Appendix C Selected First-Principle Models

This Appendix summarizes commonly used first-principles models for various physical effects. The list is obviously not exhaustive—many models are used for examples mentioned in the main text. Further information may be found in the references.

C1 Gravitational Acceleration

The gravitational potential due to a point mass is

$$U = \frac{Gm_1}{r} \tag{C1-1}$$

where G is the universal gravitational constant (6.673×10^{-11} m^3/kg-s^2), m_1 is the mass of body #1 and r is the distance from the mass. The potential U at a point outside the body (if not a point source) is defined by the position Laplacian $\nabla^2 U = 0$. The acceleration of a second body is equal to the derivative of U with respect to r:

$$\dot{\mathbf{v}} = -\left(\frac{Gm_1}{r^3}\right)\mathbf{r} \tag{C1-2}$$

where $\mathbf{r}$ is the position vector from body 1 to 2 measured in an inertial frame, $r = \|\mathbf{r}\|$ and $\mathbf{v} = \dot{\mathbf{r}}$ is the velocity vector of the second body. Hence the gravitational force between two masses is

$$\mathbf{f} = -\left(\frac{Gm_1 m_2}{r^3}\right)\mathbf{r} \tag{C1-3}$$

where m_2 is the mass of body 2. When used for modeling motion of an earth-based satellite, body 1 is the earth. The *World Geodetic System* (WGS84)—the reference for the *Global Positioning System*—uses $G\,m_e$=3.986004418$\times 10^5$ km^3/s^2 for the earth's gravitational constant (see DoD WGS84 2004). The symbol μ is often used to represent Gm_e.

For an orbital state vector consisting of position and velocity, the two-body state dynamics are

$$\begin{bmatrix} \dot{r}_1 \\ \dot{r}_2 \\ \dot{r}_3 \\ \dot{v}_1 \\ \dot{v}_2 \\ \dot{v}_3 \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ -\mu r_1 / r^3 \\ -\mu r_2 / r^3 \\ -\mu r_2 / r^3 \end{bmatrix} \tag{C1-4}$$

where $r = \sqrt{r_1^2 + r_2^2 + r_3^2}$. This is a nonlinear model, so for linearized estimation the perturbation equation is:

$$\delta\dot{\mathbf{x}}(t) = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ (\mu/r^3)(3r_1^2/r^2-1) & (\mu/r^3)3r_1r_2 & (\mu/r^3)3r_1r_3 & 0 & 0 & 0 \\ (\mu/r^3)3r_1r_2 & (\mu/r^3)(3r_2^2/r^2-1) & (\mu/r^3)3r_2r_3 & 0 & 0 & 0 \\ (\mu/r^3)3r_1r_3 & (\mu/r^3)3r_2r_3 & (\mu/r^3)(3r_3^2/r^2-1) & 0 & 0 & 0 \end{bmatrix} \delta\mathbf{x}(t) \tag{C1-5}$$

When modeling the motion of earth satellites, it is necessary to include not only the central two-body gravitation, but also the perturbing forces. These perturbations include undulations in the earth's gravitational field, gravitational forces from the sun, moon and planets, solar radiation pressure, atmospheric drag (for a low earth orbiting satellite), and thrust forces. Models for these effects are presented in Section 3.4 on satellite orbit determination.

C2 Aerodynamic Forces

The movement of a body through the air produces drag and lift forces on the body. Defining *dynamic* or *stagnation pressure* in pascals as

$$q = \frac{1}{2}\rho V^2 \tag{C2-1}$$

where ρ is the air density (kg/m^3) and V is relative air velocity (m/s), then the drag and lift forces for an airfoil are approximately modeled in the relative velocity coordinate frame as:

$$\begin{aligned} D &= qS\,(C_{D0} + C_{D\alpha}\alpha^2) \\ L &= qS\,C_{L\alpha}\alpha \end{aligned} \tag{C2-2}$$

