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FACTORS FOR UNIT CONVERSIONS

Quantity	**Equivalent Values**
Mass	1 kg = 1000 g = 0.001 metric ton = 2.20462 lb_m = 35.27392 oz
	1 lb_m = 16 oz = 5 x 10^{-4} ton = 453.593 g = 0.453593 kg
Length	1 m = 100 cm = 1000 mm = 10^6 microns (μm) = 10^{10} angstroms (Å)
	= 39.3701 in = 3.28084 ft = 1.09361 yd = 0.000621371 mile
	1 ft = 12 in. = 1/3 yd = 0.3048 m = 30.48 cm
Volume	1 m^3 = 1000 liters = 10^6 cm^3 = 10^6 ml
	= 35.31467 ft^3 = 219.969 imperial gallons = 264.172 gal
	= 1056.69 qt
	1 ft^3 = 1728 in^3 = 7.48052 gal = 0.028317 m^3 = 28.3168 liters
	= 28,316.8 cm^3
Force	1 N = 1 kg·m/s^2 = 10^5 dynes = 10^5 g·cm/s^2 = 0.22481 lb_f
	1 lb_f = 32.174 lb_m·ft/s^2 = 4.4482 N = 4.4482 x 10^5 dynes
Pressure	1 atm = 1.01325 x 10^5 N/m^2 (Pa) = 101.325 kPa = 1.01325 bars
	= 1.01325 x 10^6 dynes/cm^2
	= 760 mm Hg at 0˚ C (torr) = 10.333 m H_2O at 4˚ C
	= 14.696 lb_f/in^2 (psi) = 33.9 ft H_2O at 4˚C
	100 kPa = 1 bar
Energy	1 J = 1 N·m = 10^7 ergs = 10^7 dyne·cm
	= 2.778 x 10^{-7} kW·h = 0.23901 cal
	= 0.7376 ft·lb_f = 9.47817 x 10^{-4} Btu
Power	1 W = 1 J/s = 0.23885 cal/s = 0.7376 ft·lb_f/s = 9.47817 x 10^{-4} Btu/s = 3.4121 Btu/h
	= 1.341 x 10^{-3} hp (horsepower)
Viscosity	1 Pa·s = 1 N·s/m^2 = 1 kg/m·s
	= 10 poise = 10 dynes·s/cm^2 = 10 g/cm·s
	= 10^3 cp (centipoise)
	= 0.67197 lb_m/ft·s = 2419.088 lb_m/ft·h
Density	1 kg/m^3 = 10^{-3} g/cm^3
	= 0.06243 lb_m/ft^3
	10^3 kg/m^3 = 1 g/cm^3 = 62.428 lb_m/ft^3
Volumetric Flow	1 m^3/s= 35.31467 ft^3/s=15,850.32 gal/min (gpm)
	1 gpm = 6.30902 x 10^{-5} m^3/s=2.228009 x 10^{-3} ft^3/s=3.7854 liter/min
	1 liter/min=0.26417 gpm

Ver. 30-Oct-2014

Temperature	$T(^oC) = \frac{5}{9}\left[T(^oF) - 32\right]$
	$T(^oF) = \frac{9}{5}T(^oC) + 32 = 1.8T(^oC) + 32$
Absolute Temperature	T(K) = T(˚C) + 273.15
	T(˚R) = T(˚F) + 459.67
Temperature Interval (ΔT)	1 C˚ = 1 K = 1.8 F˚ = 1.8 R˚
	1F˚ = 1 R˚ = (5/9) C˚ = (5/9) K

USEFUL QUANTITIES

SG = ρ(20˚C)/ρ_{water} (4˚C)

ρ_{water}(4˚C) = 1000 kg/m^3 = 62.43 lb$_m$/ft^3 = 1.000 g/cm^3

ρ_{water}(25˚C) = 997.08 kg/m^3 = 62.25 lb$_m$/ft^3 = 0.99709 g/cm^3

g = 9.8066 m/s^2 = 980.66 cm/s^2 = 32.174 ft/s^2

μ_{water} (25˚C) = 8.937 x 10^{-4} Pa·s = 8.937 x 10^{-4} kg/m·s
= 0.8937 cp =0.8937 x 10^{-2} g/cm·s = 6.005 x 10^{-4} lb$_m$/ft·s

Composition of air:

N_2	78.03%
O_2	20.99%
Ar	0.94%
CO_2	0.03%
H_2, He, Ne, Kr, Xe	0.01%
	100.00%

M_{air} = 29 g/mol = 29 kg/kmol = 29 lb$_m$/lbmole

$\hat{C}_{p,water}$ (25˚C) = 4.182 kJ/kg K = 0.9989 cal/g˚C = 0.9997 Btu/lb$_m$˚F

R = 8.314 m^3·Pa/mol·K = 0.08314 liter·bar/mol·K = 0.08206 liter·atm/mol·K
= 62.36 liter·mm Hg/mol·K = 0.7302 ft^3·atm/lbmole·˚R
= 10.73 ft^3·psia/lbmole·˚R
= 8.314 J/mol·K
= 1.987 cal/mol·K = 1.987 Btu/lbmole·˚R

