that chemical.
- The TEQs for each member of the class are summed to obtain the total for the mixture, e.g., in benzo(a)pyrene equivalents for PAHs
- Soil cleanup targets for these classes are expressed in terms of index chemical equivalents.
  - Furans and dioxins share the same mode of action and are combined.

TEFs

- TEFs in Technical Report for Chapter 62-777 FAC
  - Carcinogenic PAHs (7 chemicals; Table 20)
  - Polychlorinated dioxins and furans (7 dioxins, 10 furans; Table 19)
- New TEFs are available

TEFs for PCBs

Congener	IUPAC Chlorobiphenyl Prefix	2005 WHO TEF
PCB-77	3,3',4,4'-Tetra-	0.0001
PCB-81	3,4,4',5-Tetra-	0.0003
PCB-105	2,3,3',4,4'-Penta-	0.00003
PCB-114	2,3,4,4',5-Penta-	0.00003
PCB-118	2,3',4,4',5-Penta-	0.00003
PCB-123	2,3',4,4',5'-Penta-	0.00003
PCB-126	3,3',4,4',5-Penta-	0.1
PCB-156	2,3,3',4,4',5-Hexa-	0.00003
PCB-157	2,3,3',4,4',5'-Hexa-	0.00003
PCB-167	2,3',4,4',5,5'-Hexa-	0.00003
PCB-169	3,3',4,4',5,5'-Hexa-	0.03
PCB-189	2,3,3',4,4',5,5'-Hepta-	0.00003

Life is easy …

- FDEP has developed calculator spreadsheets to facilitate expressing data in toxic equivalents.
- A spreadsheet is available for cPAHs and another is available for dioxins/furans.
- The spreadsheet will calculate total equivalents for each sample and compare with default SCTL criteria.

Additivity of Other Chemicals

- If cleanup targets are treated as not-to-exceed values, no apportionment of the cleanup goals is needed.
- If cleanup targets are compared with 95% UCL values, or alternative targets are used, cleanup targets must be apportioned such that:
  - The total excess cancer risk represented by the targets does not exceed 10^{-6}.
  - The total hazard index (HI) for all relevant toxic endpoints does not exceed 1.

