**CBE 40445**
**Fall 2020**
**Test #2**
**October 5, 2020**

## 1.  Tissue engineering (60 points)

In the 1990's, Professor Robert Langer and colleagues were culturing (rat) heart cells in laboratory dishes and creating thin cellular layers that would "beat" when electrically stimulated.  It seemed that "tissue engineering" would soon allow the synthesis of pieces of heart, liver or other tissue (*ex vivo* — outside the living creature) in a laboratory setting.  This tissue could then be transplanted into people to repair, say a portion of a damaged heart.

Soon, reality struck!  The thickness of the sheets was ultimately limited by diffusion of nutrients and perhaps most significantly by oxygen levels.  Of course this is why blood vessels infiltrate all tissue and no active cells are more than ~20 μm away from a capillary (less for heart tissue).

Even 25+ years later this limitation is a "show-stopper" despite various microfabrication techniques being applied to create artificial "pores" and specific efforts at synthesizing blood vessels.

A work around, but not at the level of functioning heart tissue is shown in figure 1.
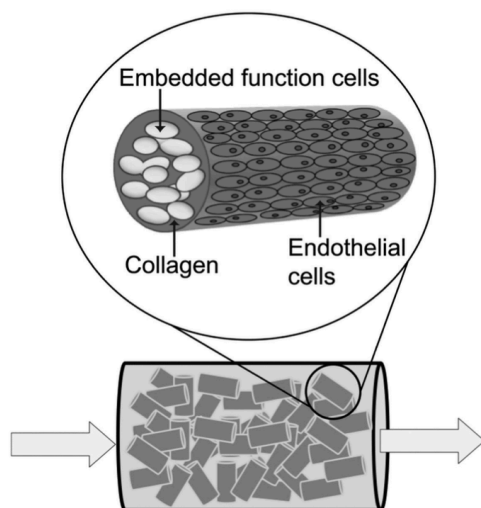
**Effectiveness factor and diffusion limitations in collagen gel modules containing HepG2 cells**

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**Figure 1.**
Modular tissue engineering. Small collagen rods containing embedded functional cells and coated with endothelial cells are randomly packed to form a "packed bed" construct. Interstitial spaces between modules allow the construct to be perfused.

In this paper they note that it had previously been assumed that cells cultured inside the collagen rods would be healthy because there would be no internal diffusion resistance. However, above a certain diameter, the cultured cells die.  They use a Thiele modulus and effectiveness factor analysis to quantify this problem.  Note that the normal assumption for oxygen as a nutrient for living cells is that the reaction is 0 order.

The authors define a Thiele modulus as

$$\phi^2 \equiv \frac{\rho_{cell}\,(OUR)\,L_p^2}{C^*\,D_{eff}}$$

where $\rho_{cell}$ is the cell density (cells/m$^3$), *OUR* is the oxygen uptake rate per cell (mole O$_2$/cell-s), $L_p$ is the characteristic length of the cylindrical modules (m), C* is the molar concentration of O$_2$ in the bulk fluid (mol O$_2$/m$^3$) and $D_{eff}$ is the effective diffusivity of oxygen in the modules (m$^2$/s).

The effectiveness factor can be defined as

$$\eta \equiv \frac{average\ volumetric\ reaction\ rate}{reaction\ rate\ with\ C\ =\ C^*\ in\ entire\ volume}$$

And we know that η can be calculated using

$$\eta = \frac{\tanh(\phi)}{\phi}$$

For this problem we would like to be able to support a cell density of 1 X10$^9$ cells/m$^3$, healthy cells have an *OUR* of 5X10$^{-15}$ mol/cell-s, $D_{eff}$ for this material is 1 X10$^{-9}$ m$^2$/s and C* = 0.001 mol/m$^3$.

a.  What is the physical meaning of the Thiele modulus?
b.  Explain how the definition here is consistent with 0 order kinetics.
c.  What is the value of the Thiele modulus for a 2 mm diameter module ($L_p$ = 5 X10$^{-4}$ m)[1] ?
d.  What are the values of the concentration in a 2 mm diameter module ($L_p$ = 5 X10$^{-4}$ m) at the center and 1/2 of the distance from the center to the surface of a module?
e.  What is the effectiveness factor for this diameter?
f.  If you want the effectiveness factor to be > 0.85, what is the largest diameter module that could be used?