Ver. 30-Oct-2014

A.2-9 Properties of Saturated Steam and Water (Steam Table), SI Units

Temperature (°C)	Vapor Pressure (kPa)	Specific Volume (m^3/kg)		Enthalpy (kJ/kg)		Entropy (kJ/kg · K)	
		Liquid	Sat'd Vapor	Liquid	Sat'd Vapor	Liquid	Sat'd Vapor
0.01	0.6113	0.0010002	206.136	0.00	2501.4	0.0000	9.1562
3	0.7577	0.0010001	168.132	12.57	2506.9	0.0457	9.0773
6	0.9349	0.0010001	137.734	25.20	2512.4	0.0912	9.0003
9	1.1477	0.0010003	113.386	37.80	2517.9	0.1362	8.9253
12	1.4022	0.0010005	93.784	50.41	2523.4	0.1806	8.8524
15	1.7051	0.0010009	77.926	62.99	2528.9	0.2245	8.7814
18	2.0640	0.0010014	65.038	75.58	2534.4	0.2679	8.7123
21	2.487	0.0010020	54.514	88.14	2539.9	0.3109	8.6450
24	2.985	0.0010027	45.883	100.70	2545.4	0.3534	8.5794
25	3.169	0.0010029	43.360	104.89	2547.2	0.3674	8.5580
27	3.567	0.0010035	38.774	113.25	2550.8	0.3954	8.5156
30	4.246	0.0010043	32.894	125.79	2556.3	0.4369	8.4533
33	5.034	0.0010053	28.011	138.33	2561.7	0.4781	8.3927
36	5.947	0.0010063	23.940	150.86	2567.1	0.5188	8.3336
40	7.384	0.0010078	19.523	167.57	2574.3	0.5725	8.2570
45	9.593	0.0010099	15.258	188.45	2583.2	0.6387	8.1648
50	12.349	0.0010121	12.032	209.33	2592.1	0.7038	8.0763
55	15.758	0.0010146	9.568	230.23	2600.9	0.7679	7.9913
60	19.940	0.0010172	7.671	251.13	2609.6	0.8312	7.9096
65	25.03	0.0010199	6.197	272.06	2618.3	0.8935	7.8310
70	31.19	0.0010228	5.042	292.98	2626.8	0.9549	7.7553
75	38.58	0.0010259	4.131	313.93	2635.3	1.0155	7.6824
80	47.39	0.0010291	3.407	334.91	2643.7	1.0753	7.6122
85	57.83	0.0010325	2.828	355.90	2651.9	1.1343	7.5445
90	70.14	0.0010360	2.361	376.92	2660.1	1.1925	7.4791
95	84.55	0.0010397	1.9819	397.96	2668.1	1.2500	7.4159
100	101.35	0.0010435	1.6729	419.04	2676.1	1.3069	7.3549
105	120.82	0.0010475	1.4194	440.15	2683.8	1.3630	7.2958
110	143.27	0.0010516	1.2102	461.30	2691.5	1.4185	7.2387
115	169.06	0.0010559	1.0366	482.48	2699.0	1.4734	7.1833
120	198.53	0.0010603	0.8919	503.71	2706.3	1.5276	7.1296
125	232.1	0.0010649	0.7706	524.99	2713.5	1.5813	7.0775
130	270.1	0.0010697	0.6685	546.31	2720.5	1.6344	7.0269
135	313.0	0.0010746	0.5822	567.69	2727.3	1.6870	6.9777
140	316.3	0.0010797	0.5089	589.13	2733.9	1.7391	6.9299
145	415.4	0.0010850	0.4463	610.63	2740.3	1.7907	6.8833
150	475.8	0.0010905	0.3928	632.20	2746.5	1.8418	6.8379
155	543.1	0.0010961	0.3468	653.84	2752.4	1.8925	6.7935
160	617.8	0.0011020	0.3071	675.55	2758.1	1.9427	6.7502
165	700.5	0.0011080	0.2727	697.34	2763.5	1.9925	6.7078
170	791.7	0.0011143	0.2428	719.21	2768.7	2.0419	6.6663
175	892.0	0.0011207	0.2168	741.17	2773.6	2.0909	6.6256
180	1002.1	0.0011274	0.19405	763.22	2778.2	2.1396	6.5857
190	1254.4	0.0011414	0.15654	807.62	2786.4	2.2359	6.5079
200	1553.8	0.0011565	0.12736	852.45	2793.2	2.3309	6.4323
225	2548	0.0011992	0.07849	966.78	2803.3	2.5639	6.2503
250	3973	0.0012512	0.05013	1085.36	2801.5	2.7927	6.0730
275	5942	0.0013168	0.03279	1210.07	2785.0	3.0208	5.8938
300	8581	0.0010436	0.02167	1344.0	2749.0	3.2534	5.7045

Source: Abridged from J. H. Keenan, F. G. Keyes, P. G. Hill, and J. G. Moore, *Steam Tables—Metric Units*. New York: John Wiley & Sons, Inc., 1969. Reprinted by permission of John Wiley & Sons, Inc.

A.3-3 Physical Properties of Air at 101.325 kPa (1 Atm Abs), SI Units

T (°C)	T (K)	ρ (kg/m³)	c_p (kJ/kg · K)	$\mu \times 10^5$ (Pa · s, or kg/m · s)	k (W/m · K)	N_{Pr}	$\beta \times 10^3$ (1/K)	$g\beta\rho^2/\mu^2$ (1/K · m³)
−17.8	255.4	1.379	1.0048	1.62	0.02250	0.720	3.92	2.79×10^8
0	273.2	1.293	1.0048	1.72	0.02423	0.715	3.65	2.04×10^8
10.0	283.2	1.246	1.0048	1.78	0.02492	0.713	3.53	1.72×10^8
37.8	311.0	1.137	1.0048	1.90	0.02700	0.705	3.22	1.12×10^8
65.6	338.8	1.043	1.0090	2.03	0.02925	0.702	2.95	0.775×10^8
93.3	366.5	0.964	1.0090	2.15	0.03115	0.694	2.74	0.534×10^8
121.1	394.3	0.895	1.0132	2.27	0.03323	0.692	2.54	0.386×10^8
148.9	422.1	0.838	1.0174	2.37	0.03531	0.689	2.38	0.289×10^8
176.7	449.9	0.785	1.0216	2.50	0.03721	0.687	2.21	0.214×10^8
204.4	477.6	0.740	1.0258	2.60	0.03894	0.686	2.09	0.168×10^8
232.2	505.4	0.700	1.0300	2.71	0.04084	0.684	1.98	0.130×10^8
260.0	533.2	0.662	1.0341	2.80	0.04258	0.680	1.87	0.104×10^8

A.2-11 Heat-Transfer Properties of Liquid Water, SI Units

T (°C)	T (K)	ρ (kg/m³)	c_p (kJ/kg · K)	$\mu \times 10^3$ (Pa · s, or kg/m · s)	k (W/m · K)	N_{Pr}	$\beta \times 10^4$ (1/K)	$(g\beta\rho^2/\mu^2) \times 10^{-8}$ (1/K · m³)
0	273.2	999.6	4.229	1.786	0.5694	13.3	−0.630	
15.6	288.8	998.0	4.187	1.131	0.5884	8.07	1.44	10.93
26.7	299.9	996.4	4.183	0.860	0.6109	5.89	2.34	30.70
37.8	311.0	994.7	4.183	0.682	0.6283	4.51	3.24	68.0
65.6	338.8	981.9	4.187	0.432	0.6629	2.72	5.04	256.2
93.3	366.5	962.7	4.229	0.3066	0.6802	1.91	6.66	642
121.1	394.3	943.5	4.271	0.2381	0.6836	1.49	8.46	1300
148.9	422.1	917.9	4.312	0.1935	0.6836	1.22	10.08	2231
204.4	477.6	858.6	4.522	0.1384	0.6611	0.950	14.04	5308
260.0	533.2	784.9	4.982	0.1042	0.6040	0.859	19.8	11 030
315.6	588.8	679.2	6.322	0.0862	0.5071	1.07	31.5	19 260

Source: Geankoplis, Transport Processes and Separation Process Principles, 4th Edition, Prentice Hall, 2003

Welty, Rorrer, Foster, “Fundamentals of Momentum, Heat, and Mass Transfer, 6th ed., Wiley 2015

Typo in value of α_{Cu} corrected, 24Feb2019.