where S is wing area (m^2), α is the angle-of-attack (radians), C_{D0} is the profile drag coefficient, $C_{D\alpha}\alpha^2$ is the induced drag coefficient (resulting from drag induced by the lift), and $C_{L\alpha}\alpha$ is the lift coefficient. The drag and lift coefficients are generally a function of the Reynolds number,

$$R_e = \rho V l / \mu , \tag{C2-3}$$

where l is body length (m) and μ is dynamic viscosity ($\text{Pa}\cdot\text{s} = \text{kg/m}\cdot\text{s}$) of the fluid. Lift and drag coefficients are sometimes tabulated as a function velocity when operating over an extended velocity range. For an airframe, drag and lift coefficients are defined for each fixed and movable surface, and the forces and torques for each surface are summed to compute the airframe total. For more information on aircraft dynamics, see Anderson (2005), Stengel (2004), or *Dynamics of the Airframe* (1952). General information on aerodynamics may be found in Avallone and Baumeister (1996, section 11.4).

For a low-earth orbit satellite moving through the atmosphere, it is often assumed that all kinetic energy of incident air molecules is completely absorbed in heating of the satellite surface. Hence the impact can be modeled as an elastic impact without reflection (Wertz, 1978, pp. 573-574). The drag force on a surface element dA with outward unit normal $\hat{\mathbf{n}}$ and relative unit velocity vector $\hat{\mathbf{v}}$ is modeled as

$$d\mathbf{f}_{\text{aero}} = -q\, C_D (\hat{\mathbf{n}} \cdot \hat{\mathbf{v}}) \hat{\mathbf{v}}\, dA \tag{C2-4}$$

The forces for all surfaces are summed to compute the total force. C_D is generally close to 2.0.

C3 Fluid Flow in Pipes or Ducts

The relationship between adiabatic pressure drop and fluid flow within a pipe is approximately modeled (see Sabersky and Acosta 1964, White 1988, or Avallone and Baumeister 1996) as:

$$p_{in} - p_{out} = 4 c_f \frac{L}{D} \left(\frac{\rho V^2}{2} \right) \tag{C3-1}$$

where

c_f is a dimensionless friction factor that is a function of Reynolds number,
L is the pipe length (m),
D is the pipe diameter (m),
V is the average flow velocity (m/s),
ρ is the density (kg/m^3), and
p_{in} and p_{out} are the pipe inlet and exit pressures (Pa).

Pipe flow is linear if the Reynolds number is less than 2000, and fully turbulent if above 3500, where the Reynolds number is defined as:

$$\mathrm{R}_{ed} = \frac{\rho V D}{\mu} \tag{C3-2}$$

and μ is dynamic viscosity in $\mathrm{Pa \cdot s = kg/m \cdot s}$. When the calculated Reynolds number is less than 2000, c_f can be approximated as $16 / \mathrm{R}_{ed}$. When R_{ed} is greater than 3500, c_f can be calculated from a Moody chart or the Colebrook formula:

$$1/\sqrt{4c_f} = -2\log_{10}\left(\frac{e/D}{3.7} + \frac{2.51}{\mathrm{R}_{ed}\sqrt{4c_f}}\right) \tag{C3-3}$$

where e/D is the pipe relative roughness ratio. Equation (C3-3) can be solved by iteration using the initial approximation

$$1/\sqrt{4c_f} = -1.8\log_{10}\left(\left(\frac{e/D}{3.7}\right)^{1.11} + \frac{6.9}{\mathrm{R}_{ed}}\right) \; . \tag{C3-4}$$

With appropriate changes in definition of the friction factor, equation (C3-1) can also be used to model gas flow within ducts (Avallone and Baumeister 1996, chapter 12).