The reaction is supposed to be 0 order so we can try a different approach to the analysis. Let's choose a differential equation that describes 0 order kinetics in a slab.

g.  What differential equation would describe diffusion with 0 order kinetics in a slab (rectangular) geometry?
h.  <u>Use a solution for this 0-order rectangular geometry case</u> to find the concentration within a rectangular slab that matches the 2mm particle (so the slab needs to be 5 X10$^{-4}$ m) that you solved for in part d. Do these match?
i.  Is there a range of φ where the match should be best? Why?

Extra credit: What would you have to know to verify that there is no external resistance in this configuration?

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[1] The author's didn't consider finite length

## 2. Analysis of a sequential reaction (30 points)

Consider a reaction scheme we have seen before for A-> M using a catalyst on a surface.
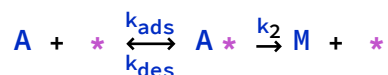
$$A + * \underset{k_{des}}{\overset{k_{ads}}{\longleftrightarrow}} A* \overset{k_2}{\rightarrow} M + *$$

It is not too hard to show that the rate of this reaction sequence is

$$r = \frac{k_2 \, K_{ads} \, [A] \, [*]_0}{1 + \frac{k_2}{k_{des}} + K_{ads} [A]},$$

where $\qquad K_{ads} \equiv \dfrac{k_{ads}}{k_{des}}$

A. For which values of which parameters could the initial adsorption step be close to equilibrium?
B. If this is not the case, could the A* concentration be approximated as being at a steady state concentration? Explain.
C. Adsorption experiments have provided a value of 10 l/mol for $K_{ads}$, also $k_{des}$ =0.1/s. Use these rate data to "<u>estimate</u>" $k_2$ and $[*]_0$.

| [A] (mol/l) | r  mol/(l-s) |
|---|---|
| 2 | 2 |
| 1 | 1.9 |
| 0.01 | 0.1 |

D. Suppose that an inert, B, is present that can also reversibly adsorb on the surface as

$$B + * \underset{k_{Bdes}}{\overset{k_{Bads}}{\longleftrightarrow}} B* \qquad K_{Bads} \equiv \frac{k_{Bads}}{k_{Bdes}}$$,

Explain why this inert will affect the observed reaction rate of A->M.

E. What you would have to know to <u>quantify</u> this effect?

### 3. A->M reaction as function of temperature. (10 points)

For the above reaction, the follow data as function of temperature are available.

| T (K) | [A] (mol/l) | r  mol/(l-s) |
|---|---|---|
| 300 | 2 | 2 |
| 320 | 2 | 3.5 |

a.  What is the apparent activation energy for this reaction?
b.  Under what conditions would you expect that this activation energy could be used to get an accurate prediction of the rate at 340 K?
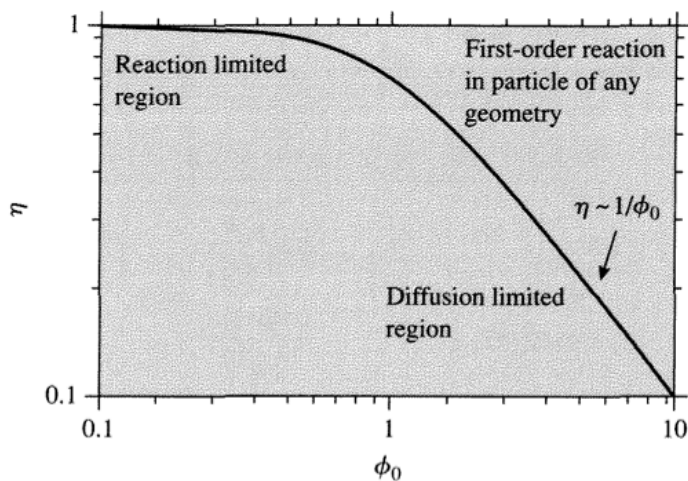
Test 2 additions to the formula sheet