Appendix H

Physical Properties of Solids

Material	ρ		c_p		α		k (Btu/h ft °F)			(W/m · K)		
	(lb_m/ft^3) (68°F)	(kg/m^3) (293 K)	(Btu/lb_m°F) (293 K)	(J/kg · 1K) $\times 10^{-2}$ (293K)	(ft^2/h) (68°F)	(m^2/s) · 10^5 (293k)	°F (68)	(212)	(572)	K (293)	(373)	(573)
Metals												
Aluminum	168.6	2,701.1	0.224	9.383	3.55	9.16	132	133	133	229	229	230
Copper	555	8,890	0.092	3.854	3.98	11.27	223	219	213	386	379	369
Gold	1206	19,320	0.031	1.299	4.52	11.66	169	170	172	293	294	298
Iron	492	7,880	0.122	5.110	0.83	2.14	42.3	39	31.6	73.2	68	54
Lead	708	11,300	0.030	1.257	0.80	2.06	20.3	19.3	17.2	35.1	33.4	29.8
Magnesium	109	1,750	0.248	10.39	3.68	9.50	99.5	96.8	91.4	172	168	158
Nickel	556	8,910	0.111	4.560	0.87	2.24	53.7	47.7	36.9	93.0	82.6	63.9
Platinum	1340	21,500	0.032	1.340	0.09	0.23	40.5	41.9	43.5	70.1	72.5	75.3
Silver	656	10,500	0.057	2.388	6.42	16.57	240	237	209	415	410	362
Tin	450	7,210	0.051	2.136	1.57	4.05	36	34	—	62	59	—
Tungsten	1206	19,320	0.032	1.340	2.44	6.30	94	87	77	160	150	130
Uranium	1167	18,700	0.027	1.131	0.53	1.37	16.9	17.2	19.6	29.3	29.8	33.9
Zinc	446	7,150	0.094	3.937	1.55	4.00	65	63	58	110	110	100
Alloys												
Aluminum 2024	173	2,770	0.230	9.634	1.76	4.54	70.2			122		
Brass (70% Cu, 30% Ni)	532	8,520	0.091	3.812	1.27	3.28	61.8	73.9	85.3	107	128	148
Constantan (60% Cu, 40% Ni)	557	8,920	0.098	4.105	0.24	0.62	13.1	15.4		22.7	26.7	
Iron, cast	455	7,920	0.100	4.189	0.65	1.68	29.6	26.8		51.2	46.4	
Nichrome V	530	8,490	0.106	4.440	0.12	0.31	7.06	7.99	9.94	12.2	13.8	17.2
Stainless steel	488	7,820	0.110	4.608	0.17	0.44	9.4	10.0	13	16	17.3	23
Steel, mild (1% C)	488	7,820	0.113	4.733	0.45	1.16	24.8	24.8	22.9	42.9	42.9	39.0
Nonmetals												
Asbestos	36	580	0.25	10.5			0.092	0.11	0.125	0.159	0.190	0.21
Brick (fire clay)	144	2,310	0.22	9.22				0.65			1.13	
Brick (masonry)	106	1,670	0.20	8.38			0.38			0.66		
Brick (chrome)	188	3,010	0.20	8.38				0.67			1.16	
Concrete	144	2,310	0.21	8.80			0.70			1.21		
Corkboard	10	160	0.4	17			0.025			0.043		
Diatomaceous earth, powdered	14	220	0.2	8.4			0.03			0.05		
Glass, window	170	2,720	0.2	8.4			0.45			0.78		
Glass, Pyrex	140	2,240	0.2	8.4			0.63	0.67	0.84	1.09	1.16	1.45
Kaolin firebrick	19	300							0.052			0.09
85% Magnesia	17	270					0.038	0.041		0.066	0.071	
Sandy loam, 4% H_2O	104	1,670	0.4	17			0.54			0.94		
Sandy loam, 10% H_2O	121	1,940					1.08			1.87		
Rock wool	10	160	0.2	8.4			0.023	0.033		0.040	0.057	
Wood, oak ⊥ to grain	51	820	0.57	23.9			0.12			0.21		
Wood, oak ∥ to grain	51	820	0.57	23.9			0.23			0.40		

Stokes-Einstein equation (for diffusion of a sphere): $D_{AB} = \frac{kT}{6\pi R\mu}$

Lumped parameter analysis characteristic length: $D_{char} = \frac{V}{A}$

Mass-Transfer Diffusion Coefficients in Binary Systems

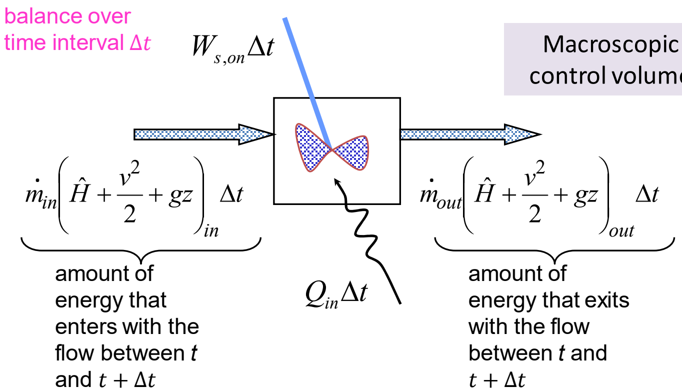
Table J.1 Binary mass diffusivities in gases†

System	T (K)	$D_{AB}P$(cm^2 atm/s)	$D_{AB}P$(m^2 Pa/s)
Air			
Ammonia	273	0.198	2.006
Aniline	298	0.0726	0.735
Benzene	298	0.0962	0.974
Bromine	293	0.091	0.923
Carbon dioxide	273	0.136	1.378
Carbon disulfide	273	0.0883	0.894
Chlorine	273	0.124	1.256
Diphenyl	491	0.160	1.621
Ethyl acetate	273	0.0709	0.718
Ethanol	298	0.132	1.337
Ethyl ether	293	0.0896	0.908
Iodine	298	0.0834	0.845
Methanol	298	0.162	1.641
Mercury	614	0.473	4.791
Naphthalene	298	0.0611	0.619
Nitrobenzene	298	0.0868	0.879
n-Octane	298	0.0602	0.610
Oxygen	273	0.175	1.773
Propyl acetate	315	0.092	0.932
Sulfur dioxide	273	0.122	1.236
Toluene	298	0.0844	0.855
Water	298	0.260	2.634
Ammonia			
Ethylene	293	0.177	1.793
Argon			
Neon	293	0.329	3.333
Carbon dioxide			
Benzene	318	0.0715	0.724
Carbon disulfide	318	0.0715	0.724
Ethyl acetate	319	0.0666	0.675

Source: Welty, Rorrer, Foster, 6th ed, 2015, Appendix J, first page only.

