

Therefore, the *dimensionless* equilibrium constant is written as:

$$K_{eq} = e^{-\Delta G_0 / \mathcal{R}T}$$

Key points to note:

There are at least three ways of writing the equilibrium constant, where it may have (strange) physical units. [\[Read page 97 of textbook.\]](#)

To compute chemical systems in equilibrium, all one has to do is to collect Gibbs free energies of the various molecules and then construct the Gibbs free energy of formation corresponding to the reaction.

Pay close attention to whether it is the specific Gibbs free energy (per unit mass) or molar Gibbs free energy.

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Appendix D: Gibbs Free Energies of Various Molecules and Reactions

We collect the molar Gibbs free energies of formation, associated with various common molecules, from the JANAF tables (<http://kinetics.nist.gov/janaf/>).

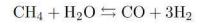
Table 6: Molar Gibbs free energies of various chemical species ($P_0 = 1$ bar)

T	H ₂ O	CH ₄	CO	CO ₂	C ₂ H ₂	C ₂ H ₄
Name	water	methane	carbon monoxide	carbon dioxide	acetylene	ethylene
(K)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)
500	-219.051	-32.741	-135.114	-394.360	197.452	80.333
600	-214.007	-22.887	-164.486	-395.182	191.735	88.017
700	-208.812	-12.643	-173.518	-395.298	186.097	95.467
800	-203.496	-2.115	-182.497	-395.586	180.534	103.180
900	-198.083	8.616	-191.416	-395.748	175.041	111.082
1000	-192.590	19.492	-200.275	-395.886	169.607	119.122
1100	-187.033	30.472	-209.075	-396.001	164.226	127.259
1200	-181.425	41.524	-217.819	-396.098	158.888	135.467
1300	-175.774	52.626	-226.509	-396.177	153.588	143.724
1400	-170.089	63.761	-235.149	-396.240	148.319	152.016
1500	-164.376	74.918	-243.740	-396.288	143.078	160.331
1600	-158.639	86.088	-252.284	-396.323	137.861	168.663
1700	-152.883	97.265	-260.784	-396.344	132.665	177.007
1800	-147.111	108.445	-269.242	-396.353	127.487	185.357
1900	-141.325	119.624	-277.658	-396.349	122.327	193.712
2000	-135.528	130.802	-286.034	-396.333	117.182	202.070
2100	-129.721	141.975	-294.372	-396.304	112.052	210.429
2200	-123.905	153.144	-302.672	-396.262	106.935	218.790
2300	-118.082	164.308	-310.936	-396.209	101.830	227.152
2400	-112.252	175.467	-319.165	-396.142	96.738	235.515
2500	-106.416	186.622	-327.358	-396.062	91.658	243.880
2600	-100.575	197.771	-335.517	-395.969	86.589	252.246
2700	-94.729	208.916	-343.643	-395.862	81.530	260.615
2800	-88.878	220.058	-351.736	-395.742	76.483	268.987
2900	-83.023	231.196	-359.797	-395.609	71.447	277.363
3000	-77.163	242.332	-367.826	-395.461	66.421	285.743

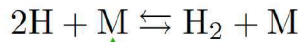
Note: The molar Gibbs free energy associated with H₂ is 0 J mol⁻¹ by definition.

Examples of tabulated Gibbs free energies from the textbook.

For example, we can use them to calculate ΔG_0 for the following chemical reaction (weighted by the stoichiometric coefficients):



Simplest possible chemical system: pure hydrogen



some third body
(not so relevant)

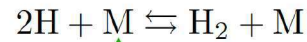
Ensure mass conservation: $n_{\text{H}} + 2n_{\text{H}_2} = n_{\text{total}}$

Write down equilibrium constant: $K'_{eq} = \frac{n_{\text{H}_2}}{n_{\text{H}}^2}$

Combine to obtain quadratic equation: $2K'_{eq}n_{\text{H}}^2 + n_{\text{H}} - n_{\text{total}} = 0$

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Simplest possible chemical system: pure hydrogen



some third body
(not so relevant)

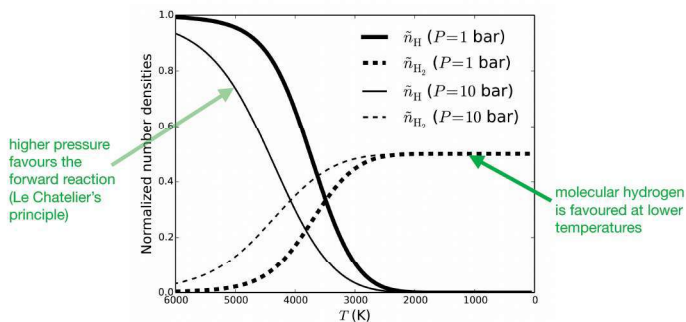
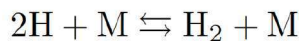
Solve for number density of atomic hydrogen:
$$n_{\text{H}} = \frac{-1 + (1 + 8K'_{eq}n_{\text{total}})^{1/2}}{4K'_{eq}}$$

The appendix of the textbook lists the Gibbs free energy of atomic hydrogen, which you can use to construct the Gibbs free energy of formation of the chemical reaction. This then allows you to relate a given (T, P) with the number density of both atomic and molecular hydrogen.

I suggest that you do this yourself as an exercise, as it is simple and builds intuition.

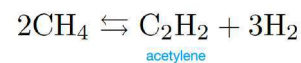
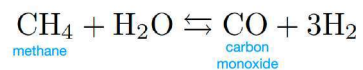
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Simplest possible chemical system: pure hydrogen



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A (still) simple chemical system: C-H-O



Write down equilibrium constants of the two reactions, where quantities with tildes are divided by n_{H_2} (volume mixing ratios):

$$K'_{eq} = \frac{n_{\text{CO}}n_{\text{H}_2}^3}{n_{\text{CH}_4}n_{\text{H}_2\text{O}}} = \frac{\tilde{n}_{\text{CO}}\tilde{n}_{\text{H}_2}^2}{\tilde{n}_{\text{CH}_4}\tilde{n}_{\text{H}_2\text{O}}},$$

$$K'_{eq,2} = \frac{n_{\text{C}_2\text{H}_2}n_{\text{H}_2}^3}{n_{\text{CH}_4}^2} = \frac{\tilde{n}_{\text{C}_2\text{H}_2}\tilde{n}_{\text{H}_2}^2}{\tilde{n}_{\text{CH}_4}^2}.$$

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