C4 Saturated Hydrological Flow

Saturated hydrological groundwater flow is modeled differently than pipe or duct flow. The water velocity vector **v** is modeled (Anderson and Woessner 1992) using Darcy's law,

$$\mathbf{v} = -\mathbf{K}\,\nabla h \tag{C4-1}$$

where **K** is the saturated hydraulic conductivity tensor for the porous medium and h is hydraulic head: $h = \rho\, g\, \Delta z$ where g is the earth gravitational acceleration and Δz is height above a reference. Using the flow relationship, the net mass flow to a unit volume is derived as

$$\nabla^T(\mathbf{K}\,\nabla h) = -q + S\frac{\partial h}{\partial t} \tag{C4-2}$$

where q is volumetric flux per unit volume to the unit, S is specific storage and t is time. Variably-saturated flow is typically modeled using a water saturation factor modification of equation (C4-2) (Huyakorn and Pinder 1983, chapter 4). Boundary conditions for finite-difference or finite-element 2-D or 3-D models include constant head, constant flux, recharge/drain, and wells.

Differential equations governing mass transport of solutes through porous media are presented in Huyakorn and Pinder (1983, chapter 5).

C5 Heat Transfer

Heat transfer occurs through convection, conduction or radiation (White 1988, Thomas 1993, Avallone and Baumeister 1996). Conductive heat transfer ($\dot{Q}_{cn}$ in Watts) was first modeled by Joseph Fourier in 1822 as

$$\dot{Q}_{cn} = -k\,A\frac{dT}{dx} \tag{C5-1}$$

where T is temperature, x is the direction of heat transfer, A is the area normal to the x direction, and k is the *thermal conductivity* of the material. The relationship is valid for all common solids, liquids, and gases.

Convective heat transfer occurs in heat exchangers where flow of one fluid is physically separated from flow of a second fluid by a metal barrier. Heat exchangers typically use pipes or ducts to separate the flow, with fins attached to increase the surface area for the heat transfer. Convective heat transfer from a surface of area A and temperature T_s to a fluid of temperature T_f is modeled using *Newton's law of cooling*:

$$\dot{Q}_{cv} = \bar{h}\,A(T_s - T_f) \tag{C5-2}$$

where $\bar{h}$ is the mean coefficient of heat transfer ($\text{W/m}^2\text{K}$). More generally the equation must be evaluated for differential areas dA since $\bar{h}$ can vary locally and with temperature. The total heat transfer is calculated as the integral over the total surface. For heat exchangers working with single-phase fluids, the total steady-state heat transfer is modeled for the hot (h) and cold (c) sides of the exchanger from the change in fluid enthalpies:

$$\begin{aligned}\dot{Q} &= (\dot{m}\,c_p)_h\,(T_{h,i} - T_{h,o}) \\ &= (\dot{m}\,c_p)_c\,(T_{c,o} - T_{c,i})\end{aligned} \tag{C5-3}$$

where $T_{h,i}$ and $T_{h,o}$ are the hot fluid input and output temperatures, $T_{c,i}$ and $T_{c,o}$ are the cold fluid input and output temperatures, $\dot{m}$ is the fluid flow rate (kg/s), and c_p is the fluid constant-pressure specific heat by mass (J/kg-K). The *capacity rates* $(\dot{m}\,c_p)_h$ and $(\dot{m}\,C_p)_c$ are parameters of the heat exchanger that can be used to relate total heat transfer to flow and temperatures.

Total radiant heat transfer $\dot{Q}_r$ (Watts) from a hot body is generally modeled as:

$$\dot{Q}_r = \varepsilon_b\,A\sigma\,T_h^4 \tag{C5-4}$$

where

ε_b = emissivity of hot body
A = surface area (m^2)
σ = Stephan-Boltzman constant (5.67×10^{-8} $\mathrm{W/m^2K^4}$)
T_h = hot object temperature (K)

The variation in ε_b with temperature can be quite large over small temperature ranges, so the exponent of T_h can be greater or smaller than four for limited temperature ranges. When modeling the heat transfer between two bodies—such as from hot gases to chamber walls in a boiler—it may be important to also model the radiation back from the colder object to the hotter:

$$\dot{Q}_r = \varepsilon_b A\sigma[T_h^4 - T_c^4] \qquad \text{(C5-5)}$$

where T_c is the cold temperature.

