1 Green Process Efficiency

$\eta_{\text{atom},i} = \frac{\nu_{i,\text{desired product}}}{\nu_{i,\text{reactants}}}$ $\eta_{\text{mass}} = \frac{(n\check{m})_{\text{desired product}}}{\sum_{\text{reactants}} (n_i \check{m}_i)}$

2 Emissions

Leaks: $E_{\text{VOC}} = f_E w_{\text{TOC}} N_{\text{equipment}} \frac{w_{\text{TOC}} - w_{\text{Et}} - w_{\text{Me}}}{w_{\text{TOC}} - w_{\text{Me}}}$

2.1 Charging an Empty Vessel

$n_i = \frac{V_{\text{disp}}\rho_i}{\check{m}_i} x_i$ $E_i = \frac{p_i V_{\text{disp}}}{RT} \check{m}_i$

Pure or mixed solvent: $P = \sum_i p_i + p_{\text{inert}}$ $p_i = \gamma_i x_i p_i^\star$

2.2 Charging a Partially Filled Vessel

$\phi_A = 1 + \frac{n_B}{n_A} \ln \frac{n_B}{n_A + n_B}$ $\phi_B = -\frac{n_B}{n_A} \ln \frac{n_B}{n_A + n_B}$

Above surface: $p_i = x_i p_i^\star$

Subsurface: $\langle x_A \rangle = x_{A,\text{ inlet}} \phi_A + x_{A,\text{ tank}} \phi_B$ $p_i = \langle x_i \rangle p_i^\star$

Immiscible, $\{x_i = 1\} : p_i = p_i^\star$

3 Theoretical Oxygen Demand (ThOD)

Carbonaceous: $\mathrm{C_a H_b O_c N_d} + \left(\mathrm{a} + \frac{\mathrm{b}}{4} - \frac{\mathrm{c}}{2} - \frac{3\mathrm{d}}{4}\right) \mathrm{O_2} \longrightarrow$
$\mathrm{aCO_2} + \left(\frac{\mathrm{b}}{2} - \frac{3\mathrm{d}}{2}\right) \mathrm{H_2O} + \mathrm{dNH_3}$

Nitrogenous: $\mathrm{dHN_3} + (2\mathrm{d})\mathrm{O_2} \longrightarrow \mathrm{dHNO_3} + \mathrm{dH_2O}$

4 Environmental Fate of a Chemical

$\check{V}_{\text{w}} = 1.8\text{E}{-5} \frac{\text{m}^3}{\text{mol}}$ $p_i = c_i RT$ $x_i = c_{\text{w},i} \check{V}_{\text{w}}$ $m_i = C_i V_i$

Lipid-H_2O partition:

$K_{\text{ow}} = \frac{C_{\text{octanol}}}{C_{\text{water}}}$ $m_{\text{T}} = C_{\text{o}} V_{\text{o}} + C_{\text{w}} V_{\text{w}} = C_{\text{w}} (K_{\text{ow}} V_{\text{o}} + V_{\text{w}})$

Biomass-H_2O partition:

$K_{\text{d}} = \frac{C_{\text{soil/sediment}}}{C_{\text{w}}}$ $K_{\text{oc}} = \frac{100 K_{\text{d}}}{\%\text{ organic carbon}}$ $\text{BCF} = \frac{C_{\text{organism}}}{C_{\text{w}}}$

Air-H_2O partition:

$\mathcal{H}_{px} \equiv \frac{p_i}{x_i} [\text{atm}]$ $\mathcal{H}_{cc} \equiv \frac{c_{\text{air},i}}{c_{\text{w},i}}$

$\mathcal{H}_{pc} \equiv \frac{p_i}{c_{\text{w},i}} = \mathcal{H}_{cc} RT = \mathcal{H}_{px} \check{V}_{\text{w}} \left[\frac{\text{atm m}^3}{\text{mol}}\right]$

Mass balance: water, air, solids, sediment, fish

$E_{\text{T}} = E_{\text{a}} + E_{\text{w}} + E_{\text{s}} = \sum C_{\text{x}} V_{\text{x}}$ $\text{x} \in \{\text{w, a, s, t, f}\}$

$C_{\text{a}} = C_{\text{w}} \mathcal{H}_{cc}$ $C_{\text{s}} = C_{\text{w}} K_{\text{d}}$ $C_{\text{t}} = C_{\text{w}} K'_{\text{d}}$ $C_{\text{f}} = C_{\text{w}} \text{BCF}$

$\sum C_{\text{x}} V_{\text{x}} = C_{\text{w}} \left(\mathcal{H}_{cc} V_{\text{a}} + V_{\text{w}} + K_{\text{d}} V_{\text{s}} + K'_{\text{d}} V_{\text{t}} + \text{BCF} \cdot V_{\text{f}}\right)$

5 Industrial Hygiene

$Y = k_1 + k_2 \ln V$ $\%(Y) = 50 \left(1 + \frac{Y-5}{|Y-5|} \text{erf} \frac{|Y-5|}{\sqrt{2}}\right)$