Unsteady Macroscopic Energy Balance

see Felder and Rousseau or Himmelblau



Unsteady Macroscopic Energy Balance

accumulation = input − output

Q_{in} = Heat ***in***to the chosen macroscopic control volume

$$\frac{d}{dt}\left(U_{sys}+E_{k,sys}+E_{p,sys}\right)=-\Delta H-\Delta E_k-\Delta E_p+Q_{in}+W_{s,on}$$

$Q_{in}=\sum_i q_{in,i}$ comes from a variety of sources:

Signs must match transfer from outside (bulk fluid) to inside (metal)

- Thermal conduction: $q_{in}=-kA\frac{dT}{dx}$
- Convection: $q_{in}=hA(T_b-T)$
- Radiation: $q_{in}=\varepsilon\sigma A\left(T_{surroundings}^4-T_{surface}^4\right)$
- Electric current: $q_{in}=I^2R_{elec}L$
- Chemical Reaction: $q_{in}=S_{rxn}V_{sys}$

$S[=]\frac{\text{energy}}{\text{time volume}}$

Unsteady Macroscopic Energy Balance

$$\frac{d}{dt}\left(U_{sys}+E_{k,sys}+E_{p,sys}\right)=-\Delta H-\Delta E_k-\Delta E_p+Q_{in}+W_{s,on}$$

$Q_{in}=\sum_i q_{in,i}$ comes from a variety of sources:

- **Thermal conduction: $q_{in}=-kA\frac{dT}{dx}$**
  e.g. device held by bracket; a solid phase that extends through boundaries of control volume
- **Convection: $q_{in}=hA(T_b-T)$**
  e.g. device dropped in stirred liquid; forced air stream flows past, natural convection occurs outside system; phase change at boundary
- **Radiation: $q_{in}=\varepsilon\sigma A\left(T_{surroundings}^4-T_{surface}^4\right)$**
  e.g. device at high temp. exposed to a gas/vacuum; hot enough to produce nat. conv.=possibly hot enough for radiation
- **Electric current: $q_{in}=I^2R_{elec}L$**
  e.g. if electric current is flowing within the device/control volume/ system
- **Chemical Reaction: $q_{in}=S_{rxn}V_{sys}$**
  e.g. if a homogeneous reaction is taking place throughout the device/ control volume/system

S-B constant: $\sigma=5.676\times10^{-8}\frac{W}{m^2K^4}$

Table: Emissivity ε of solids $(300K)$

Material	ε
Aluminum foil	0.04
Asbestos board	0.96
Brass, polished	0.03
Brass, dull plate	0.22
Cast iron, turned and heated	0.60-0.70
Concrete	0.85
Ice, smooth	0.966
Ice, rough	0.985
Plaster	0.98
Roofing paper	0.91
Sand	0.76
Steel, Oxidized	0.79
Wrought Iron	0.94

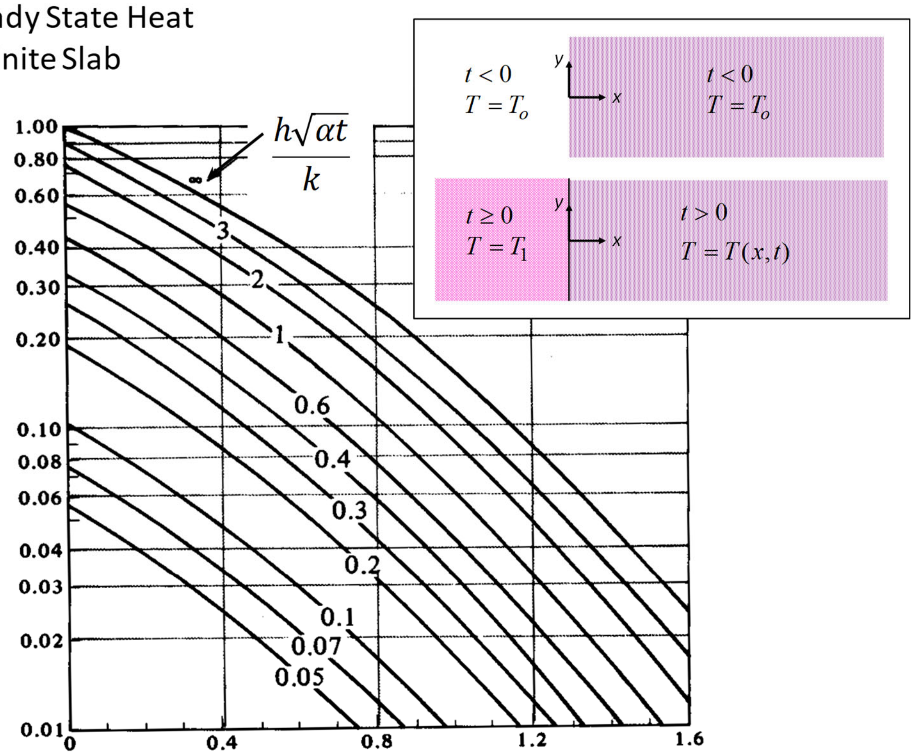
Reference: Engineering Toolbox, *www.engineeringtoolbox.com/emissivity-coefficients-d_447.html*

Mechanical Energy Balance:

$$\frac{P_2-P_1}{\rho}+\frac{\langle v\rangle_2^2-\langle v\rangle_1^2}{2\alpha}+g(z_2-z_1)+F_{21}=\frac{W_{s,on,21}}{\dot{m}}$$

