Institut für Technische Verbrennung
RWTH AACHEN UNIVERSITY

Formelsammlung

Technische Verbrennung I

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Kapitel 2
Thermodynamik von Verbrennungsprozessen

Molenbruch:

$$n_s = \sum_{i=1}^{n} n_i$$

$$X_i = \frac{n_i}{n_s}$$

Massenbruch:

$$m_i = M_i n_i$$

$$m = \sum_{i=1}^{n} m_i$$

$$Y_i = \frac{m_i}{m}$$

$$m = M n_s$$

$$M = \sum_{i=1}^{n} M_i X_i = \left[\sum_{i=1}^{n} \frac{Y_i}{M_i}\right]^{-1}$$

$$Y_i = \frac{M_i}{M} X_i$$

Massenbruch
der Elemente:

$$Z_j = \sum_{i=1}^{n} \frac{a_{ij} M_j}{M_i} Y_i$$

$$Z_j = \frac{M_j}{M} \sum_{i=1}^{n} a_{ij} X_i$$

Konzentration:

$$C_i = \frac{n_i}{V}$$

Volumenanteil:

$$v_i = \frac{V_i}{V} = X_i$$

Gasgesetz:

$$p = \frac{\rho \mathcal{R} T}{M} = C_s \mathcal{R} T, \quad \mathcal{R} = 8.31451 \frac{kJ}{kmol \cdot K}$$

stöchiometrischer Koeffizient:

$$\nu_i = \nu_i'' - \nu_i'$$

$$0 = \sum_{i=1}^{n} \nu_{ik}[X_i]$$

Umsatzgleichung:

$$\frac{dn_i}{\nu_i} = \frac{dn_1}{\nu_1}, \quad \frac{dm_i}{\nu_i M_i} = \frac{dm_1}{\nu_1 M_1}, \quad \frac{dY_i}{\nu_i M_i} = \frac{dY_1}{\nu_1 M_1}$$

$$\frac{Y_{O_2} - Y_{O_2,u}}{\nu'_{O_2} M_{O_2}} = \frac{Y_B - Y_{B,u}}{\nu'_B M_B}$$

Mindestluftbedarf:

$$l_{min} = \frac{o_{min}}{Y_{O_2,Luft}}, \quad l_{min,m} = \frac{o_{min,m}}{X_{O_2,Luft}}$$

Luftzahl:

$$\lambda = \frac{l}{l_{min}} = \frac{l_m}{l_{min,m}}, \quad \phi = \frac{1}{\lambda}$$

Restsauerstoff:

$$n_{O_2,Rest} = (\lambda - 1)\frac{\nu'_{O_2}}{\nu'_B} n_{B,u}, \quad m_{O_2,Rest} = (\lambda - 1)\frac{\nu'_{O_2} M_{O_2}}{\nu'_B M_B} m_{B,u}$$

1.Hauptsatz der Thermodynamik:

$$E = U + E_{\text{kin}} + E_{\text{pot}}$$

Innere Energie und Enthalpie:

$$H = U + pV$$

$$U = \sum_{i=1}^{n} m_i u_i, \quad U = \sum_{i=1}^{n} n_i u_{i,m}$$

$$H = \sum_{i=1}^{n} m_i h_i, \quad H = \sum_{i=1}^{n} n_i h_{i,m}$$

$$c_v = \sum_{i=1}^{n} Y_i c_{vi}, \quad c_{v,m} = \sum_{i=1}^{n} X_i c_{vi,m}$$

$$c_p = \sum_{i=1}^{n} Y_i c_{pi}, \quad c_{p,m} = \sum_{i=1}^{n} X_i c_{pi,m}$$

Reaktionsenthalpie und Heizwert:

$$h_u = \frac{(-\Delta h_m)}{\nu'_B M_B}$$

$$h_d = \Delta h_m = \sum_{i=1}^{n} \nu_i h_{i,m}$$

NASA-Polynome:

$$\frac{c_{p,m}}{\mathcal{R}} = a_1 + a_2 T/K + a_3 (T/K)^2 + a_4 (T/K)^3 + a_5 (T/K)^4$$

$$\frac{h_m}{\mathcal{R}T} = a_1 + a_2 \frac{T/K}{2} + a_3 \frac{(T/K)^2}{3} + a_4 \frac{(T/K)^3}{4} + a_5 \frac{(T/K)^4}{5} + \frac{a_6}{T/K}$$

$$\frac{s_m}{\mathcal{R}} = a_1 ln(T/K) + a_2 T/K + a_3 \frac{(T/K)^2}{2} + a_4 \frac{(T/K)^3}{3} + a_5 \frac{(T/K)^4}{4} + a_7 + ln \frac{p}{p_0}$$

adiabate Flammentemperatur:

$$T_b = T_u + \frac{(-\Delta h_m)_{ref} Y_{B,u}}{c_p \nu'_B M_B}$$

chemisches Gleichgewicht:

$$0 = \sum_{i=1}^{n} \nu_i \mu_i$$

Massenwirkungsgesetz:

$$K_{pk} = \prod_{i=1}^{n} \left(\frac{p_i}{p_0}\right)^{\nu_{ik}}$$

$$\pi_i(T) = \pi_{i,A} + \pi_{i,B} lnT$$

$$K_p(T) = \text{exp}\left(\frac{-\sum\limits_{i=1}^{n} \nu_i \mu_i^0}{\mathcal{R}T}\right) = \text{exp}\left(\frac{-\sum\limits_{i=1}^{n} \nu_i h_{i,m_{ref}}}{\mathcal{R}T}\right) \text{exp}\left(\sum_{i=1}^{n} \nu_i \pi_i\right)$$

$$K_{pk} = B_{pk} T^{n_{pk}} \text{exp}\left(\frac{-\Delta h_{k,m,ref}}{\mathcal{R}T}\right) \qquad \text{(Arrhenius-Ansatz)}$$

$$B_{pk} = \text{exp}\left(\sum_{i=1}^{n} \nu_{ik} \pi_{iA}\right)$$

$$n_{pk} = \sum_{i=1}^{n} \nu_{ik} \pi_{iB}$$

Kapitel 3
Reaktionskinetik homogener Gasreaktionen

chem. Reaktionsgeschw.:

$$\frac{dC_A}{dt} = -\nu'_A k_f C_A^{\nu'_A} C_B^{\nu'_B} + \nu'_A k_b C_C^{\nu''_C} C_D^{\nu''_D} = \nu_A w_f - \nu_A w_b = \nu_A w$$

$$k_i = B_i T^{n_i} \text{exp}\left(-\frac{E_i}{\mathcal{R}T}\right)$$

Konzentration inerter Stoßpartner:

$$C_{M'} = \sum_{i=1}^{n} z_i C_i$$

Gleichgewichtskonstante:

$$K_C = \frac{k_f(T)}{k_b(T)}$$

chem. Produktionsdichte:

$$\dot{m}_i = M_i \sum_{k=1}^{r} \nu_{ik} w_k$$

reduzierter Methan-Mechanismus

$$\begin{aligned}
I: &\quad CH_4 + 2H^\circ + H_2O &= CO + 4H_2 \\
II: &\quad CO + H_2O &= CO_2 + H_2 \\
III: &\quad 2H^\circ + M &= H_2 + M \\
IV: &\quad 3H_2 + O_2 &= 2H^\circ + 2H_2O
\end{aligned}$$

Kapitel 4
Zünd- und Löschvorgänge in homogenen Systemen

Verbrennung bei konst. Volumen:

$$\frac{du}{dt} = 0$$

Temperaturgleichung:

$$\rho c_v \frac{dT}{dt} = -\sum_{i=1}^{n} u_i M_i \sum_{k=1}^{r} \nu_{ik} w_k = -\sum_{i=1}^{n} u_i \, \dot{m}_i = -\sum_{k=1}^{r} \left(\sum_{i=1}^{n} M_i u_i \nu_{ik} \right) w_k$$

$$= \sum_{k=1}^{r} (-\Delta u_{k,m}) w_k$$

adiabate therm. Explosion:

$$w = B \left(\frac{\rho Y_B}{M_B} \right) \left(\frac{\rho Y_{O_2}}{M_{O_2}} \right) \text{exp} \left(-\frac{E}{\mathcal{R}T} \right)$$

Zündverzugszeit:

$$t_i = \frac{\mathcal{R}T_0^2}{E} \frac{c_v}{(-\Delta u_m) B \rho} \left(\frac{M_B}{Y_{B,0}} \right) \left(\frac{M_{O_2}}{Y_{O_2,0}} \right) \text{exp} \left(\frac{E}{\mathcal{R}T_0} \right)$$

$$\frac{t_{i,q}}{t_i} = \int_0^{\infty} \frac{dz}{\text{exp}(z) - \alpha z}, \qquad \alpha = \frac{t_i}{t_q}$$

Reaktorgleichungen:

$$\frac{dY^*}{dt^*} = 1 - Y^* - Da\, Y^* \, \text{exp} \left(-\frac{E^*}{T^*} \right)$$

$$\frac{dT^*}{dt^*} = 1 - T^* + Q^* \, Da\, Y^* \, \text{exp} \left(-\frac{E^*}{T^*} \right)$$

$$Y^* = \frac{Y}{Y_u}, \quad Da = \frac{t_v}{t_r}, \quad E^* = \frac{E}{\mathcal{R}T_u}, \quad T^* = \frac{T}{T_u}, \quad t^* = \frac{t}{t_v},$$

$$Q^* = \frac{(-\Delta h_m) Y_u}{c_p M T_u}$$

Kapitel 6
Laminare und turbulente Vormischflammen

Brennstoff-Luft-Verhältnis:

$$\phi = \frac{Z}{1-Z}\frac{1-Z_{st}}{Z_{st}}$$

$$T_b = aT_u + b + c\phi + d\phi^2 + e\phi^3$$

Approximationsformel:

$$s_L = Y_{B,u}^m A(T_0)\frac{T_u}{T_0}\left(\frac{T_b - T_0}{T_b - T_u}\right)^n, \qquad \phi \leq 1$$

$$A(T_0) = F\ \text{exp}(-G/T_0)$$

$$T_0 = -\frac{\tilde{E}}{ln(p/B)}$$

Zeldovich-Zahl:

$$\text{Ze} = n\left(\frac{T_b - T_u}{T_b - T_0} - 1\right) = \frac{E}{\mathcal{R}}\frac{T_b - T_u}{T_b^2}$$