5.1 Volatiles

Vapour: $C_{\text{ppm}} = 0.08205 \left[\frac{\text{atm L}}{\text{K mol}}\right] \left(\frac{T[\text{K}]}{P[\text{atm}] \check{m}[\text{g mol}^{-1}]}\right) C \left[\frac{\text{mg}}{\text{m}^3}\right]$

$\text{TWA} = \frac{1}{8} \int_0^{t_w} C(t)\, dt = \frac{1}{8} \sum_i C_i t_i$

$(\text{TLV-TWA})_{\text{mix}} = \sum_i C_i \left(\sum_i \frac{C_i}{(\text{TLV-TWA})_i}\right)^{-1}$

$C_{\text{ppm}} = \frac{\dot{m} RT}{\varepsilon_{\text{m}} \dot{V} P \check{m}} \times 10^6$ $0.1 \le \varepsilon_{\text{m}} \le 0.5$ $C\% = C_{\text{ppm}} \times 10^4$

5.2 Vapourisation

$C_{\text{ppm}} = \frac{k A p^\star}{\varepsilon_{\text{m}} \dot{V} P}$ $k = k^\ominus \left(\frac{\check{m}^\ominus}{\check{m}}\right)^{1/3}$

5.3 Filling

$\dot{m}_i = \dot{m}_{\text{evap}} + \dot{m}_{\text{disp}} = \frac{\check{m}_i p_i^\star}{RT} (\varepsilon_{\text{f}} \dot{V}_i + k_i A_\sigma)$ $\varepsilon_{\text{f}} {=1, \text{ splash} \atop =0.5, \text{ subsfc.}}$

$\{T = T_{(\text{l})}\}: C_{\text{ppm}} = \frac{p_i^\star}{\varepsilon_{\text{m}} V_i P} (\varepsilon_{\text{f}} \dot{V} + k_i A_\sigma) \times 10^6$

5.4 Miscellany

$\dot{V}_{\text{hood}} = A_\sigma \vec{v}$ $0.406 \le \vec{v} \le 0.610$ [m/s] $L_I = -10 \log \frac{I}{I_0}$

6 Fluid Mechanics

$\frac{\Delta P}{\rho} + \frac{\Delta(\vec{v}^2)}{2\alpha} + g\Delta z + \sum \hat{F} = \frac{\dot{W}_{\text{s,by}}}{\dot{m}}$ $\alpha {\approx 1, \text{ turbulent} \atop = 0.5, \text{ laminar}}$

$\dot{V} = A_\sigma \langle \vec{v} \rangle = \frac{\dot{m}}{\rho}$ $(\rho \vec{v}) = \frac{\dot{m}}{A_\sigma}$ $\rho_1 A_{\sigma 1} \langle \vec{v}_1 \rangle = \rho_2 A_{\sigma 2} \langle \vec{v}_2 \rangle$

Hydrostatic column: $P_\perp = P_\top + \rho g \hbar$

6.1 Force Losses

$\text{Re} = \frac{\langle \vec{v} \rangle \rho \varnothing}{\mu}$ $f = \frac{\varnothing}{\ell} \frac{\Delta P}{2\rho \langle \vec{v} \rangle^2}$

$f_{\text{smooth, lam}} = 16/\text{Re}$ $f_{\text{smooth, trb}} = 0.079\text{Re}^{-0.25}$

$\hat{F}_{\text{straight pipe}} = 4f \frac{\ell}{\varnothing} \frac{\langle \vec{v} \rangle^2}{2} = \frac{\Delta P}{\rho}$ $\hat{F}_{\text{fitting}} = K_{\text{f}} \frac{\langle \vec{v} \rangle^2}{2}$ $K_{\text{f, straight}} = \frac{4 f \ell}{\varnothing}$

$\sum \hat{F} = \sum_i 4 f_i \frac{\ell_i}{\varnothing_i} \left(\frac{\langle \vec{v} \rangle_i^2}{2}\right) + \sum_j K_{\text{f},j} \left(\frac{\langle \vec{v} \rangle_j^2}{2}\right)$ $\tilde{H}_i = \frac{\hat{F}_i}{g}$ $\tilde{H} = \frac{\Delta P}{\rho g}$

7 Source Models

$\langle \vec{v} \rangle = C_0 \sqrt{\frac{2 P_{\text{gauge}}}{\rho}}$ $C_0 {=1, \text{ laminar} \atop =0.61, \text{ turbulent}}$

$\dot{m}_{\text{hole}} = \rho A \langle \vec{v} \rangle = C_0 A \sqrt{2\rho \Delta P}$ $\dot{V}_{\text{hole}} = C_0 A \sqrt{\frac{2\Delta P}{\rho}}$