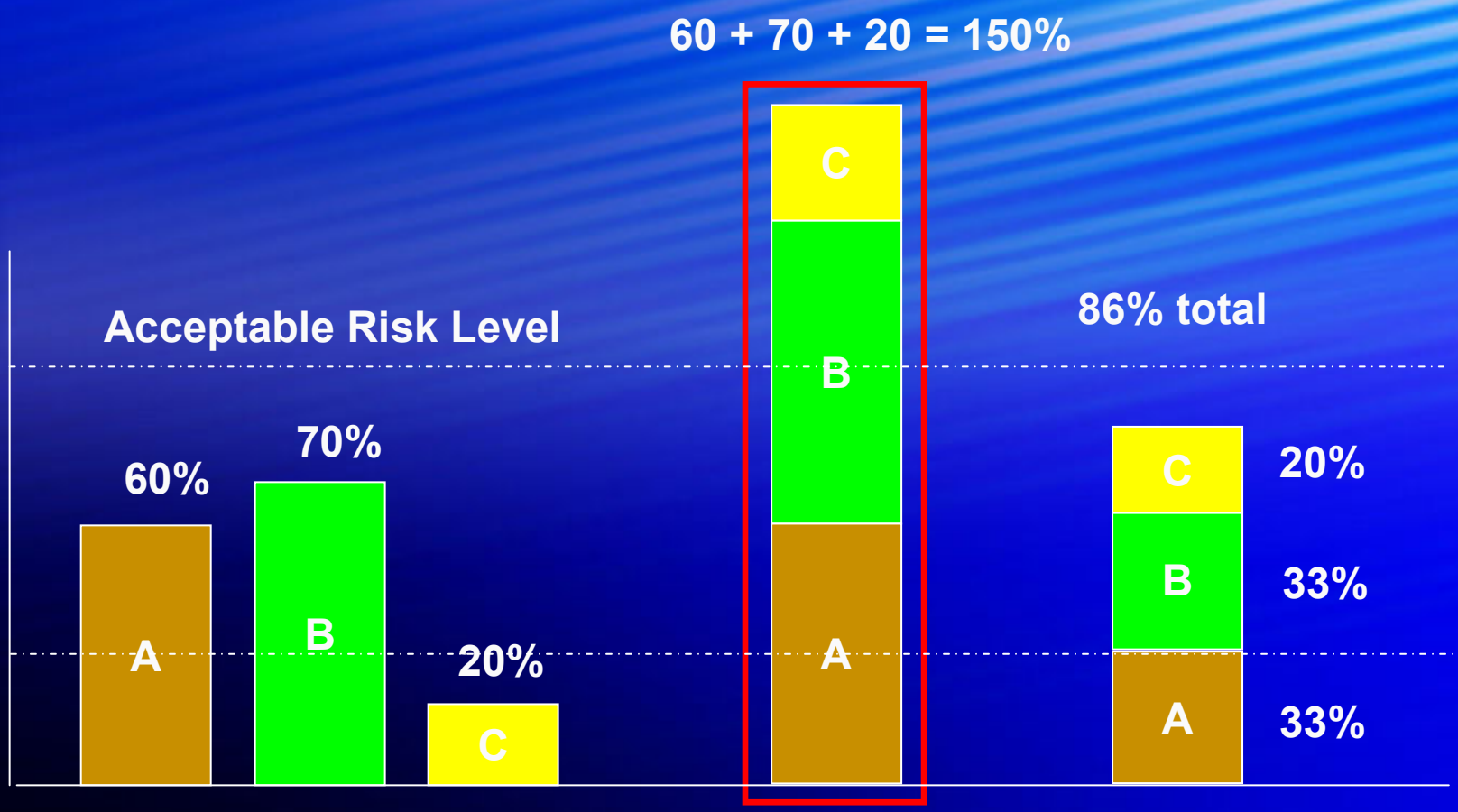
What to add …

- The effects of carcinogens are assumed to be additive.
- For non-carcinogens, additive effects are assumed if the chemicals affect the same target organ/system or produce the same effect.
  - e.g., liver, kidney, skin, body weight