$$N_{Ax} = -D_{AB} \frac{dC_A}{dx}$$

$$Sh = \frac{\bar{k}_c (2R_p)}{D_{AB}}$$

$$-\frac{dN_A}{dx} = \frac{2k_s}{R_{pore}} C_A$$

$$N_A = -D_{TA} \frac{dC_A}{dx}$$

$$\frac{d^2C_A}{dx^2} - \frac{2k_s}{D_{TA}R_{pore}} C_A = 0$$

$$\frac{d^2C_A}{d\chi^2} - \phi^2 C_A = 0$$

$$r_{obs} = 4\pi (R_p)^2 D_{TA}^e \frac{dC_A}{d\bar{r}} \bigg|_{\bar{r}=R_p}$$

$$\eta = \frac{r_{obs}}{r_{max}} = \frac{4\pi (R_p)^2 D_{TA}^e \frac{dC_A}{d\bar{r}}\big|_{\bar{r}=R_p}}{\frac{4}{3}\pi (R_p)^3 kC_{AS}} = \frac{3}{R_p} \frac{D_{TA}^e}{k} \frac{\frac{dC_A}{d\bar{r}}\big|_{\bar{r}=R_p}}{C_{AS}}$$



$$\phi_0 = L_p \sqrt{\frac{k}{D_{TA}^e}}$$

$$L_p = \frac{V_p}{S_p}$$

$$\eta = \frac{\tanh(\phi_0)}{\phi_0}$$

**Figure 6.3.9 |**
Effectiveness factor $[\eta = \tanh(\phi_0)/\phi_0]$ for a first-order
reaction in a catalyst as a function of the Thiele modulus
with generalized length parameter.

**Table 6.3.2** | Characteristic length parameters of common pellet shapes.

| | $L_p$ |
|---|---|
| Slab | Length of pore, $x_p$ |
| Cylinder | $R_p/2$ |
| Sphere | $R_p/3$ |

$$\phi_0 = \frac{V_p}{S_p}\sqrt{\frac{k}{D_{TA}^e}} = \left[\frac{R_p}{\dfrac{R_p}{x_p} + 2}\right]\sqrt{\frac{k}{D_{TA}^e}}$$

$$\phi_0 = \frac{V_p}{S_p}\sqrt{\frac{n+1}{2}\frac{kC_{AS}^{n-1}}{D_{TA}^e}} \qquad n > -1$$

$$r_{obs} = \eta k C_{AS}^n$$

In[138]:= `TrigToExp[Cosh[ϕ ω]]`

Out[138]= $\dfrac{e^{-\phi\,\omega}}{2} + \dfrac{e^{\phi\,\omega}}{2}$

In[139]:= `TrigToExp[Sinh[ϕ ω]]`

Out[139]= $-\dfrac{1}{2}\,e^{-\phi\,\omega} + \dfrac{e^{\phi\,\omega}}{2}$

In[141]:= `Together[TrigToExp[Tanh[ϕ ω]]]`

Out[141]= $\dfrac{-1 + e^{2\,\phi\,\omega}}{1 + e^{2\,\phi\,\omega}}$

In[142]:= `D[Cosh[ϕ ω], ω]`

Out[142]= $\phi\,\mathrm{Sinh}[\phi\,\omega]$

In[143]:= `D[Sinh[ϕ ω], ω]`

Out[143]= $\phi\,\mathrm{Cosh}[\phi\,\omega]$

In[144]:= `D[Tanh[ϕ ω], ω]`

Out[144]= $\phi\,\mathrm{Sech}[\phi\,\omega]^{2}$

In[145]:= `1 / Sech[ϕ ω]`

Out[145]= $\mathrm{Cosh}[\phi\,\omega]$

$\omega \equiv x/L_P,$
$\psi[\omega] \equiv C_{O2}[\omega]/C^{*}$
Outside surface is x=1.  Middle of particle is x=1.

