Cheming cheatsheet

A handy guide containing the most important equations that a chemical engineer will need in practical life. For a few selected equations, their derivation process is outlined, but only in *very* brief points. Czech names are in violet.
Unit conversions are not included; see [this tool](#) that will tackle anything you come across.
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Contents

Reaction quantification

E, P stands for an extensive quantity for educts (reaktanty) and products, such as n_i, m_i, $\dot{n}_i$.
When certain conditions are met, also intensive quantities may be balanced: c_i, p_i, w_i etc...
ν_i is the stoichiometric coefficient of a component i.

Extent of reaction (reakční rozsah) for a component i ξ

$$\xi = \frac{n_i - n_i^0}{\nu_i} \qquad \xi_V = \frac{n_i - n_i^0}{V \nu_i} \tag{1}$$

Conversion

$$X = \frac{E^0 - E}{E^0} \tag{2}$$

Yield (výtěžek)

$$Y = \frac{P}{E^0} \frac{\nu_\mathrm{E}}{\nu_\mathrm{P}} = X \cdot S \tag{3}$$

Selectivity (of one reaction with st. coeffs $\nu_\mathrm{E}, \nu_\mathrm{P}$ against all other reactions)

$$S = \frac{P}{E^0 - E} \frac{\nu_\mathrm{E}}{\nu_\mathrm{P}} \tag{4}$$

Relative selectivity (of two parallel reactions $\mathrm{E} \to \mathrm{P}, \mathrm{P}*$ with st. coeffs $\nu_\mathrm{P}, \nu_{\mathrm{P}*}$)

$$S_{\mathrm{P}/\mathrm{P}*} = \frac{P}{P*} \frac{\nu_\mathrm{P}*}{\nu_\mathrm{P}} = \frac{r_\mathrm{P}}{r_{\mathrm{P}*}} \tag{5}$$

Reaction kinetics

Various definitions of **reaction rate** (reakční rychlost):

$$R = \frac{\mathrm{d}\xi}{\mathrm{d}\tau} \tag{6}$$

$$R_i = R\nu_i \tag{7}$$

$$r = \frac{\mathrm{d}R}{\mathrm{d}V} = \frac{\mathrm{d}\xi_V}{\mathrm{d}\tau} = \frac{1}{V\nu_i}\frac{\mathrm{d}n_i}{\mathrm{d}\tau} \tag{8}$$

$$r_i = r\nu_i = \frac{\mathrm{d}R_i}{\mathrm{d}V} = \frac{1}{V}\frac{\mathrm{d}n_i}{\mathrm{d}\tau} \tag{9}$$

CSTR balance for reactor 1, component A (F is volume flow rate, assuming constant ρ):

$$FC_{\mathrm{A0}} - FC_{\mathrm{A1}} + \nu_{\mathrm{A}} r(C_{\mathrm{A1}})V = 0 \tag{10}$$

Power law with equilibrium for reaction A + B $\rightleftharpoons$ C + D, where R is backwards reaction:

$$r = kc_{\mathrm{A}}^a c_{\mathrm{B}}^b - k_{\mathrm{R}} c_{\mathrm{C}}^c c_{\mathrm{D}}^d \tag{11}$$

Langmuir-Hinschelwood for surface reaction A + B $\rightleftharpoons$ C:

$$r = k_1 q_{\mathrm{A}} q_{\mathrm{B}} - k_2 q_{\mathrm{C}} = k_1 K_{\mathrm{A}} c_{\mathrm{A}} K_{\mathrm{B}} c_{\mathrm{B}} q^2 - k_2 K_{\mathrm{c}} c_{\mathrm{c}} q \tag{12}$$

Where q (surface conc. of free active sites $[\frac{\mathrm{mol}}{\mathrm{m}^2}]$) is following ($Q$ is total surface conc.):

$$q = \frac{Q}{1 + K_{\mathrm{A}} c_{\mathrm{A}} + K_{\mathrm{B}} c_{\mathrm{B}} + K_{\mathrm{C}} c_{\mathrm{C}}} \tag{13}$$