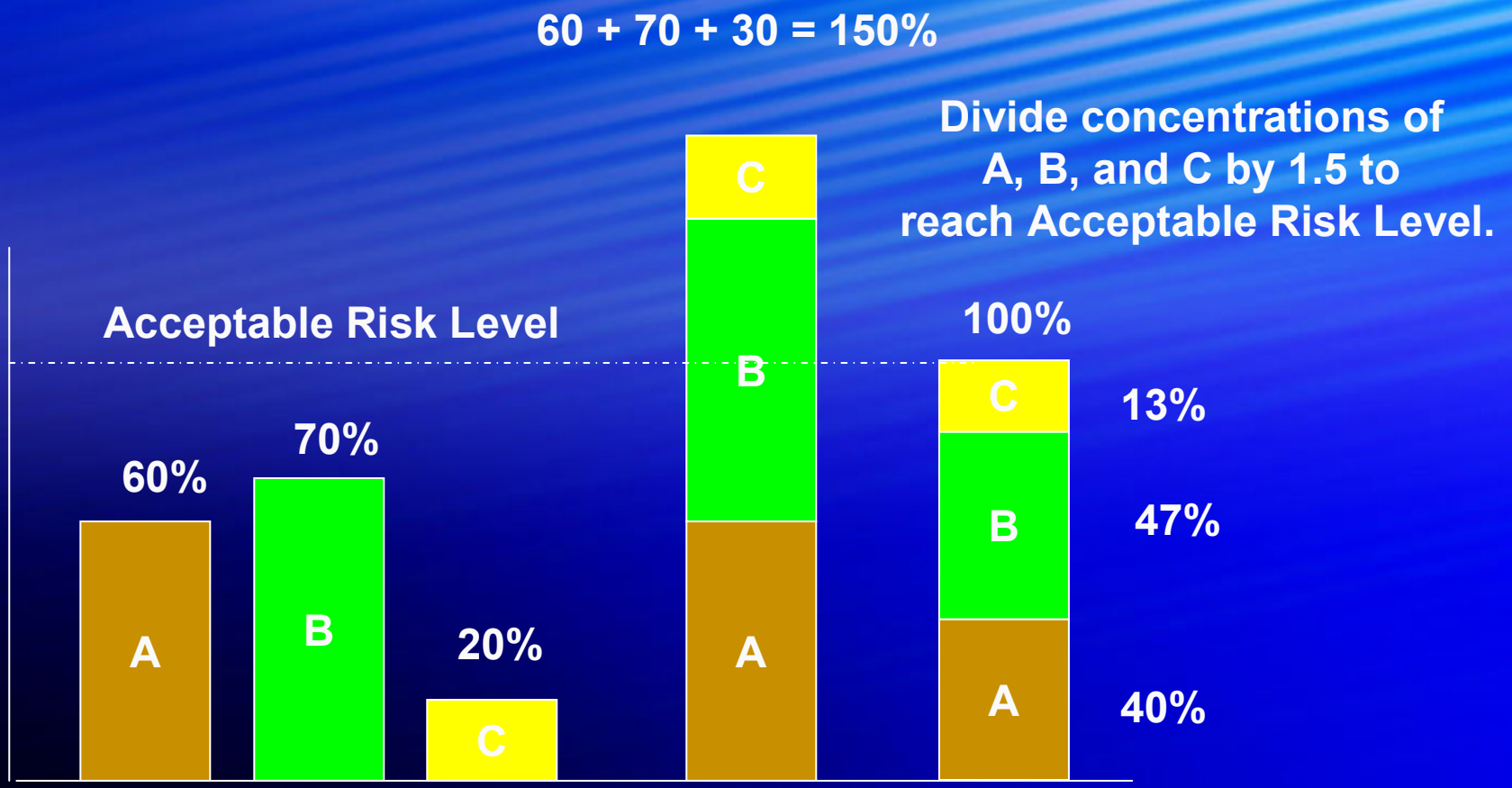
Different Ways to Apportion

- Simple apportionment - Divide the default SCTL for each of the chemicals with the same target organs/systems or effects by the number of chemicals.
  - Calculation is simple, but often overly conservative
- Weighted apportionment - Results in SCTLs that achieve more precisely FDEP risk goals.
  - Takes into consideration the concentrations of chemicals present at the site
  - Distributes risk among chemicals with the same effect
  - Weighting can be tailored to the site