In[152]:= `DSolve[{ D[ψ[ω], {ω, 2}] - ϕ^2 ψ[ω] == 0, ψ[1] == 1, ψ'[0] == 0}, ψ[ω], ω]`

Out[152]= $\left\{\left\{\psi[\omega] \to \dfrac{e^{\phi-\phi\,\omega}\left(1 + e^{2\,\phi\,\omega}\right)}{1 + e^{2\,\phi}}\right\}\right\}$

In[153]:= `ψ[ω] /. %[[1]]`

Out[153]= $\dfrac{e^{\phi-\phi\,\omega}\left(1 + e^{2\,\phi\,\omega}\right)}{1 + e^{2\,\phi}}$

In[154]:= `FullSimplify[ExpToTrig[%]]`

Out[154]= $\mathrm{Cosh}[\phi\,\omega]\,\mathrm{Sech}[\phi]$

In[155]:= `(1 / ϕ^2 D[Cosh[ϕ ω] Sech[ϕ], ω]) /. ω → 1`

Out[155]= $\dfrac{\mathrm{Tanh}[\phi]}{\phi}$

Potentially useful formulae:

$$\Delta G - \Delta G^0 = R_g T \sum_{i=1}^{NCOMP} v_i \ln a_i = R_g T \ln\left(\prod_i a_i^{v_i}\right) \qquad \Delta G^0 = -R_g T \ln\left[\frac{a_W^{\overline{w}} a_S^{\overline{s}}\cdots}{a_A^{\overline{a}} a_B^{\overline{b}}\cdots}\right] = -R_g T \ln K_a$$

equilibrium constant.

$$\left[\frac{\partial(\ln K_a)}{\partial T}\right]_P = \frac{\Delta H^0}{R_g T^2} \qquad K_a = \exp\left[-\Delta G^0/(R_g T)\right]$$

$$a = \bar{f}_i/\bar{f}_i^0 \qquad \bar{f}_i = X_i \bar{\phi}_i P \qquad K_a = \left[\frac{X_W^{\overline{w}} X_S^{\overline{s}}\cdots}{X_A^{\overline{a}} X_B^{\overline{b}}\cdots}\right]\left[\frac{\overline{\phi}_W^{\overline{w}} \overline{\phi}_S^{\overline{s}}\cdots}{\overline{\phi}_A^{\overline{a}} \overline{\phi}_B^{\overline{b}}\cdots}\right] P^{\overline{w}+\overline{s}+\cdots-\overline{a}-\overline{b}\cdots}$$

The fractional conversion is defined as:

$$f(t) = \frac{\Phi(t)}{\Phi_{\max}} \tag{1.2.9}$$

and can be calculated from Equations (1.2.3) and (1.2.8):

$$f_\ell = (-v_\ell)\frac{\Phi}{n_\ell^0} = 1 - \frac{n_\ell}{n_\ell^0} \tag{1.2.10}$$

Equation (1.2.10) can be rearranged to give:

$$n_\ell = n_\ell^0(1 - f_\ell) \tag{1.2.11}$$

where $0 \leq f_\ell \leq 1$. When the thermodynamics of the system limit $\Phi$ such that it cannot reach $\Phi_{\max}$ (where $n_\ell = 0$), $\Phi$ will approach its equilibrium value $\Phi^{eq}$ ($n_\ell \neq 0$ value of $n_\ell$ determined by the equilibrium constant). When a reaction is limited by

This expression is either positive or equal to zero if the system has reached equilibrium. The reaction rate, like $\Phi$, is an extensive property of the system. A specific rate called the *volumic rate* is obtained by dividing the reaction rate by the volume of the system, $V$:

$$r = \frac{1}{V}\frac{d\Phi}{dt} \qquad \left(\frac{mol}{time\cdot volume}\right) \tag{1.3.2}$$