Derivation: ($q, q_{\mathrm{A}}, q_{\mathrm{B}}, q_{\mathrm{C}}$ are unknowns, $Q, K_{\mathrm{A}}, K_{\mathrm{B}}, K_{\mathrm{C}}$ are parameters)

$$Q = q + q_{\mathrm{A}} + q_{\mathrm{B}} + q_{\mathrm{C}} \tag{14}$$

$$K_i = \frac{q_i}{c_i q} \tag{15}$$

Michaelis-Menten for enzymatic reaction E + S $\rightleftharpoons$ ES $\rightarrow$ P:

$$r_{\mathrm{P}} = k_{\mathrm{MAX}} \frac{c_{\mathrm{S}}}{k_{\mathrm{A}} + c_{\mathrm{S}}} \tag{16}$$

Derivation: $\mathrm{d}c_{\mathrm{ES}}/\mathrm{d}\tau = 0, \quad c_{\mathrm{E}} = c_{\mathrm{E}}^0 - c_{\mathrm{ES}}$

Thermodynamics

Antoine equation for vapor pressure of pure component i (tlak sytých par):

$$\log_{10} p_i^\circ = A - \frac{B}{T + C} \tag{17}$$

Dependence of various constants on temperature:

$$\frac{\mathrm{d}\ln k}{\mathrm{d}T} = \frac{\Delta H}{RT^2} \tag{18}$$

constant	equilibrium	reaction rate	p°	Henry	adsorption
enthalpy	reaction	activation energy	evaporation	dissolution	adsorption

Dimensionless numbers

Reynolds = ratio of momentum (hybnost) / viscous forces (vazké síly).
Eq. 19 for pipe (or a particle, then $d = d_p$), 20 for rotary component:

$$\mathrm{Re} = \frac{\rho v d}{\eta} \tag{19}$$

$$\mathrm{Re} = \frac{\rho f d^2}{\eta} \tag{20}$$

Note: $\mathrm{Re} < 2300$ laminar, $\mathrm{Re} > 10000$ turbulent.

Schmidt = ratio of convective diffusion / molecular diffusion:

$$\mathrm{Sc} = \frac{\nu}{D} = \frac{\eta}{\rho D} \tag{21}$$

Prandtl = ratio of viscosity / thermal diffusivity (teplotní difuzivita),
where λ is thermal conductivity (tepelná vodivost) $[\frac{\mathrm{W}}{\mathrm{m\cdot K}}]$:

$$\mathrm{Pr} = \frac{\nu}{D_\mathrm{T}} = \frac{\eta/\rho}{\lambda/C_\mathrm{p}/\rho} = \frac{\eta C_\mathrm{p}}{\lambda} \tag{22}$$

Grasshof describes the combined effect of gravity + thermal expansion (the free convection):

$$\mathrm{Gr} = \frac{gL^3}{\nu^2}\beta\Delta T \qquad\qquad \beta = \frac{1}{V_m}\frac{\partial V_m}{\partial T} \tag{23}$$

Nusselt = ratio of convection / conduction (vedení), α is heat transfer coeff:

$$\mathrm{Nu} = \frac{\alpha d}{\lambda} \tag{24}$$

Usually $\mathrm{Nu} = \mathrm{Nu}(\mathrm{Re}, \mathrm{Pr}, \mathrm{Gr})$; for a smooth tubular pipe you may use the Dittus-Boelter correlation: $\mathrm{Nu} = 0.023\mathrm{Re}^{0.8}\mathrm{Pr}^n$, where n is 0.3 when cooling, 0.4 when heating.

Sherwood = ratio of convection / diffusion, β is mass transfer coeff (koef. přestupu hmoty):

$$\mathrm{Sh} = \frac{\beta d}{D} \tag{25}$$

Power number for a rotary component:

$$\mathrm{N_P} = \frac{P}{\rho d^5 f^3} \tag{26}$$

Péclet relates to axial dispersion coeff E:

$$\mathrm{Pe} = \frac{lv}{E} \tag{27}$$

Damköhler = ratio of component A formation rate / convective transport rate in a tubular reactor, generally and for first order reaction:

$$\mathrm{Da} = \frac{Lr}{vc_\mathrm{A}} \qquad\qquad = \frac{Lk}{v} \tag{28}$$

Hydraulics

Bernoulli equation in various dimensions for *incompressible* flow.
Equation 29 serves no practical purpose, but is a great mnemotechnic.
Divide it with either m, V, mg to obtain equations 30, 31, 32.