C6 Thermodynamics for a Control Volume

The first law of thermodynamics for a control volume (see Van Wylen and Sonntag 1986) is

$$\dot{Q}_{c.v.} + \sum \dot{m}_i (h_i + \frac{V_i^2}{2} + gZ_i) = \frac{dE_{c.v.}}{dt} + \sum \dot{m}_e (h_e + \frac{V_e^2}{2} + gZ_e) + \dot{W}_{c.v.} \qquad \text{(C6-1)}$$

where

$\dot{Q}_{c.v.}$ is the rate of heat transfer (W = J/s) to the system,
$\dot{W}_{c.v.}$ is the rate of work (W) done by the system,
$\frac{dE_{c.v.}}{dt}$ is the rate of change of energy in the system,
$\dot{m}$ is the fluid flow rate (kg/s),
h is fluid enthalpy (J/kg),
V is the fluid flow velocity (m/s),
g is the acceleration due to gravity (m/s^2),
Z is the elevation (m) of the system above a reference, and
i and o designate input and output respectively.

The first law is commonly used to calculate relationships between heat transfer, work performed, or change in fluid enthalpy for various subsystems involving continuous (steady or non-steady) fluid flow.

C.6.1 Turbine Thermodynamics

Gas and steam turbines employ convergent/divergent nozzles to convert the thermodynamic energy of the working fluid to kinetic energy, which is transferred to the output turbine shaft using turbine “buckets.” As shown in Figure C6-1, the fluid converges until reaching the throat, and then expands in the nozzle. Flow though convergent-divergent nozzles operating in a “choked-flow” mode (throat Mach number = 1.0) is usually computed assuming isentropic expansion, with an efficiency correction at the nozzle exit to account for irreversible losses (see Salisbury 1974, Van Wylen and Sonntag 1986, Avallone and Baumeister 1996).

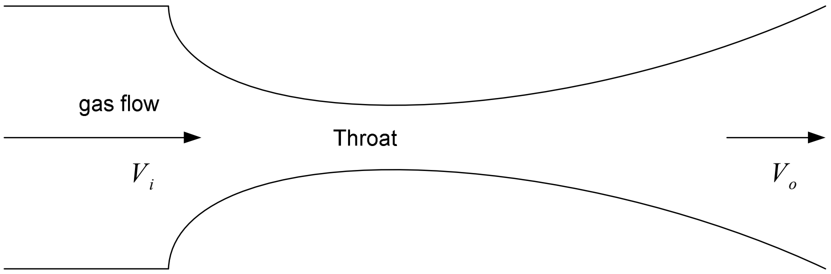

Figure C6-1: Convergent-divergent nozzle.

The flow equation is derived using the first law of thermodynamics for a steady-flow adiabatic process, with assumptions that potential energy is unchanged, the initial velocity is zero, and no work is done. The result is $V_o = \sqrt{2(h_i - h_o)}$ where V_o is the exit velocity (m/s), h_i is the input enthalpy (J/kg), and h_o is the output enthalpy (J/kg). Enthalpy for an ideal gas is $u + Pv = u + RT$, where u (internal energy) is only a function of temperature and v is specific volume. Constant-pressure specific heat by mole (C_p) is assumed constant so that h is a linear function of temperature. It is also assumed that the gas undergoes isentropic expansion and that the expansion can be modeled as an ideal gas ($Pv^k = \text{constant}$). This leads to

$$\frac{v_o}{v_i} = \left(\frac{P_o}{P_i}\right)^{-1/k} \qquad \text{(C6-2)}$$

and

$$\frac{T_o}{T_i} = \left(\frac{P_o}{P_i}\right)^{(k-1)/k} \qquad \text{(C6-3)}$$

where v_i and v_o are input and output specific volume (m^3/kg), P_i and P_o are input and output absolute pressure (Pa), T_i and T_o are input and output absolute temperature (K), and $k = C_p / C_v$ is the ratio of constant-pressure and constant-volume specific heats. Typically $k \cong 1.3$ for high-pressure steam. The other required relationship is the “continuity" equation $\dot{m} = AV / v = \text{constant}$, where $\dot{m}$ is fluid flow in kg/s. For $k = 1.3$, the gas flow through the nozzle is