Differentiation of Equation (1.2.3) gives:

$$dn_i = v_i \, d\Phi \tag{1.3.3}$$

Substitution of Equation (1.3.3) into Equation (1.3.2) yields:

$$r = \frac{1}{v_i V}\frac{dn_i}{dt} \tag{1.3.4}$$

tion (1.2.1), then the number of moles of component $A_i$ at any time $t$ will be given by the equation:

$$n_i(t) = n_i^0 + \nu_i \Phi(t) \tag{1.2.3}$$

that is an expression of the *Law of Definitive Proportions* (or more simply, a mole balance) and defines the parameter, $\Phi$, called the *extent of reaction*. The extent of reaction is a function of time and is a natural reaction variable.

concentrations, $C_i$, is desired. Since $C_i = n_i/V$, Equation (1.3.4) can be written as:

$$r = \frac{1}{\nu_i V} \frac{d}{dt}(C_i V) = \frac{1}{\nu_i} \frac{dC_i}{dt} + \frac{C_i}{\nu_i V} \frac{dV}{dt} \tag{1.3.6}$$

Note that only when the volume of the system is constant that the volumic rate can be written as:

$$r = \frac{1}{\nu_i} \frac{dC_i}{dt}, \text{ constant } V \tag{1.3.7}$$

When it is not possible to write a stoichiometric equation for the reaction, the

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### Rule II

The rate of an irreversible (one-way) reaction can generally be written in the form:

$$r = k(T)\overline{F}(C_i,T) \tag{1.4.1}$$

where $\overline{F}(C_i,T)$ is a function that depends on the composition of the system as expressed by the concentrations $C_i$.

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### Rule III

The rate constant generally depends on the absolute temperature, $T$, following the law first proposed by Arrhenius in 1889:

$$k = \overline{A} \exp\left[\frac{-E}{R_g T}\right] \tag{1.4.2}$$

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### Rule IV

Frequently, the function $\overline{F}(C_i)$ in the expression $r = k\overline{F}(C_i)$ can approximately be written as:

$$\overline{F}(C_i) = \prod_i C_i^{\alpha_i}$$

Consider the unimolecular reaction:

$$A \rightarrow products \qquad (1.5.1)$$

Using the Guldberg-Waage form of the reaction rate to describe this reaction gives:

$$r = kC_A \qquad (1.5.2)$$

From Equations (1.3.4) and (1.5.2):

$$r = \frac{1}{v_i V} \frac{dn_i}{dt} = \frac{-1}{V} \frac{dn_A}{dt} = kC_A$$

$$\frac{dn_A}{dt} = -kn_A \qquad \text{(variable } V) \qquad (1.5.3)$$

$$\frac{df_A}{dt} = k(1 - f_A) \qquad [\text{using Equation (1.2.11)}] \qquad (1.5.4)$$

Consider the bimolecular reaction:

$$A + B \rightarrow products \qquad (1.5.7)$$

Using the Guldberg-Waage form of the reaction rate to describe this reaction gives:

$$r = kC_A C_B \qquad (1.5.8)$$

$$r = \frac{1}{v_i V} \frac{dn_i}{dt} = \frac{-1}{V} \frac{dn_A}{dt} = kC_A C_B$$

$$r = \left(\frac{\overline{k}T}{h}\right) \exp\left[\frac{\Delta S_0^{\ddagger}}{R_g}\right] \exp\left[\frac{-\Delta H_0^{\ddagger}}{R_g T}\right] C_A C_B$$

$$\frac{dn_i}{dt} = 0 - 0 + (v_i r V)$$

accumulation     input     output     amount produced by reaction

The material balance can also be written in terms of the fractional conversion and it is:

$$n_i^0 \frac{df_i}{dt} = -(v_i r)V^0(1 + \varepsilon_i f_i) \quad \text{with } f_i = 0 \text{ @ } t = 0 \qquad (3.2.2)$$

where $|\varepsilon_i| > 0$ for nonconstant volume.