$$\tfrac{1}{2}mv_1^2 + mgh_1 + p_1V = \tfrac{1}{2}mv_2^2 + mgh_2 + p_2V \qquad [\mathrm{J}] \tag{29}$$
$$\tfrac{1}{2}v_1^2 + gh_1 + p_1/\rho = \tfrac{1}{2}v_2^2 + gh_2 + p_2/\rho \qquad [\mathrm{J/kg}] \tag{30}$$
$$\tfrac{1}{2}\rho v_1^2 + \rho gh_1 + p_1 = \tfrac{1}{2}\rho v_2^2 + \rho gh_2 + p_2 \qquad [\mathrm{Pa}] \tag{31}$$
$$\tfrac{1}{2}\tfrac{v_1^2}{g} + h_1 + \tfrac{p_1}{\rho g} = \tfrac{1}{2}\tfrac{v_2^2}{g} + h_2 + \tfrac{p_2}{\rho g} \qquad [\mathrm{m}] \tag{32}$$

Energy dissipation can be added to the left-hand side of 30 for either a straight pipe section of length L and diameter d, or generally any pipe fitting (tvarovka či armatura):

$$e_{\mathrm{dis}} = \lambda\frac{Lv^2}{2d} \qquad = \zeta\frac{v^2}{2} \qquad [\mathrm{J/kg}] \tag{33}$$

Note 1: friction coeff λ and local resistance coeff ζ are dimensionless
Note 2: for laminar flow and straight tubular pipe, $\lambda = 64/Re$

By combining eqs 30, 33 and $v = F/A$, we get pressure drop as function of flow rate F:

$$\Delta p = e_{\mathrm{dis}}\rho = \lambda\rho\frac{8LF^2}{\pi^2 d^5} \tag{34}$$

Valve sizing:
C_V means such flow rate F [gal/min] of water at 60°F, that $\Delta P = 1$ psi
K_V means such flow rate F [m^3/h] of water at 16°C, that $\Delta P = 1$ bar
$K_V \doteq 0.8650 C_V$
By combining eqs 30, 33, and $\rho_{\mathrm{r}} = \rho/\rho_{\mathrm{H_2O}}$ we get the pressure drop in bars:

$$\frac{\Delta p}{\mathrm{bar}} = \rho_{\mathrm{r}}\frac{F^2}{K_V^2} \tag{35}$$

Note: make sure to use the same units for K_V and F.

Ergun equation for Δp along axis x in packed columns (výplňové kolony), where ε is void fraction (mezerovitost), d_{e} is equivalent particle diameter, v_x is superficial velocity.
For *compressible* flow: $\mu = \mu(x), \rho = \rho(x)$, but for *incompressible* we may simplify: $\frac{\partial p}{\partial x} = \frac{\Delta p}{L}$

$$\frac{\partial p}{\partial x} = \frac{150\mu}{d_{\mathrm{e}}^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}v_x + \frac{7}{4}\frac{\rho}{d_{\mathrm{e}}}\frac{(1-\varepsilon)}{\varepsilon^3}v_x|v_x| \tag{36}$$

Particle settling (usazování částic) in *laminar* flow (calculate settling velocity from Re):

$$\mathrm{Re} = \frac{\mathrm{Ar}^2}{18^3} \qquad \mathrm{Ar} = \frac{d_p^3 g}{\nu^2}\frac{(\rho_p - \rho)}{\rho} \tag{37}$$

Note: verify that $\mathrm{Re} < 2300$ (otherwise use more complex calculation)

Mass & heat effects

Adiabatic reaction exotherm (nárůst teploty), where $\hat{C}_{p,\mathrm{sp}}$ $[\frac{\mathrm{J}}{\mathrm{kg \cdot K}}]$:

$$\Delta T_{\mathrm{ad}} = \frac{-\Delta H_{\mathrm{R}}}{\hat{C}_{p,\mathrm{sp}}} \frac{c_{\mathrm{A}}^0}{\rho} X \tag{38}$$