1D Heat Transfer: Unsteady State Heat Conduction in a Semi-Infinite Slab

$$1 - Y = \left(\frac{T - T_0}{T_1 - T_0}\right)$$

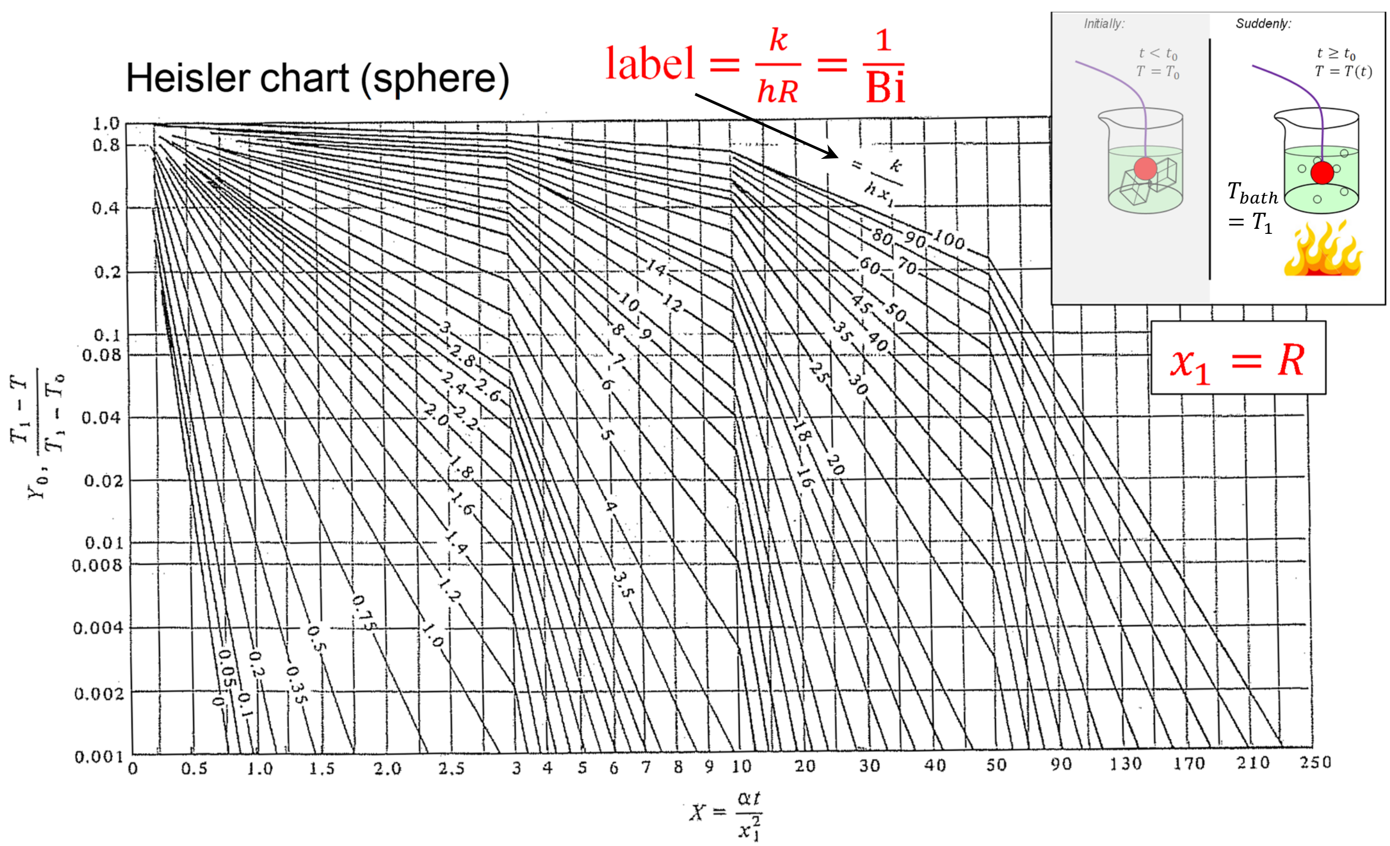


$$\zeta = \frac{x}{2\sqrt{\alpha\, t}}$$

Geankoplis 4th ed.,
Figure 5.3-3, page 364

Heisler chart (sphere)

$$\text{label} = \frac{k}{hR} = \frac{1}{\text{Bi}}$$



$$x_1 = R$$

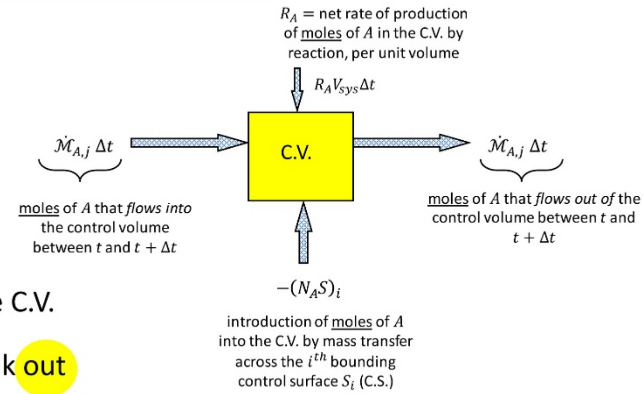
FIGURE 5.3-10. *Chart for determining the temperature at the center of a sphere for unsteady-state heat conduction. [From H. P. Heisler, Trans. A.S.M.E., 69, 227 (1947). With permission.]*

From Geankopolis, 4th edition, page 374

MOLES

accumulation = net flow in + production + introduction

$$\frac{d}{dt}\left(\mathcal{M}_{A,sys}\right) = -\Delta\dot{\mathcal{M}}_A + R_A V_{sys} - \sum_i (N_A S)_i$$



$\mathcal{M}_{A,sys} = c_A V_{sys}$ = total moles of A in the C.V.

$\Delta\dot{\mathcal{M}}_A = \sum_{j,outs}\dot{\mathcal{M}}_{A,j} - \sum_{j,ins}\dot{\mathcal{M}}_{A,j}$ = bulk out

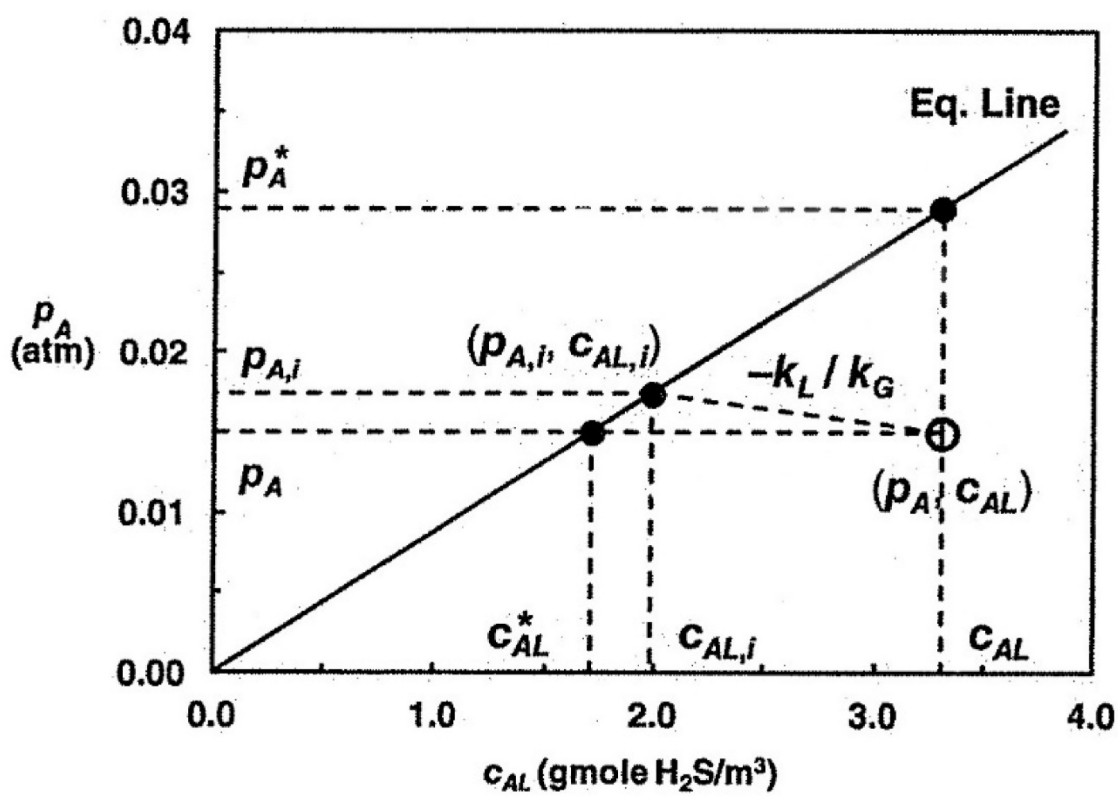
R_A = net rate of production of moles of A in the C.V. by reaction, per unit volume