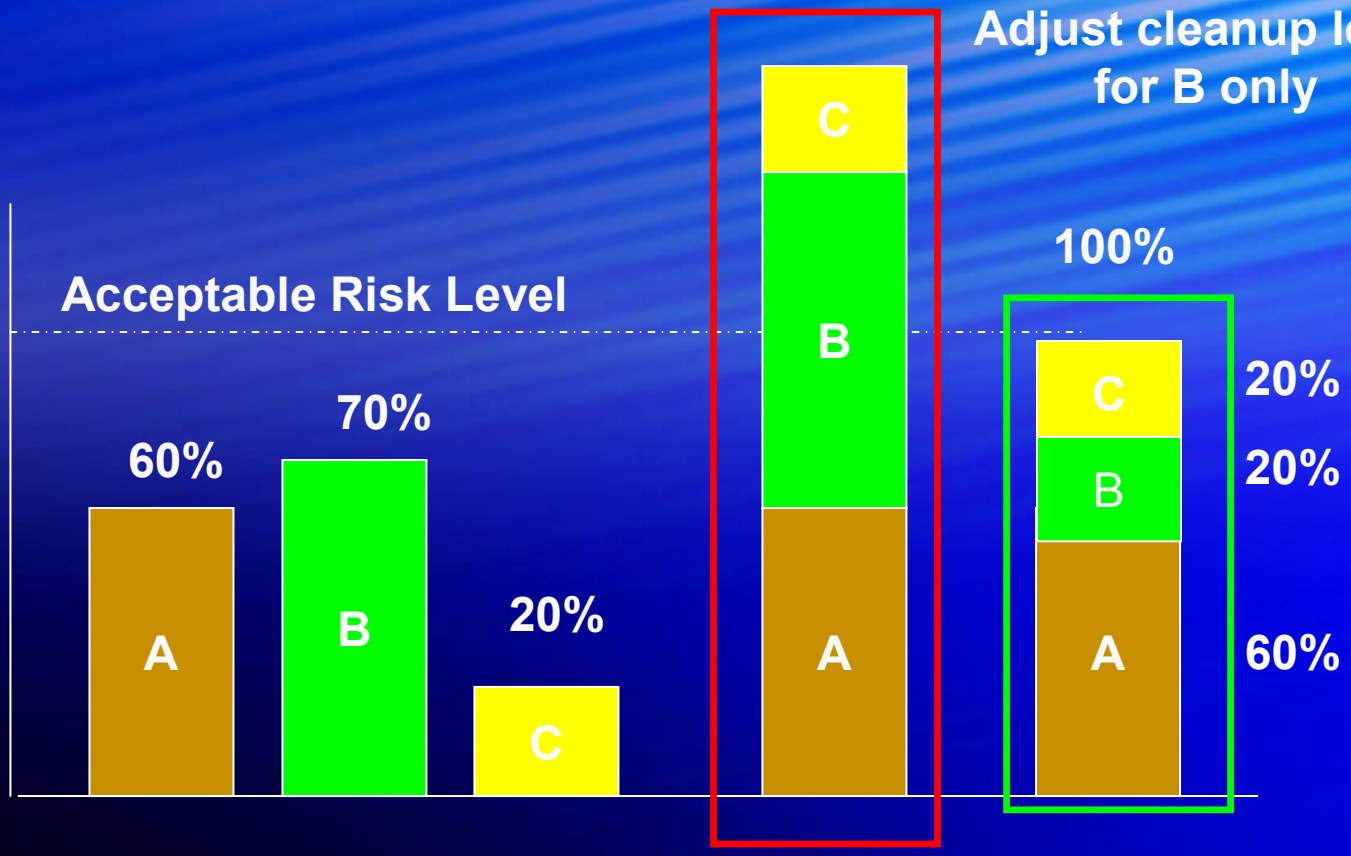
Simple Apportioning



Weighted Apportioning



Selective Apportioning



Apportionment Process

- The process is based on standard risk assessment principles
- Apportionment is the trade-off for using 95% UCL or alternative cleanup goals.
  - If you want to use more refined approaches to evaluate risk, you have to take a balanced approach.
- The process is developed in a way that allows maximum flexibility to meet the Department's risk goals.
  - The process is not simple (except for simple apportionment, which is seldom recommended).

Apportionment Process

- This example apportionment process is for soils.
- Purpose is to illustrate the steps needed to develop apportioned SCTLs and some of the considerations.
- Basic steps are:
  - Identify the “automatic” SCTLs
  - Screening of chemicals
  - Construct additivity groups
  - Calculate initial apportioned SCTLs
  - Reapportion SCTLs, if needed
  - Develop a final list of SCTLs

"Automatic" SCTLs

- These are SCTLs that are not subject to the apportionment process.
  - Lead - because cleanup criteria are developed differently than for other chemicals.
  - TRPH - because this is a complex mixture that represents a variety of toxic endpoints.
  - Acute toxicity SCTLs for residential scenarios (namely, barium, cadmium, copper, cyanide, fluoride, nickel, phenol, vanadium)
- If the maximum concentration on site is above the default SCTL, add the default SCTL to the list of final SCTLs.