Since the reactor is at steady-state, the difference in $F_i^0$ (input) and $F_i$ (output) must be due to the reaction. (In this text, the superscript 0 on flow rates denotes the input to the reactor.) The material balance on a CSTR is written as:

$$\begin{array}{ccccccc} 0 & = & F_i^0 & - & F_i & + & (v_i r)V \\ \text{accumulation} & & \begin{array}{c}\text{input}\\\text{of } i\end{array} & & \begin{array}{c}\text{output}\\\text{of } i\end{array} & & \begin{array}{c}\text{amount}\\\text{produced}\\\text{by reaction}\end{array} \end{array} \qquad (3.3.1)$$

$$V \frac{d\,C_i}{dt} = q_i\,C_{i0} - q\,C_i + v_i\,r\,V$$

$$f_l = \frac{n_l^0 - n_l}{n_l^0} = \frac{F_l^0 - F_l}{F_l^0}$$

2.2.4) into Equation (3.3.2) yields:
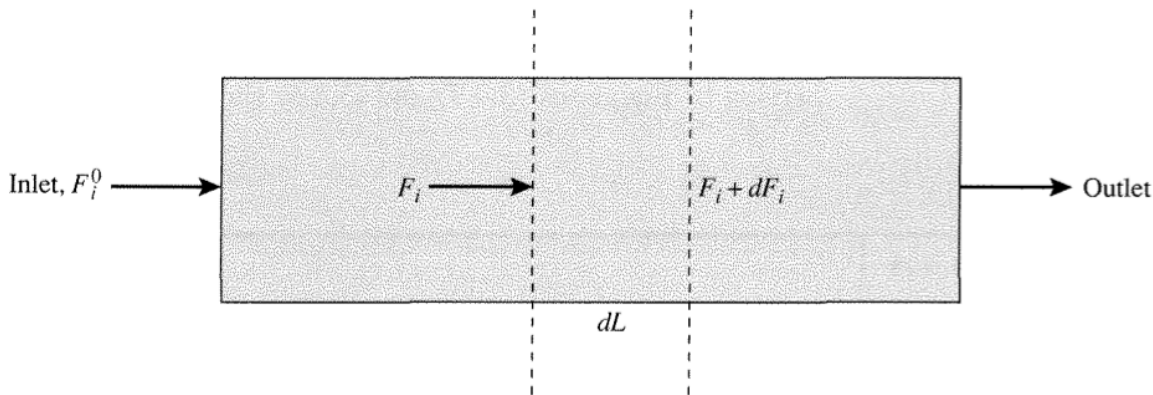


**Figure 3.4.1 |**
Tubular reactor.

$$\begin{array}{ccccc} 0 & = & F_i & - & (F_i + dF_i) + v_i r A_C\, dL \\ \text{(accumulation)} & = & \text{(input)} & - & \begin{array}{c}\text{(output)}\end{array} \begin{array}{c}+ \text{(amount produced}\\\text{by reaction)}\end{array} \end{array} \qquad (3.4.1)$$

where $A_C$ is the cross-sectional area of the tube. Also, $A_C dL = dV_R$, so Equation (3.4.1) can be written as:

$$\frac{dF_i}{dV_R} = v_i \mathbf{r} \tag{3.4.2}$$

or

$$F_i^0 \frac{df_i}{dV_R} = -v_i \mathbf{r} \tag{3.4.3}$$

Integration of Equation (3.4.3) gives:

$$\frac{V_R}{F_i^0} = \int_{f_i^0}^{f_i^{\text{outlet}}} \frac{df_i}{(v_i \mathbf{r})} \quad \text{or} \quad \tau = \frac{V_R}{v} = C_i^0 \int_{f_i^0}^{f_i^{\text{outlet}}} \frac{df_i}{(v_i \mathbf{r})} \tag{3.4.4}$$