V_{sys} = system volume

$N_{A_i} = k_c(c_A - c^*_{Ai})$ =molar flux of A out through the i^{th} C.S.

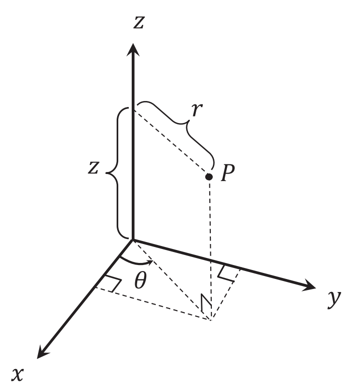
$S_{sys} = \sum_i S_i$
Δ is "out"- "in"
C.S. = control surface
C.V. = control volume

Example:
WRF Example 1 page 604 (solution in text)

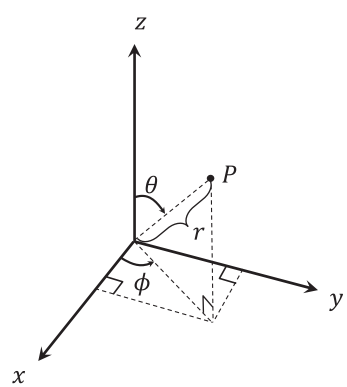


The equations in F. A. Morrison, ***An Introduction to Fluid Mechanics*** (Cambridge, 2013) assume the following definitions of the cylindrical and spherical coordinate systems.

Cylindrical Coordinate System: Note that the θ-coordinate swings around the z-axis



Spherical Coordinate System: Note that the θ-coordinate swings down from the z-axis; this is different from its definition in the cylindrical system above.



Typical values of the convection heat transfer coefficient. From Incropera et al., Fundamentals of Heat and Mass Transfer, 6th edition, Wiley, 2007.

Process		$h\left(\frac{W}{m^2K}\right)$
Free convection	Gases	2-25
	Liquids	50-1000
Forced convection	Gases	25-250
	Liquids	100-20,000
Convection with phase change	Boiling or condensation	2500-10^5

The **Equation of Energy** in Cartesian, cylindrical, and spherical coordinates for Newtonian fluids of constant density, with source term S. Source could be electrical energy due to current flow, chemical energy, etc. Two cases are presented: the general case where thermal conductivity may be a function of temperature (vector flux $\underline{\tilde{q}} = \underline{q}/A$ appears in the equations); and the more usual case, where thermal conductivity is constant.

Fall 2013 Faith A. Morrison, Michigan Technological University

Microscopic energy balance, in terms of flux; Gibbs notation

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = -\nabla \cdot \underline{\tilde{q}} + S$$

Microscopic energy balance, in terms of flux; Cartesian coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = -\left(\frac{\partial \tilde{q}_x}{\partial x} + \frac{\partial \tilde{q}_y}{\partial y} + \frac{\partial \tilde{q}_z}{\partial z} \right) + S$$

Microscopic energy balance, in terms of flux; cylindrical coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = -\left(\frac{1}{r} \frac{\partial (r\tilde{q}_r)}{\partial r} + \frac{1}{r} \frac{\partial \tilde{q}_\theta}{\partial \theta} + \frac{\partial \tilde{q}_z}{\partial z} \right) + S$$

Microscopic energy balance, in terms of flux; spherical coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + \frac{v_\phi}{r \sin\theta} \frac{\partial T}{\partial \phi} \right) = -\left(\frac{1}{r^2} \frac{\partial (r^2 \tilde{q}_r)}{\partial r} + \frac{1}{r \sin\theta} \frac{\partial (\tilde{q}_\theta sin\theta)}{\partial \theta} + \frac{1}{r \sin\theta} \frac{\partial \tilde{q}_\phi}{\partial \phi} \right) + S$$

Fourier's law of heat conduction, Gibbs notation: $\underline{\tilde{q}} = -k \nabla T$

Fourier's law of heat conduction, Cartesian coordinates: $\begin{pmatrix} \tilde{q}_x \\ \tilde{q}_y \\ \tilde{q}_z \end{pmatrix}_{xyz} = \begin{pmatrix} -k \frac{\partial T}{\partial x} \\ -k \frac{\partial T}{\partial y} \\ -k \frac{\partial T}{\partial z} \end{pmatrix}_{xyz}$

Fourier's law of heat conduction, cylindrical coordinates: $\begin{pmatrix} \tilde{q}_r \\ \tilde{q}_\theta \\ \tilde{q}_z \end{pmatrix}_{xyz} = \begin{pmatrix} -k \frac{\partial T}{\partial r} \\ -\frac{k}{r} \frac{\partial T}{\partial \theta} \\ -k \frac{\partial T}{\partial z} \end{pmatrix}_{r\theta z}$

Fourier's law of heat conduction, spherical coordinates: $\begin{pmatrix} \tilde{q}_r \\ \tilde{q}_\theta \\ \tilde{q}_\phi \end{pmatrix}_{xyz} = \begin{pmatrix} -k \frac{\partial T}{\partial r} \\ -\frac{k}{r} \frac{\partial T}{\partial \theta} \\ -\frac{k}{r \sin\theta} \frac{\partial T}{\partial \phi} \end{pmatrix}_{r\theta\phi}$

The **Equation of Energy** for systems with **constant k**

Microscopic energy balance, constant thermal conductivity; Gibbs notation

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = k \nabla^2 T + S$$

Microscopic energy balance, constant thermal conductivity; Cartesian coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + S$$

Microscopic energy balance, constant thermal conductivity; cylindrical coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right) + S$$

Microscopic energy balance, constant thermal conductivity; spherical coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial T}{\partial \phi} \right)$$
$$= k \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial T}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 T}{\partial \phi^2} \right) + S$$

Reference: F. A. Morrison, "Web Appendix to *An Introduction to Fluid Mechanics*," Cambridge University Press, New York, 2013. On the web at www.chem.mtu.edu/~fmorriso/IFM_WebAppendixCD2013.pdf

The **Equation of Species Mass Balance** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the mass flux with respect to mass-average velocity ($\underline{j}_A$) appears (p. 1), and the more usual case (p. 2), where the diffusion coefficient is constant and Fick's law has been incorporated.