Screening

- For inorganics, eliminate any that are present at background concentrations.
- Eliminate any chemical with a maximum concentration $\leq$ 1/10 the default SCTL.
- Eliminate any chemical that is infrequently detected. All criteria must be met:
  - Detected in 5% or fewer samples out of 20 or more, or no more than 1 sample out of 10 or more
  - Detected in low concentrations (< default SCTL)
  - There is no reason to believe that the chemical may be present due to historical site activities.

Screening Example

	max	SCTL	1/10 SCTL	2x BG	Freq	PCC?
arsenic	4.5	2.1	0.21	1.4	20/20	yes
dieldrin	0.32	0.06	0.006	NA	15/20	yes
DDT	4.7	2.9	0.29	NA	9/20	yes
chlordane	0.25	2.8	0.28	NA	5/20	no
captan	12	230	23	NA	7/20	no
chloroform	0.3	0.4	0.04	NA	1/20	no

Construct Additivity Groups

- Group chemicals by target organ/effect.
  - Default target organs/effects listed in Tables 2 and 6 of the technical report for Ch. 62-777.
  - cPAHs and dioxins should be reported as B(a)P and TCDD equivalents, respectively
  - Carcinogens should be grouped only based on carcinogenicity (not also on their non-cancer effects)
- Calculate the exposure point concentration (EPC) for each chemical.
  - 95% UCL if sufficient data are available; use the maximum concentration if data are limited.

Calculate Apportioned SCTL

- Calculate an Exceedance Ratio (ER) for each chemical in each group.
  - The ER is the EPC/default SCTL for that chemical
- Calculate the total ER for each additivity group
- Divide the EPC for each chemical by the total ER for the group to calculate an initial apportioned SCTL.

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1		
dieldrin	0.32	0.15	0.15	0.06		
DDT	4.7	2.4	2.4	2.9		

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1		
dieldrin	0.32	0.15	0.15	0.06		
DDT	4.7	2.4	2.4	2.9		

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1		
dieldrin	0.32	0.15	0.15	0.06		
DDT	4.7	2.4	2.4	2.9		

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	
dieldrin	0.32	0.15	0.15	0.06		
DDT	4.7	2.4	2.4	2.9		

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	
dieldrin	0.32	0.15	0.15	0.06	2.5	
DDT	4.7	2.4	2.4	2.9	0.83	
					4.71	

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	
dieldrin	0.32	0.15	0.15	0.06	2.5	
DDT	4.7	2.4	2.4	2.9	0.83	
					4.71	

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	
dieldrin	0.32	0.15	0.15	0.06	2.5	
DDT	4.7	2.4	2.4	2.9	0.83	
					4.71	

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	0.616
dieldrin	0.32	0.15	0.15	0.06	2.5	
DDT	4.7	2.4	2.4	2.9	0.83	
					4.71	

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	0.616
dieldrin	0.32	0.15	0.15	0.06	2.5	
DDT	4.7	2.4	2.4	2.9	0.83	
					4.71	

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	0.616
dieldrin	0.32	0.15	0.15	0.06	2.5	0.032
DDT	4.7	2.4	2.4	2.9	0.83	
					4.71	

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	0.616
dieldrin	0.32	0.15	0.15	0.06	2.5	0.032
DDT	4.7	2.4	2.4	2.9	0.83	0.509
					4.71	

Apportioned SCTL

- Compare each initial apportioned SCTL with background (if applicable) and PQL.
  - If it is less, set the SCTL at background or PQL (as appropriate) and remove it from the additivity group.
  - Recalculate the total ER and apportioned SCTLs for the remainder of the group.