Liquid: $\dot{m} = \rho A_{\text{hole}} C_0 \sqrt{2 \left(\frac{P_{\text{gauge}}}{\rho} + g\hbar_L\right)}$

$$\dot{m}(t) = \rho A_{\text{hole}} C_0 \sqrt{2 \left(\frac{P_{\text{gauge}}}{\rho} + g\hbar_0\right)} - \frac{\rho g C_0^2 A_{\text{hole}}^2}{A_{\sigma,\text{tank}}} t$$

$$\hbar_L(t) = \hbar_0 - t \frac{A_{\text{hole}} C_0}{A_{\sigma,\text{tank}}} \sqrt{\frac{P_{\text{gauge}}}{\rho} + 2g\hbar_0} + \frac{g}{2} \left(\frac{C_0 A_{\text{hole}}}{A_{\sigma,\text{tank}}} t\right)^2$$

$$t_{\text{empty}} = \frac{1}{C_0 g} \frac{A_{\sigma,\text{tank}}}{A_{\text{hole}}} \left[\sqrt{2 \left(\frac{P_{\text{gauge}}}{\rho} + g\hbar_0\right)} - \sqrt{\frac{2 P_{\text{gauge}}}{\rho}}\right]$$

Gas: $\dot{m} = \rho A_{\text{hole}} C_0 \sqrt{\frac{2\check{m}}{R T_G} \frac{\gamma}{\gamma - 1} \left[\left(\frac{P}{P_G}\right)^{\frac{2}{\gamma}} - \left(\frac{P}{P_G}\right)^{\frac{\gamma+1}{\gamma}}\right]}$

$$\dot{m}_{\text{choked}} = P_G A_{\text{hole}} C_0 \sqrt{\frac{\gamma \check{m}}{R T_G} \left(\frac{2}{\gamma - 1}\right)^{\frac{(\gamma+1)}{(\gamma-1)}}}$$

Breather vent: $m = \frac{\check{m} p^\star U}{R T_{\text{L}}} \left(\frac{T_{\text{H}}}{T_{\text{L}}} - 1\right)$

8 Dispersion Models

Puff with instantaneous point source at $\hbar_{\text{R}}$ above ground level and coordinate system on ground that moves with puff:

$$\langle C \rangle(x, y, z, t) = \frac{m}{(2\pi)^{1.5} \sigma_x \sigma_y \sigma_z} e^{-0.5\left(\frac{y}{\sigma_y}\right)^2} \times \left[e^{-0.5\left(\frac{z - \hbar_{\text{R}}}{\sigma_z}\right)^2} + e^{-0.5\left(\frac{z + \hbar_{\text{R}}}{\sigma_z}\right)^2}\right]$$

Plume with continuous steady-state source at $\hbar_{\text{R}}$ above ground level and wind moving in x direction at $\vec{v}_{\text{wind}}$:

$$\langle C \rangle(x, y, z) = \frac{\dot{m}}{\pi \sigma_y \sigma_z \vec{v}_{x,\text{wind}}} e^{-0.5\left(\frac{y}{\sigma_y}\right)^2} \times \left[e^{-0.5\left(\frac{z - \hbar_{\text{R}}}{\sigma_z}\right)^2} + e^{-0.5\left(\frac{z + \hbar_{\text{R}}}{\sigma_z}\right)^2}\right]$$

9 Fires and Explosions

$L = \left(\sum_i \frac{y_i}{L_i}\right)^{-1}$ $L \in \{\text{LFL}, \text{UFL}\}$

$L(T) = L(25°\text{C}) - \frac{0.75}{\Delta_{\text{c}} H} (T - 25°\text{C})$ $\Delta_{\text{c}} \check{H} = \sum_i y_i \Delta_{\text{c}} \check{H}_i \frac{\text{kcal}}{\text{mol}}$

$\mathrm{C_a H_b O_c} + \mathrm{zO_2} \longrightarrow \mathrm{aCO_2} + \frac{\mathrm{b}}{2} \mathrm{H_2O}$ $z \equiv a + \frac{b}{4} - \frac{c}{2}$

$\text{LOC} = \text{LFL} \frac{n_{\text{O}_2}}{n_{\text{fuel}}} = z(\text{LFL})$

$z_{\text{e}} \equiv \frac{r}{m_{\text{TNT}}^{1/3}}$ $m_{\text{TNT}} = \frac{\eta_{\text{explosion}} m_{\text{hydrocarbon}} \Delta_{\text{c}} \hat{H}}{E_{\text{TNT}}}$ $P^* = \frac{\text{peak overpressure}}{P_{\text{ambient}}}$

$E = RT \left[\ln \frac{P_g}{P} - 1 + \frac{P}{P_g}\right]$

9.1 Purging

$y_i - y_{\text{oxygen}} = \left(\frac{P_{\text{L}}}{P_{\text{H}}}\right)^i (y_0 - y_{\text{oxygen}})$ $\Delta n_{\text{nitrogen}} = i(P_{\text{H}} - P_{\text{L}}) \frac{V}{RT}$

$\dot{V}_{\text{inert}} t = V \ln \frac{C_1 - C_0}{C_2 - C_0}$ $\text{OSFC} = \frac{\text{LOC}}{z - z \frac{\text{LOC}}{21}}$

References

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