If changes in volume due to reaction are negligible, then $[F_i = C_i v;$ moles of $i$/time $=$ (moles of $i$/volume) (volume/time)]:

$$\frac{dC_i}{d\tau} = \frac{dC_i}{d(V_R/v)} = v_i \mathbf{r} \tag{3.4.5}$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$-\int_{C_{A0}}^{C_A} \frac{1}{\xi^2} d\xi = \frac{1}{C_A} - \frac{1}{C_{A0}}$$

$$\int_{x_0}^{x} \frac{1}{(\xi - \alpha)} d\xi = \ln\left(\frac{x - \alpha}{x_0 - \alpha}\right)$$

$$\int_{x_0}^{x} \frac{1}{\xi} d\xi = \ln\left(\frac{x}{x_0}\right)$$

# Periodic table of the elements

**Legend:**
- Alkali metals
- Alkaline-earth metals
- Transition metals
- Other metals
- Other nonmetals
- Halogens
- Noble gases
- Rare-earth elements (21, 39, 57–71) and lanthanoid elements (57–71 only)
- Actinoid elements

| period | group 1* | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 H | | | | | | | | | | | | | | | | | 2 He |
| 2 | 3 Li | 4 Be | | | | | | | | | | | 5 B | 6 C | 7 N | 8 O | 9 F | 10 Ne |
| 3 | 11 Na | 12 Mg | | | | | | | | | | | 13 Al | 14 Si | 15 P | 16 S | 17 Cl | 18 Ar |
| 4 | 19 K | 20 Ca | 21 Sc | 22 Ti | 23 V | 24 Cr | 25 Mn | 26 Fe | 27 Co | 28 Ni | 29 Cu | 30 Zn | 31 Ga | 32 Ge | 33 As | 34 Se | 35 Br | 36 Kr |
| 5 | 37 Rb | 38 Sr | 39 Y | 40 Zr | 41 Nb | 42 Mo | 43 Tc | 44 Ru | 45 Rh | 46 Pd | 47 Ag | 48 Cd | 49 In | 50 Sn | 51 Sb | 52 Te | 53 I | 54 Xe |
| 6 | 55 Cs | 56 Ba | 57 La | 72 Hf | 73 Ta | 74 W | 75 Re | 76 Os | 77 Ir | 78 Pt | 79 Au | 80 Hg | 81 Tl | 82 Pb | 83 Bi | 84 Po | 85 At | 86 Rn |
| 7 | 87 Fr | 88 Ra | 89 Ac | 104 Rf | 105 Db | 106 Sg | 107 Bh | 108 Hs | 109 Mt | 110 Ds | 111 Rg | 112 Cn | 113 Nh | 114 Fl | 115 Mc | 116 Lv | 117 Ts | 118 Og |

| lanthanoid series 6 | 58 Ce | 59 Pr | 60 Nd | 61 Pm | 62 Sm | 63 Eu | 64 Gd | 65 Tb | 66 Dy | 67 Ho | 68 Er | 69 Tm | 70 Yb | 71 Lu |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| actinoid series 7 | 90 Th | 91 Pa | 92 U | 93 Np | 94 Pu | 95 Am | 96 Cm | 97 Bk | 98 Cf | 99 Es | 100 Fm | 101 Md | 102 No | 103 Lr |

*Numbering system adopted by the International Union of Pure and Applied Chemistry (IUPAC). © Encyclopædia Britannica, Inc.

# UNITS

**Mass**
$1 \text{ kg} = 1000 \text{ g} = 0.001 \text{ metric ton} = 2.20462 \text{ lb}_m$
$1 \text{ lb}_m = 16 \text{ oz} = 5\text{E-4 ton} = 453.59 \text{ g} = 0.45359 \text{ kg}$

**Length**
$1 \text{ m} = 100 \text{ cm} = 1000 \text{ mm} = 1\text{E6 } \mu\text{m} = 1\text{E9 nm} = 39.370 \text{ in} = 3.2808 \text{ ft} = 1.0936 \text{ yd}$
$1 \text{ ft} = 12 \text{ in} = 0.30480 \text{ m} = 30.480 \text{ cm}$
$1 \text{ in} = 2.5400 \text{ cm}$

