

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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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

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

Conversion

$$X = \frac{E^0 - E}{E^0} \qquad (2)$$

Yield (**výtěžek**)

$$Y = \frac{P}{E^0} \frac{\nu_E}{\nu_P} = X \cdot S \qquad (3)$$

Selectivity (of one reaction with st. coeffs ν_E, ν_P against all other reactions)

$$S = \frac{P}{E^0 - E} \frac{\nu_E}{\nu_P} \qquad (4)$$

Relative selectivity (of two parallel reactions $E \rightarrow P, P^*$ with st. coeffs ν_P, ν_{P^*})

$$S_{P/P^*} = \frac{P}{P^*} \frac{\nu_{P^*}}{\nu_P} = \frac{r_P}{r_{P^*}} \qquad (5)$$

Reaction kinetics

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

$$R = \frac{d\xi}{d\tau} \quad (6)$$

$$R_i = R\nu_i \quad (7)$$

$$r = \frac{dR}{dV} = \frac{d\xi_V}{d\tau} = \frac{1}{V\nu_i} \frac{dn_i}{d\tau} \quad (8)$$

$$r_i = r\nu_i = \frac{dR_i}{dV} = \frac{1}{V} \frac{dn_i}{d\tau} \quad (9)$$

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

$$FC_{A0} - FC_{A1} + \nu_A r(C_{A1})V = 0 \quad (10)$$

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

$$r = kc_A^a c_B^b - k_R c_C^c c_D^d \quad (11)$$

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

$$r = k_1 q_A q_B - k_2 q_C = k_1 K_A c_A K_B c_B q^2 - k_2 K_C c_C q \quad (12)$$

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

$$q = \frac{Q}{1 + K_A c_A + K_B c_B + K_C c_C} \quad (13)$$

Derivation: (q, q_A, q_B, q_C are unknowns, Q, K_A, K_B, K_C are parameters)

$$Q = q + q_A + q_B + q_C \quad (14)$$

$$K_i = \frac{q_i}{c_i q} \quad (15)$$

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

$$r_P = k_{\text{MAX}} \frac{c_S}{k_A + c_S} \quad (16)$$

Derivation: $dc_{ES}/d\tau = 0$, $c_E = c_E^0 - c_{ES}$

Thermodynamics

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

$$\ln p_i^\circ = A - \frac{B}{T + C} \quad (17)$$

Dependence of various constants on temperature:

$$\frac{d \ln k}{dT} = \frac{\Delta H}{RT^2} \quad (18)$$

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:

$$\text{Re} = \frac{\rho v d}{\eta} \quad (19)$$

$$\text{Re} = \frac{\rho f d^2}{\eta} \quad (20)$$

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

Schmidt = ratio of convective diffusion / molecular diffusion:

$$\text{Sc} = \frac{\nu}{D} = \frac{\eta}{\rho D} \quad (21)$$

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

$$\text{Pr} = \frac{\nu}{D_T} = \frac{\eta/\rho}{\lambda/C_p/\rho} = \frac{\eta C_p}{\lambda} \quad (22)$$

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

$$\text{Gr} = \frac{g L^3}{\nu^2} \beta \Delta T \quad \beta = \frac{1}{V_m} \frac{\partial V_m}{\partial T} \quad (23)$$

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

$$\text{Nu} = \frac{\alpha d}{\lambda} \quad (24)$$

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

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

$$\text{Sh} = \frac{\beta d}{D} \quad (25)$$

Power number for a rotary component:

$$\text{Np} = \frac{P}{\rho d^5 f^3} \quad (26)$$

Péclet relates to axial dispersion coeff E :

$$\text{Pe} = \frac{lv}{E} \quad (27)$$

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

$$\text{Da} = \frac{Lr}{vc_A} = \frac{Lk}{v} \quad (28)$$

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.

$$\frac{1}{2}mv_1^2 + mgh_1 + p_1V = \frac{1}{2}mv_2^2 + mgh_2 + p_2V \quad [\text{J}] \quad (29)$$

$$\frac{1}{2}v_1^2 + gh_1 + p_1/\rho = \frac{1}{2}v_2^2 + gh_2 + p_2/\rho \quad [\text{J/kg}] \quad (30)$$

$$\frac{1}{2}\rho v_1^2 + \rho gh_1 + p_1 = \frac{1}{2}\rho v_2^2 + \rho gh_2 + p_2 \quad [\text{Pa}] \quad (31)$$

$$\frac{1}{2}\frac{v_1^2}{g} + h_1 + \frac{p_1}{\rho g} = \frac{1}{2}\frac{v_2^2}{g} + h_2 + \frac{p_2}{\rho g} \quad [\text{m}] \quad (32)$$

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**):

$$e_{\text{dis}} = \lambda \frac{Lv^2}{2d} = \zeta \frac{v^2}{2} \quad [\text{J/kg}] \quad (33)$$

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 :

$$\Delta p = e_{\text{dis}}\rho = \lambda\rho \frac{8LF^2}{\pi^2 d^5} \quad (34)$$

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 [m³/h] of water at 16°C, that $\Delta P = 1$ bar

$K_V \doteq 0.8650C_V$

By combining eqs 30, 33, and $\rho_r = \rho/\rho_{\text{H}_2\text{O}}$ we get the pressure drop in bars:

$$\frac{\Delta p}{\text{bar}} = \rho_r \frac{F^2}{K_V^2} \quad (35)$$

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: $\frac{\partial p}{\partial x} = \frac{\Delta p}{L}$

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

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

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

Note: verify that $Re < 2300$ (otherwise use more complex calculation)

Mass & heat effects

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

$$\Delta T_{ad} = \frac{-\Delta H_R c_A^0}{\hat{C}_{p,sp} \rho} X \quad (38)$$

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 [$\frac{W}{m^2 K}$]:

$$\dot{Q} = K A \Delta T \quad (39)$$

$$\frac{1}{K} = \frac{1}{\alpha_1} + \frac{d}{\lambda} + \frac{1}{\alpha_2} \quad (40)$$

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

$$\dot{Q} = K_L L \Delta T \quad (41)$$

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

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:

$$\Delta T_{ls} = \frac{\Delta T_A - \Delta T_B}{\ln \frac{\Delta T_A}{\Delta T_B}} \quad (43)$$

Mass transfer of component i from fluid phase x to fluid phase y through phase interface, expressed for c_i [mol/m³], where K are mass transfer coeffs [m/s],

m is distribution coeff at interface: $m = c_{y,eq}/c_{x,eq}$

$$\dot{n}_i = K_x A (c_x - c_y/m) \quad \dot{n}_i = K_y A (c_x m - c_y) \quad (44)$$

$$\frac{1}{K_x} = \frac{1}{\beta_x} + \frac{1}{\beta_y m} \quad \frac{1}{K_y} = \frac{1}{\beta_x/m} + \frac{1}{\beta_y} \quad (45)$$

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

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}_{feed} is mean molar mass, $p^\circ = \text{atm}$, $T^\circ = 273.15\text{K}$

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

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

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

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

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

$$\dot{V} = \beta \frac{A \Delta p}{L \eta} \quad (49)$$

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

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

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