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Poster BOHS OH2014

OEL of lead component in mixtures

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- www.dohsbase.com

Simultaneous exposure to chemicals

Approach:

1. Sum score
2. Non-ideal fugacity/evaporation

Combined exposure

- Not included in:
  - ECETOC-TRA, Stoffenmanager (first tier modelling)
- Included in:
  - ACGIH-TLV for Mixtures
  - Advanced REACH tool (higher tier modelling)
- Still unclear in REACH ES for mixtures (DPD+).

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Additive Mixture Formula (Sum-score)

ACGIH-TLV for Mixtures

$$\sum_{i=1}^{i=n} \left(\frac{C_i}{OELV_i}\right) \leq 1$$

Case: mixture compliance

Phenol (p), Butanol (b) & Cumene (c) **are respiratory irritants (R37/Scoel)**. Therefore their exposures must be combined:

$$\sum_{i=1}^{i=3}\left(\frac{C_i}{STEL_i}\right)=\sum_{i=1}^{i=3}\left(\frac{C_p}{16}+\frac{C_b}{45}+\frac{C_c}{250}\right)\leq 1$$

C_p, C_b and C_p are:

1. determined by their vapour pressure p_i and
2. mutual dependant through Raoult's law.

How much lower is $STEL_{i,mix}$ compared to $STEL_i$?

Vapor pressure of mixtures of liquids

Raoult's law : the pressure of a single-phase mixture is *(in theory)* equal to the mole-fraction-weighted sum of the components' vapor pressures:

$$p_{tot}=\sum_{i=1}^{i=n} (pi * X_i)$$

where ***p*** is the mixture's vapor pressure, ***i*** is one of the components of the mixture and ***X*** is the mole fraction of that component in the liquid mixture.

$p_i * X_i$ is the partial pressure of component ***i*** in the mixture

Raoult's partial vapor pressures and OELs of components in the mixture

Component composition of a 1:1:1 Molar liquid mixture	Component vapor pressure in Pa	Component mol fraction in the mixture	Component partial vp in the mixture in Pa (ideal)	Component regular STEL in mg/m3	Component ideal partial vp STEL for the mixture air composition in mg/m3
n-Butanol	891,10	0,33	297,03	45	26,74
Phenol	9,98	0,33	3,33	16	0,11
Cumene	598,5	0,33	199,50	250	99,78
Mixture		Σ=	500	Σ=	127

$$STEL_{c,\ part} = vp_c^{*}/vp_t^{*} STEL_c = 199/500*250 = 99,8$$

$$\sum_{i=1}^{i=3} \left(\frac{STEL_{i\ part}}{STEL_i}\right) \leq 1 \qquad \sum_{i=1}^{i=3} \left(\frac{26,7}{45} + \frac{0,11}{16} + \frac{99,8}{250}\right) = 1$$

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Non-ideal liquid mixtures

Estimate (partial) vapor pressures using [XLUNIFAC]:

$$VP_{tot}=\sum_{i=1}^{i=n} (vp_i * X_i * a_i)$$

where ***a*** is the mixture's non-ideal vapor pressure activity coefficient and $a_i * vp_i * X_i$ is the adjusted partial vapor pressure vp_i of component ***i*** in the mixture

UNIFAC partial vapor pressures and OELs of components in the workshop mixture

Component composition of a 1:1:1 Molar liquid mixture	Component partial vp in the mixture in Pa (ideal)	Component UNIFAC activity coefficient	Component partial UNIFAC vp in the mixture in Pa	Component regular STEL in mg/m3	Component STEL for the mixture UNIFAC air mass composition in mg/m3
n-Butanol	297,03	0,7593	225,53	45	16,53
Phenol	3,33	0,6411	2,13	16	0,06
Cumene	199,50	1,9361	386,25	250	157,29
Mixture	Σ = 500	Σ=	613,91	Σ=	173,88

$$STEL_{c,\ part} = vp_c{*}/vp_t{*}STEL_c = 386/614*250 = 157{,}3$$

$$\sum_{i=1}^{i=3} \left(\frac{STEL_{i\ part}}{STEL_i}\right) \leq 1 \qquad \sum_{i=1}^{i=3} \left(\frac{16{,}5}{45} + \frac{0{,}06}{16} + \frac{157{,}3}{250}\right) = 1$$

Conclusion

- non-ideal behavior of components in liquid mixture:
  - enhances & inhibits evaporation.
- Based on precautionary:
  - use the lowest Raoult or UNIFAC adjusted component OEL, to test compliance for the whole mixture
- to test irritation risk of example mixture, use
  - Cumene Raoult STEL 99,8 mg/m3/15min or
  - n-Butanol UNIFAC STEL 17 mg/m3/15min

Phenol adjusted OEL is <LoD