$$\begin{aligned}\dot{m} &= A_t\sqrt{\eta}P_i\sqrt{\frac{k}{RT_i}}\Big/\left(\frac{k+1}{2}\right)^{(k+1)/2(k-1)} \\ &= \frac{0.667A_t\sqrt{\eta}P_i}{\sqrt{RT_i}}\end{aligned} \tag{C6-4}$$

where A_t is the nozzle throat area (m^2), η is nozzle efficiency, P_i is the inlet pressure (Pa), T_i is the nozzle inlet temperature (K), and R is the gas constant (J/kg-K) for the given gas mixture.

The isentropic nozzle efficiency η is typically about 0.90 for individual stages of a gas or steam turbine utilizing convergent-divergent nozzles. Since irreversible losses from one stage are extra heat available for the next stage, overall turbine efficiency can be 0.95.

C.6.2 Combustion

The first law of thermodynamics within a control volume for a steady-state, steady-flow process that involves reacting systems with negligible changes in kinetic and potential energy can be written as

$$Q_{c.v.} + \sum_{react} n_i(\bar{h}_f^o + \Delta\bar{h})_i = W_{c.v.} + \sum_{prod} n_e(\bar{h}_f^o + \Delta\bar{h})_e \tag{C6-5}$$

where

n_i is the number of moles of reactant i involved in the combustion,

n_e is the number of moles of product e involved in the combustion,

$\bar{h}_f^o$ is the heat (enthalpy) of formation for the given reactant or product at the reference temperature

$\Delta\bar{h}$ is the change in enthalpy due to the change in temperature from the reference for the given reactant or product

$Q_{c.v.}$ is the heat added to the system, and

$W_{c.v.}$ is the work done by the system.

For example, consider the reaction of gaseous methane and air, with gaseous carbon dioxide, nitrogen, and liquid water as products:

$$\mathrm{CH_4} + 2(\mathrm{O_2} + 3.76\,\mathrm{N_2}) \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O}(l) + 7.52\,\mathrm{N_2} \tag{C6-6}$$

Air is assumed to have 3.76 moles of N_2 for every mole of O_2 with no water vapor. Thermodynamic properties of the reactants and products are listed in Table C6-1 (from Van Wylen and Sonntag 1986, tables A.8SI, A11SI, A.13SI). The energy released by the combustion is calculated as

$$-74873+2(0+3.76\cdot 0)-\left[-393522+2(-285838)+7.52\cdot 0\right]=890325\text{ J} \ .$$

Table C6-1: Selected Thermodynamic Properties

Compound	$\bar{h}_f^o$ (J/mol) at 25 °C	$\bar{C}_p$ (J/(mol-K) at 25 °C	Molecular Weight (kg/mol)
CH_4	-74873	36.15	16.04
O_2	0	29.48	31.999
N_2	0	29.15	28.013
CO_2	-393522	37.11	44.01
H_2O (gas)	-241827	33.66	18.015
H_2O (liquid)	-285838	75.32	18.015

If all energy is used to heat the surroundings, or it is completely converted into work, the temperature of the products will not rise above the initial temperature of 25°C. However, if $Q_{c.v.}=W_{c.v.}=0$, the temperature of the products must rise until the total product enthalpy equals the enthalpy of the reactants. The temperature at which $H_{\text{reactants}}=H_{\text{products}}$ is called the adiabatic flame temperature. If specific heat C_p is constant and the product water is gaseous:

$$-74873\text{ J}=\left[-393522+\Delta\text{T}\cdot 37.11+2(-241827+\Delta\text{T}\cdot 33.66)+\Delta\text{T}\cdot 7.52\cdot 29.15\right]\text{ J}$$

or

$$\Delta\text{T}=802\,303\text{ J}/(37.11+2\cdot 33.66+7.52\cdot 29.15)=2479\text{ K} \ .$$