Flammendicke:

$$l_F = \frac{D}{s_L} = \frac{\lambda_b}{c_p \rho_u s_L}$$

Flammenzeit:

$$t_F = \frac{l_F}{s_L}$$

chem. Flammenzeit:

$$t_c = \frac{\rho_u E^2 (T_b - T_u)^2}{2B\rho_b^2(\mathcal{R}T_b^2)^2 S}\ \text{exp}\left(\frac{E}{\mathcal{R}T_b}\right)$$

$$s_L = \sqrt{\frac{D}{t_c}}$$

Brennstoff	B [bar]	$\tilde{E}$ [K]	F [cm/s]	G [K]	m	n
CH_4	$3,1557 \times 10^8$	$23873,0$	$2,21760 \times 10^1$	$-6444,27$	$0,565175$	$2,5158$
C_2H_2	$5,6834 \times 10^4$	$11344,4$	$3,77466 \times 10^4$	$1032,36$	$0,907619$	$2,5874$
C_2H_4	$3,7036 \times 10^5$	$14368,7$	$9,97890 \times 10^3$	$263,23$	$0,771333$	$2,3998$
C_2H_6	$4,3203 \times 10^6$	$18859,0$	$1,90041 \times 10^3$	$-506,97$	$0,431345$	$2,1804$
C_3H_8	$2,2501 \times 10^6$	$17223,5$	$1,27489 \times 10^3$	$-1324,78$	$0,582214$	$2,3970$
CH_3OH	$2,1100 \times 10^6$	$17657,5$	$9,99557 \times 10^3$	$1088,85$	$0,91$	$2,263$
n-C_7H_{16}	$1,7000 \times 10^6$	$17508,0$	$7,95600 \times 10^3$	$912,00$	$0,52$	$2,30$
i-C_8H_{18}	$3,8000 \times 10^7$	$20906,0$	$2,92600 \times 10^3$	$-25,60$	$0,5578$	$2,5214$

Table 1: Koeffizienten zur Berechnung der laminaren Brenngeschwindigkeit für magere bis stöchiometrische Gemische

Brennstoff	a	b [K]	c [K]	d [K]	e [K]	Le
CH_4	$0,627$	1270,15	$-2449,0$	6776	-3556	$0,91$
C_2H_2	$0,52$	1646,0	$-2965,0$	8187	-4160	$1,68$
C_2H_4	$0,44$	602,0	$880,0$	2686	-1891	$1,21$
C_2H_6	$0,526$	1437,0	$-2967,0$	7538	-3873	$1,32$
C_3H_8	$0,53$	1434,0	$-2952,0$	7518	-3856	$1,63$
CH_3OH	$0,77$	1260,0	$-2449,0$	6797	-3594	$1,68$
n-C_7H_{16}	$0,49$	758,7	$-277,8$	4269	-2642	$2,056$
i-C_8H_{18}	$0,61$	936,0	$-1127,0$	5326	-3044	$2,55$

Table 2: Koeffizienten zur Berechnung der adiabaten Flammentemperatur sowie Zahlenwerte für die Lewis-Zahl

Kapitel 7
Laminare und turbulente Diffusionsflammen

Mischungsbruch:

$$Z = \frac{\dot{m}_1}{\dot{m}_1 + \dot{m}_2}$$

$\dot{m}_1$ Brenngasstrom

$\dot{m}_2$ Oxidatorstrom

$$Y_{B,u} = Y_{B,1} Z$$

$$Y_{O2,u} = Y_{O_2,2}(1 - Z)$$

$$Z_{st} = \left[1 + \nu \frac{Y_{B,1}}{Y_{O_2,2}}\right]^{-1} = \left[1 + \frac{\nu'_{O_2} M_{O_2} Y_{B,1}}{\nu'_B M_B Y_{O_2,2}}\right]^{-1}$$

$$\lambda = \frac{Z_{st}}{Z} \frac{1 - Z}{1 - Z_{st}}$$

adiabate Flammentemperatur:

$$T_b(Z) = T_u(Z) + \frac{(-\Delta h_m)_{ref} Y_{B,1}}{c_p \nu'_B M_B} Z, \qquad 0 \leq Z \leq Z_{st}$$

$$T_u(Z) = T_2 + Z(T_1 - T_2)$$

Burke-Schumann-Lösung:

$$T(Z) = T_u(Z) + \frac{Z}{Z_{st}} \left[T_{st} - T_u(Z_{st})\right], \qquad 0 \leq Z \leq Z_{st}$$

$$T(Z) = T_u(Z) + \frac{1 - Z}{1 - Z_{st}} \left[T_{st} - T_u(Z_{st})\right], \qquad Z_{st} \leq Z \leq 1$$