Example

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	1.38	0.616
dieldrin	0.32	0.15	0.15	0.06	2.5	0.032
DDT	4.7	2.4	2.4	2.9	0.83	0.509
					4.71	

Apportion w/o arsenic …

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	NA	NA
dieldrin	0.32	0.15	0.15	0.06	2.5	
DDT	4.7	2.4	2.4	2.9	0.83	

Apportion w/o arsenic …

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	NA	NA
dieldrin	0.32	0.15	0.15	0.06	2.5	
DDT	4.7	2.4	2.4	2.9	0.83	
					3.33	

Apportion w/o arsenic …

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	NA	NA
dieldrin	0.32	0.15	0.15	0.06	2.5	0.045
DDT	4.7	2.4	2.4	2.9	0.83	
					3.33	

Apportion w/o arsenic …

	max	95% UCL	EPC	SCTL	ER	SCTLwa
arsenic	4.5	2.9	2.9	2.1	NA	NA
dieldrin	0.32	0.15	0.15	0.06	2.5	0.045
DDT	4.7	2.4	2.4	2.9	0.83	0.721
					3.33	

Chemicals in Multiple Groups

- Determine whether there are any chemicals that appear in more than one group. If so:
  - Identify the lowest apportioned SCTL for that chemical. This will become its final SCTL.
  - [Optional] Modify other additivity groups based on selection of the lowest SCTL.
    - Replace the original apportioned SCTL with the lower, final SCTL. Recalculate the ER and distribute remaining risk to other chemicals in the group.

Reapportion SCTLs, if needed

- [Optional] Evaluate all remaining additivity groups. Redistribute risk among chemicals within a group using selective apportionment if warranted by site-specific conditions.
  - Example: If contaminants are not co-located, it may be more cost-effective to concentrate remediation on one or a few chemicals rather than the whole group.

Selective Apportioning

	SCTL	SCTLwa	ER	SCTLsla	ER
arsenic	2.1	NA	NA	NA	NA
dieldrin	0.06	0.0451	0.751		
DDT	2.9	0.721	0.249		
			1.00		

Selective Apportioning

	SCTL	SCTLwa	ER	SCTLsla	ER
arsenic	2.1	NA	NA	NA	NA
dieldrin	0.06	0.0451	0.751		0.5
DDT	2.9	0.721	0.249		0.5
			1.00		1.00

Selective Apportioning

	SCTL	SCTLwa	ER	SCTLsla	ER
arsenic	2.1	NA	NA	NA	NA
dieldrin	0.06	0.0451	0.751		0.5
DDT	2.9	0.721	0.249		0.5
			1.00		1.00

Selective Apportioning

	SCTL	SCTLwa	ER	SCTLsla	ER
arsenic	2.1	NA	NA	NA	NA
dieldrin	0.06	0.0451	0.751		0.5
DDT	2.9	0.721	0.249		0.5
			1.00		1.00

Selective Apportioning

	SCTL	SCTLwa	ER	SCTLsla	ER
arsenic	2.1	NA	NA	NA	NA
dieldrin	0.06	0.0451	0.751	0.03	0.5
DDT	2.9	0.721	0.249		0.5
			1.00		1.00

Selective Apportioning

	SCTL	SCTLwa	ER	SCTLsla	ER
arsenic	2.1	NA	NA	NA	NA
dieldrin	0.06	0.0451	0.751	0.03	0.5
DDT	2.9	0.721	0.249	1.45	0.5
			1.00		1.00

Develop a final list of SCTLs

- Include SCTLs from the "automatics"
  - Lead, TRPH, and acute toxicity SCTLs, if appropriate
- Include SCTLs based on PQL and background
- Include SCTLs based on apportioned risk
  - Either from weighted or selective apportioning
- Include SCTLs based on leaching, if warranted by site conditions.

Comparing with the SCTLs

- Leachability, acute toxicity, and PQL SCTLs are not-to-exceed values.
- Background - stat or non-stat approaches
- Apportioned risk SCTLs should be compared with the EPC. The maximum concentration should be compared with 3x the SCTL.
  - For RMO 1 and 2, 3x the default SCTL
  - For RMO 3, 3x the apportioned, alternative SCTL (or something else, if justified to the department)

Apportionment for Groundwater

- Additional issues for apportionment
  - Apportioned alternative GCTLs cannot be less than the standard (if there is one)
  - Apportioning should be performed on health-based criteria (not primary standards, organoleptic criteria, etc.)
  - Class C carcinogens
  - Exposure point concentration is not an average