Thus $\text{T}=273+25+2479=2777\text{ K}$. The actual adiabatic flame temperature will be lower because the change in enthalpy with temperature is not linear over this temperature range. The enthalpy of formation ($\Delta\bar{h}$) of $CO_2, H_2O(g)$ and N_2 are, respectively, 67007, 109671, and 88295 J/mol at 2300 K (Van Wylen and Sonntag 1986, table A.11SI). Hence the enthalpy of the products is calculated as -87022 J, which is close to the -74873 J of the reactants. By interpolation, the adiabatic flame temperature is calculated as 2328 K. This is much greater than the actual flame temperature of natural gas-fired furnaces. The actual flame temperature will be lower because of incomplete combustion and disassociation reactions. Furthermore, much heat will be transferred to the furnace walls, which is generally the purpose of a furnace. Hence the average flame temperature will be much lower than 2328 K. The average flame temperature can be computed iteratively using radiant heat transfer equations and a constant C_p appropriate for the higher temperature.

C7 Electrical Circuits

The linear relationships between applied voltage (v) and current (i) for resistors, capacitors, and inductors are, respectively,

$$v = iR \tag{C7-1}$$

$$i = C\frac{dv}{dt} \tag{C7-2}$$

$$v = L\frac{di}{dt} \tag{C7-3}$$

where R is resistance (ohms), C is capacitance (farads), and L is inductance (henrys). In the Laplace transform domain, the relationships for capacitors and inductors are

$$i(s) = s\,C\,v(s) \tag{C7-4}$$

$$v(s) = s\,L\,i(s) \quad . \tag{C7-5}$$

Consider the RLC circuit of Figure C9-1.

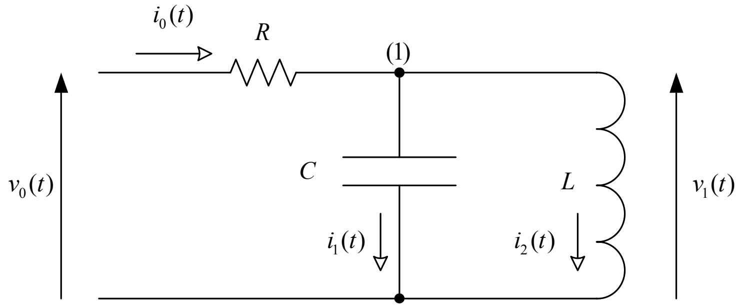

Figure C7-1: RLC circuit.

Summing the net current to node (1) gives

$$\frac{v_0 - v_1}{R} = C\frac{dv_1}{dt} + \frac{1}{L}\int v_1 dt \tag{C7-6}$$

in the time domain, or

$$\dot{v}_0 = RC\,\ddot{v}_1 + \dot{v}_1 + (R/L)v_1 \quad . \tag{C7-7}$$

The Laplace transfer function is

$$\frac{v_1(s)}{v_0(s)} = \frac{s}{RC(s^2 + s/RC + 1/LC)} \tag{C7-8}$$

where the undamped natural frequency of the circuit is $\omega_0 = \sqrt{1/LC}$ and the damping ratio is

$$\zeta = \frac{1}{2RC\omega_0} = \frac{\sqrt{L/C}}{2R} \; .$$

This is a band-pass filter: the output voltage approaches zero at very low and high frequencies. Of course, real inductors have small internal resistance, so the response is not zero at zero frequency.

Active devices such as transistors can be modeled as quasi-linear over limited operating ranges. Depending on the associated circuitry, junction transistors are sometimes modeled as current-controlled current sources, and field effect transistors modeled as voltage-controlled current sources. However, manufacturer data should be used for specific devices.

Electromechanical devices such as motors, actuators, and sensors must be modeled in control applications. Again specific design information should be used because characteristics vary greatly. Two general sources of information are Avallone and Baumeister (1996) and Levine (1996, section XVII).