Spring 2019 Faith A. Morrison, Michigan Technological University

In terms of mass flux, $\underline{j}_A$

Microscopic species mass balance, in terms of mass flux; Gibbs notation

$$\rho\left(\frac{\partial \omega_A}{\partial t}+\underline{v}\cdot\nabla\omega_A\right)=-\nabla\cdot\underline{j}_A+r_A$$

WRF 25-10

Microscopic species mass balance, in terms of mass flux; Cartesian coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_x\frac{\partial \omega_A}{\partial x}+v_y\frac{\partial \omega_A}{\partial y}+v_z\frac{\partial \omega_A}{\partial z}\right)=-\left(\frac{\partial j_{A,x}}{\partial x}+\frac{\partial j_{A,y}}{\partial y}+\frac{\partial j_{A,z}}{\partial z}\right)+r_A$$

Microscopic species mass balance, in terms of mass flux; cylindrical coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_r\frac{\partial \omega_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta}+v_z\frac{\partial \omega_A}{\partial z}\right)=-\left(\frac{1}{r}\frac{\partial (r j_{A,r})}{\partial r}+\frac{1}{r}\frac{\partial j_{A,\theta}}{\partial \theta}+\frac{\partial j_{A,z}}{\partial z}\right)+r_A$$

Microscopic species mass balance, in terms of mass flux; spherical coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t}+v_r\frac{\partial \omega_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}\right)=-\left(\frac{1}{r^2}\frac{\partial (r^2 j_{A,r})}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial (j_{A,\theta}\sin\theta)}{\partial \theta}+\frac{1}{r\sin\theta}\frac{\partial j_{A,\phi}}{\partial \phi}\right)+r_A$$

Fick's law of diffusion, Gibbs notation: $\underline{j}_A=-\rho D_{AB}\nabla\omega_A$

WRF 24-17

$$=\rho\omega_A(\underline{v}_A-\underline{v})$$

Fick's law of diffusion, Cartesian coordinates:
$$\begin{pmatrix} j_{A,x}\\ j_{A,y}\\ j_{A,z}\end{pmatrix}_{xyz}=\begin{pmatrix}-\rho D_{AB}\frac{\partial \omega_A}{\partial x}\\ -\rho D_{AB}\frac{\partial \omega_A}{\partial y}\\ -\rho D_{AB}\frac{\partial \omega_A}{\partial z}\end{pmatrix}_{xyz}$$

Fick's law of diffusion, cylindrical coordinates:
$$\begin{pmatrix} j_{A,r}\\ j_{A,\theta}\\ j_{A,z}\end{pmatrix}_{r\theta z}=\begin{pmatrix}-\rho D_{AB}\frac{\partial \omega_A}{\partial r}\\ -\frac{\rho D_{AB}}{r}\frac{\partial \omega_A}{\partial \theta}\\ -\rho D_{AB}\frac{\partial \omega_A}{\partial z}\end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:
$$\begin{pmatrix} j_{A,r}\\ j_{A,\theta}\\ j_{A,\phi}\end{pmatrix}_{r\theta\phi}=\begin{pmatrix}-\rho D_{AB}\frac{\partial \omega_A}{\partial r}\\ -\frac{\rho D_{AB}}{r}\frac{\partial \omega_A}{\partial \theta}\\ -\frac{\rho D_{AB}}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}\end{pmatrix}_{r\theta\phi}$$

The **Equation of Species Mass Balance, constant ρD_{AB}.** For binary systems, and Fick's law has been incorporated. Good for dilute liquid solutions at constant temperature and pressure.

In terms of Diffusivity, D_{AB}

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

$$\rho\left(\frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A\right) = \rho D_{AB} \nabla^2 \omega_A + r_A$$

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_x \frac{\partial \omega_A}{\partial x} + v_y \frac{\partial \omega_A}{\partial y} + v_z \frac{\partial \omega_A}{\partial z}\right) = \rho D_{AB}\left(\frac{\partial^2 \omega_A}{\partial x^2} + \frac{\partial^2 \omega_A}{\partial y^2} + \frac{\partial^2 \omega_A}{\partial z^2}\right) + r_A$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_r \frac{\partial \omega_A}{\partial r} + \frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta} + v_z \frac{\partial \omega_A}{\partial z}\right) = \rho D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \omega_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 \omega_A}{\partial \theta^2} + \frac{\partial^2 \omega_A}{\partial z^2}\right) + r_A$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_r \frac{\partial \omega_A}{\partial r} + \frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}\right)$$
$$= \rho D_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \omega_A}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \omega_A}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 \omega_A}{\partial \phi^2}\right) + r_A$$

$cx_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$ $\left(\text{units: } c[=]\frac{mol\ mix}{vol\ soln}; \rho[=]\frac{mass\ mix}{vol\ soln}; c_A[=]\frac{mol\ A}{vol\ soln}; \rho_A[=]\frac{mass\ A}{vol\ soln}\right)$

$\underline{j}_A \equiv$ mass flux of species A relative to a mixture's mass average velocity, $\underline{v}$ $\left(\text{units: } \underline{j}_A[=]\frac{mass\ A}{area\cdot time}\right)$

$= \rho_A(\underline{v}_A - \underline{v})$

$\underline{j}_A + \underline{j}_B = 0$, i.e. these fluxes are measured relative to the mixture's center of mass

$\underline{n}_A \equiv \rho_A \underline{v}_A = \underline{j}_A + \rho_A \underline{v} =$ combined mass flux relative to stationary coordinates

$\underline{n}_A + \underline{n}_B = \rho \underline{v}$

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

$\underline{v} = \omega_A \underline{v}_A + \omega_B \underline{v}_B \equiv$ mass average velocity; same velocity as in the microscopic momentum and energy balances

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002.
(p. 515, 584)

The **Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B.

The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.