**Volume**
$1 \text{ m}^3 = 1000 \text{ L} = 1\text{E6 cm}^3 = 1\text{E6 ml} = 35.315 \text{ ft}^3 = 264.17 \text{ gal}$
$1 \text{ ft}^3 = 1728.0 \text{ in}^3 = 7.4805 \text{ gal} = 0.028317 \text{ m}^3 = 28.317 \text{ L} = 28317 \text{ ml}$

**Force**
$1 \text{ N} = 1 \text{ kg-m/s}^2 = 1\text{E5 dynes} = 1\text{E5 g-cm/s}^2 = 0.22481 \text{ lb}_f$
$1 \text{ lb}_f = 32.174 \text{ lb}_m\text{-ft/s}^2 = 4.4482 \text{ N}$

**Pressure**
$1 \text{ atm} = 1.01325\text{E5 N/m}^2(\text{Pa}) = 1.01325 \text{ bar} = 760 \text{ mm}_{\text{Hg at 0°C}} = 33.9 \text{ ft}_{\text{H2O at 4°C}}$
$1 \text{ atm} = 14.696 \text{ psia}$
$1 \text{ bar} = 0.1 \text{ MPa} = 0.98692 \text{ atm} = 14.504 \text{ psia} = 750.06 \text{ mm}_{\text{Hg at 0°C}} = 10.197 \text{ m}_{\text{H2O at 4°C}}$

**Energy**
$1 \text{ J} = 1 \text{ N-m} = 1 \text{ MPa-cm}^3 = 1 \text{ kgm}^2/\text{s}^2 = 0.23901 \text{ cal} = 0.73756 \text{ ft-lb}_f$
$1 \text{ J} = 1\text{E7 ergs} = 1\text{E7 g-cm}^2/\text{s}^2$
$1 \text{ kJ} = 0.94781 \text{ Btu}^{\text{(see note 1)}} = 2.7778\text{E-4 kW-h} = 0.23901 \text{ food calorie}$

**Power**
$1 \text{ W} = 1 \text{ J/s} = 0.2390 \text{ cal/s}^{\text{(see note 2)}} = 0.73756 \text{ ft-lb}_f/\text{s} = 3.4121 \text{ Btu/h}^{\text{(see note 1)}}$
$1 \text{ hp} = 550 \text{ ft-lb}_f/\text{s} = 0.70726 \text{ Btu/s}^{\text{(see note 1)}} = 0.74570 \text{ kW}$

**Gas Constant, $R$**
$= 8.31447 \text{ J/mole-K} = 8.31447 \text{ cm}^3\text{-MPa/mole-K} = 8.31447 \text{ m}^3\text{-Pa/mole-K}$
$= 8{,}314.47 \text{ cm}^3\text{-kPa/mole-K} = 83.1447 \text{ cm}^3\text{-bar/mole-K} = 1.9859 \text{ Btu/lbmole-R}^{\text{(see note 1)}}$
$= 82.057 \text{ cm}^3\text{-atm/mole-K} = 1.9872 \text{ cal/mole-K}^{\text{(see note 2)}} = 10.731 \text{ ft}^3\text{-psia/lbmole-R}$

**Gravitational Constants at sea level**
$g = 9.8066 \text{ m/s}^2 \quad g/g_c = 9.8066 \text{ N/kg} \quad g_c = 1 \text{ (kg-m/s}^2)/\text{N}$
$g = 32.174 \text{ ft/s}^2 \quad g/g_c = 1 \text{ lb}_f/\text{lb}_m \quad g_c = 32.174 \text{ (lb}_m\text{-ft/s}^2)/\text{lb}_f$

**Faraday's Constant**
$F = 96{,}485 \text{ J/V}$

**IUPAC Standard Conditions of Temperature and Pressure**
$T = 0°\text{C} = 273.15 \text{ K}; \ P = 0.1 \text{ MPa}; \ V(\text{ideal gas}) = 22711 \text{ cm}^3/\text{mole};$
$\rho(\text{water}) = 0.99984 \text{ g/cm}^3 = 8.3441 \text{ lb}_m/\text{gal}$

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1. The International Steam Table (IT) BTU.
2. The thermochemical calorie.