Plate exchanger (deskový výměník) heat transfer from fluid 1 to fluid 2 through solid wall of surface A, where K, α are heat transfer coeffs $[\frac{\mathrm{W}}{\mathrm{m^2 K}}]$:

$$\dot{Q} = KA\Delta T \tag{39}$$

$$\frac{1}{K} = \frac{1}{\alpha_1} + \frac{d}{\lambda} + \frac{1}{\alpha_2} \tag{40}$$

Tube exchanger (trubkový výměník) with inner tube diameter d_1, outer d_2,
where K_L is heat transfer coeff per length $[\frac{\mathrm{W}}{\mathrm{m \cdot K}}]$:

$$\dot{Q} = K_L L \Delta T \tag{41}$$

$$\frac{2\pi}{K_L} = \frac{1}{d_1\alpha_1} + \frac{1}{\lambda} \ln \frac{d_2}{d_1} + \frac{1}{d_2\alpha_2} \tag{42}$$

ΔT in countercurrent exchange between points A, B, where ΔT_A is the temp. difference between *the two mediums* at point A, and analog. for B:

$$\Delta T_{\mathrm{ls}} = \frac{\Delta T_{\mathrm{A}} - \Delta T_{\mathrm{B}}}{\ln \frac{\Delta T_{\mathrm{A}}}{\Delta T_{\mathrm{B}}}} \tag{43}$$

Mass transfer of component i from fluid phase x to fluid phase y through phase interface,
expressed for $c_i[\mathrm{mol/m^3}]$, where K are mass transfer coeffs [m/s],
m is distribution coeff *at interface*: $m = c_{y,\mathrm{eq}}/c_{x,\mathrm{eq}}$

$$\dot{n}_i = K_x A \left(c_x - c_y/m\right) \qquad \dot{n}_i = K_y A \left(c_x m - c_y\right) \tag{44}$$

$$\frac{1}{K_x} = \frac{1}{\beta_x} + \frac{1}{\beta_y m} \qquad \frac{1}{K_y} = \frac{1}{\beta_x/m} + \frac{1}{\beta_y} \tag{45}$$

Note: choose only one from eqs 44, as they are lin. dependent; $K_x = mK_y$

Porous solids and catalysis

Throughput (zatížení) of a fixed-bed catalytic reactor is often expressed via $LHSV$ [h^{-1}] (liquid hourly space velocity) for liquid feed *incl. trickle-bed (skrápěné lože)*,
and for gas feed via $GHSV$, where $\bar{M}_{\text{feed}}$ is mean molar mass, $p^\circ = \text{atm}, T^\circ = 273.15\text{K}$

$$LHSV = \frac{\dot{V}_{\text{feed}}}{V_{\text{cat}}} = \frac{\dot{m}_{\text{feed}}}{\rho_{\text{feed}} V_{\text{cat}}} \tag{46}$$

$$GHSV = \frac{\dot{V}^\circ_{\text{feed}}}{V_{\text{cat}}} = \frac{\dot{n}_{\text{feed}}}{V_{\text{cat}}} \frac{RT^\circ}{p^\circ} = \frac{\dot{m}_{\text{feed}}}{V_{\text{cat}}} \frac{RT^\circ}{\bar{M}_{\text{feed}} p^\circ} \tag{47}$$

Thiele modulus (dimensionless) = ratio of surface reaction rate / mass transfer, $c_{\text{A,S}}$ is c at catalyst surface, d_p is radius of particle. The second form is simplification when $r = kSc_{\text{A,S}}$, with S being the specific surface [m^{-1}].

$$\kappa = d_p \sqrt{\frac{r}{c_{\text{A,S}} D_{\text{eff}}}} = d_p \sqrt{\frac{kS}{D_{\text{eff}}}} \tag{48}$$

Viscous flow in a porous particle or membrane, where β is the permeability [m^2]

$$\dot{V} = \beta \frac{A}{L} \frac{\Delta p}{\eta} \tag{49}$$

Freundlich isotherm (adsorption of component i) with parameters K, n:

$$\frac{m_i}{m_{\text{adsorbent}}} = K p^{\frac{1}{n}} \tag{50}$$

Langmuir-Hinschelwood: see **eq 12** *(which integrates the isotherm in the reaction rate formula)*