Spring 2019 Faith A. Morrison, Michigan Technological University

In terms of total molar flux, $\underline{N}_A$

Microscopic species mass balance, in terms of molar flux; Gibbs notation

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

WRF 25-11

Microscopic species mass balance, in terms of combined molar flux; Cartesian coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; cylindrical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{A,r})}{\partial r} + \frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{A,r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{A,\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{A,z}}{\partial \phi}\right) + R_A$$

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

$$= c_A \underline{v}^* - cD_{AB}\nabla x_A$$

WRF 24-22

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB}\frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB}\frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

NOTES:

- If component A has no sink, $\underline{N}_A = 0$.
- If A diffuses through stagnant B, $\underline{N}_B = 0$.
- If a binary mixture of A and B are undergoing steady equimolar counterdiffusion, $\underline{N}_A = -\underline{N}_B$.
- If, for example, two moles of A diffuse to a surface at which a rapid, irreversible reaction coverts it to one mole of B, then at steady state $-0.5\underline{N}_A = \underline{N}_B$.

$cx_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$ $\left(\text{units: } c[=]\frac{mol\ mix}{vol\ soln}; \rho[=]\frac{mass\ mix}{vol\ soln}; c_A[=]\frac{mol\ A}{vol\ soln}; \rho_A[=]\frac{mass\ A}{vol\ soln}\right)$

$\underline{J}_A^* \equiv$ molar flux relative to a mixture's molar average velocity, $\underline{v}^*$ $\left(\text{units: } \underline{J}_A^*[=]\frac{mole\ A}{area{\cdot}time}\right)$

$= c_A(\underline{v}_A - \underline{v}^*)$

$\underline{J}_A^* + \underline{J}_B^* = 0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ combined molar flux relative to stationary coordinates

$\underline{N}_A + \underline{N}_B = c\underline{v}^*$

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

$\underline{v}^* = x_A\underline{v}_A + x_B\underline{v}_B \equiv$ molar average velocity

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002.
(p. 515, 584)

The **Equation of Species Mass Balance in Terms of Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. Two cases are presented: the general case, where the molar flux with respect to molar velocity ($\underline{J}_A^*$) appears (p. 1), and the more usual case (p. 2), where the diffusion coefficient is constant and Fick's law has been incorporated.

Spring 2019 Faith A. Morrison, Michigan Technological University

In terms of molar flux, $\underline{J}_A^*$

Microscopic species mass balance, in terms of molar flux; Gibbs notation

$$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^* \cdot \nabla x_A\right) = -\nabla \cdot \underline{J}_A^* + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, in terms of molar flux; Cartesian coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_x^* \frac{\partial x_A}{\partial x} + v_y^* \frac{\partial \omega_A}{\partial y} + v_z^* \frac{\partial x_A}{\partial z}\right) = -\left(\frac{\partial J_{A,x}^*}{\partial x} + \frac{\partial J_{A,y}^*}{\partial y} + \frac{\partial J_{A,z}^*}{\partial z}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, in terms of molar flux; cylindrical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + v_z^* \frac{\partial x_A}{\partial z}\right) = -\left(\frac{1}{r}\frac{\partial (r J_{A,r}^*)}{\partial r} + \frac{1}{r}\frac{\partial J_{A,\theta}^*}{\partial \theta} + \frac{\partial J_{A,z}^*}{\partial z}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, in terms of molar flux; spherical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_r^* \frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + \frac{v_\phi^*}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\right) = -\left(\frac{1}{r^2}\frac{\partial (r^2 J_{A,r}^*)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (J_{A,\theta}^* \sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial J_{A,\phi}^*}{\partial \phi}\right) + (x_B R_A - x_A R_B)$$

Fick's law of diffusion, Gibbs notation: $\underline{J}_A^* = -cD_{AB}\nabla x_A$

WRF 24-16

$$= c x_A(\underline{v}_A - \underline{v}^*)$$

Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} J_{A,x}^* \\ J_{A,y}^* \\ J_{A,z}^* \end{pmatrix}_{xyz} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial x} \\ -cD_{AB}\frac{\partial x_A}{\partial y} \\ -cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$

Fick's law of diffusion, cylindrical coordinates: $\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,z}^* \end{pmatrix}_{r\theta z} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial r} \\ -\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ -cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$

Fick's law of diffusion, spherical coordinates: $\begin{pmatrix} J_{A,r}^* \\ J_{A,\theta}^* \\ J_{A,\phi}^* \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} -cD_{AB}\frac{\partial x_A}{\partial r} \\ -\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ -\frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$

The **Equation of Species Mass Balance in Terms of Molar Quantities, constant cD_{AB}.** For binary systems, and Fick's law has been incorporated. Good for low density gases at constant temperature and pressure.

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

$$c\left(\frac{\partial x_A}{\partial t}+\underline{v}^*\cdot\nabla x_A\right)=cD_{AB}\nabla^2 x_A+(x_B R_A-x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$c\left(\frac{\partial x_A}{\partial t}+v_x^*\frac{\partial x_A}{\partial x}+v_y^*\frac{\partial x_A}{\partial y}+v_z^*\frac{\partial x_A}{\partial z}\right)=cD_{AB}\left(\frac{\partial^2 x_A}{\partial x^2}+\frac{\partial^2 x_A}{\partial y^2}+\frac{\partial^2 x_A}{\partial z^2}\right)+(x_B R_A-x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$c\left(\frac{\partial x_A}{\partial t}+v_r^*\frac{\partial x_A}{\partial r}+\frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta}+v_z^*\frac{\partial x_A}{\partial z}\right)=cD_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x_A}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 x_A}{\partial \theta^2}+\frac{\partial^2 x_A}{\partial z^2}\right)+(x_B R_A-x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$c\left(\frac{\partial x_A}{\partial t}+v_r^*\frac{\partial x_A}{\partial r}+\frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta}+\frac{v_\phi^*}{r\sin\theta}\frac{\partial x_A}{\partial \phi}\right)$$
$$=cD_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial x_A}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial x_A}{\partial \theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2 x_A}{\partial \phi^2}\right)+(x_B R_A-x_A R_B)$$

In terms of Diffusivity, D_{AB}

$cx_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$ $\left(\text{units: } c[=]\frac{mol\ mix}{vol\ soln}; \rho[=]\frac{mass\ mix}{vol\ soln}; c_A[=]\frac{mol\ A}{vol\ soln}; \rho_A[=]\frac{mass\ A}{vol\ soln}\right)$

$\underline{J}_A^* \equiv$ molar flux relative to a mixture's molar average velocity, $\underline{v}^*$ $\left(\text{units: } \underline{J}_A^*[=]\frac{mole}{area\cdot time}\right)$

$= c_A(\underline{v}_A-\underline{v}^*)$

$\underline{J}_A^*+\underline{J}_B^*=0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^*+c_A\underline{v}^* =$ combined molar flux relative to stationary coordinates

$\underline{N}_A+\underline{N}_B = c\underline{v}^*$

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

$\underline{v}^* = x_A\underline{v}_A + x_B\underline{v}_B \equiv$ molar average velocity

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002. (p. 515, 584)