1 Derivation of the Heat Equation for Fluid Flow Problems

The purpose of this writeup is to obtain the differential equation for the temperature $T(\mathbf{x}, t)$ which will be used in the discussion of finite-volume methods as well is in example problems using STAR-CCM+. This will involve first using the first law of thermodynamics to obtain a differential equation for the total energy per unit mass, e, and from this an equation for the internal energy, $\hat{u}$, and finally from this an equation for the temperature T.

1.1 The equation for the total energy per unit mass e

Consider the energy equation (the first law of thermodynamics) for a control volume:

$$\underbrace{\frac{d}{dt}\iiint_{V} \rho\, e\, d\mathcal{V}}_{(i)} = \underbrace{\dot{W}}_{(ii)} + \underbrace{\dot{Q}}_{(iii)} - \underbrace{\iint_{CS} \rho\, e(\mathbf{V}\cdot\mathbf{n})d\mathcal{A}}_{(iv)}\,, \tag{1}$$

where ρ is the density and $\mathbf{V}$ is the velocity vector. The scalar e is the total energy per unit mass, given by

$$e = \hat{u} + \frac{1}{2}|\mathbf{V}|^2 + gz\,, \tag{2}$$

where $\hat{u}$ is the internal energy per unit mass, $\frac{1}{2}|\mathbf{V}|^2$ is the kinetic energy per unit mass, and gz is the potential energy per unit mass; g is the usual gravitational acceleration, and z is the coordinate in the direction opposite to the force of gravity. The term $\dot{Q}$ is the rate that heat is being added to the control volume, and $\dot{W}$ is the rate that work is done on the control volume. The rate of work is often split into three parts,

$$\dot{W} = \dot{W}_{\text{shaft}} + \dot{W}_{\text{pressure}} + \dot{W}_{\text{viscous}}\,, \tag{3}$$

where $\dot{W}_{\text{shaft}}$ is the rate of work done by a shaft internal to the control volume; $\dot{W}_{\text{pressure}}$ is the rate of work by pressure forces acting at the control surfaces; and $\dot{W}_{\text{viscous}}$ is the rate of work by viscous forces acting on the control surfaces. No internal shaft in the control volume will be considered, so that $\dot{W}_{\text{shaft}} = 0$. Also $\dot{W}_{\text{viscous}}$ will be neglected, assuming that the Mach number is small.

The pressure forces act at the surfaces of the control volume. In a local region of the surface of area $d\mathcal{A}$, with outward normal $\mathbf{n}$, the pressure force is $-p\,\mathbf{n}\,d\mathcal{A}$. The rate of work of the pressure force is then $-p\,\mathbf{n}\,d\mathcal{A}\cdot\mathbf{V} = -p\,(\mathbf{V}\cdot\mathbf{n})\,d\mathcal{A}$, where $\mathbf{V}$ is the local fluid velocity. Therefore, integrating over the entire control surface gives the rate of work by the pressure forces as

$$\dot{W}_{\text{pressure}} = -\iint_{CS} p(\mathbf{V}\cdot\mathbf{n})d\mathcal{A}\,. \tag{4}$$

In Equation (1), in addition to terms (ii) and (iii) already explained, term (i) represents the rate-of-change of total energy in the control volume, and term (iv) represents the net rate of energy flux across the control surfaces.

When applying Equation (1) to a differential control volume, as done in class, where the volume is $d\mathcal{V} = dx\,dy\,dz$, the result is, for terms (i) and (iv) in this equation, as well as for Equation (4):

- $\frac{d}{dt}\iiint\limits_{V} \rho\, e\, d\mathcal{V} = \frac{\partial}{\partial t}(\rho\, e)\, d\mathcal{V}\,;$
- $-\iint\limits_{CS} \rho\, e(\mathbf{V}\cdot\mathbf{n})d\mathcal{A} = \nabla\cdot(\rho\, e\mathbf{V})\, d\mathcal{V}\,;$
- $\dot{W}_{\text{pressure}} = -\iint\limits_{CS} p\,(\mathbf{V}\cdot\mathbf{n})\, d\mathcal{A} = -\nabla\cdot(p\mathbf{V})\, d\mathcal{V}$ using Equation (4).

Using these results in Equation (1) gives, after dividing by $d\mathcal{V}$,

$$\rho\frac{De}{Dt} = \dot{Q}_{uv} - \nabla\cdot(p\mathbf{V}) = \dot{Q}_{uv} - p(\nabla\cdot\mathbf{V}) - \mathbf{V}\cdot\nabla p\,, \tag{5}$$

using the fact that, with the continuity equation,

$$\begin{aligned}\frac{\partial}{\partial t}\rho\, e + \nabla\cdot(\rho\, e\mathbf{V}) &= \rho\,\frac{\partial e}{\partial t} + \rho\,\mathbf{V}\cdot\nabla e \\ &+ \underbrace{e\left(\frac{\partial\rho}{\partial t} + \rho\,\nabla\cdot\mathbf{V}\right)}_{=0 \text{ from continuity}} \\ &= \rho\,\frac{De}{Dt}\end{aligned}$$

where $\dot{Q}_{uv} = \dot{Q}/d\mathcal{V}$ is the heat flux per unit volume. This is the differential equation for the total energy e.

1.2 The equation for the internal energy per unit mass $\hat{u}$

The differential equation for the mechanical energy can be obtained by take the dot product of the velocity vector $\mathbf{V}$ with the momentum equation giving:

$$\rho\,\mathbf{V}\cdot\frac{D\mathbf{V}}{Dt} = -\mathbf{V}\cdot\nabla p + \mathbf{V}\cdot(\rho\,\mathbf{g}) + \mathbf{V}\cdot\mathbf{F}_{\text{viscous}}\,, \tag{6}$$

where $\mathbf{F}_{\text{viscous}}$ is the viscous force. Taking $\mathbf{g} = -g\mathbf{e}_z = -\nabla(gz)$, then

$$\rho\,\mathbf{V}\cdot\mathbf{g} = \rho\mathbf{V}\cdot\nabla(-gz) = \rho\left(\underbrace{\frac{\partial}{\partial t}(-gz)}_{=0} + \mathbf{V}\cdot\nabla(-gz)\right) = \rho\,\frac{D}{Dt}(-gz)\,,$$

so Equation (6) becomes

$$\rho\frac{D}{Dt}\left(\frac{1}{2}|\mathbf{V}|^2 + gz\right) = -\mathbf{V}\cdot\nabla p + \mathbf{V}\cdot\mathbf{F}_{\text{viscous}}\,. \tag{7}$$

Next, subtracting Equation (7) from Equation (5) gives, using Equation (2), gives:

$$\rho\frac{D\hat{u}}{Dt} = \dot{Q}_{uv} - p\nabla\cdot\mathbf{V}\,, \tag{8}$$

the differential equation for the internal energy per unit mass, $\hat{u}$. Note that the viscous term $\mathbf{V}\cdot\mathbf{F}_{\text{viscous}}$ has been neglected, assuming low Mach number flow.

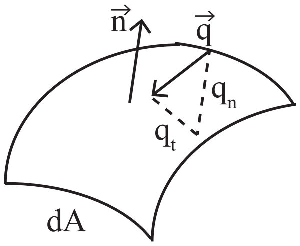

Figure 1: Heat flux across the surface area dA.

1.3 The equation for the temperature T

The next step is to determine $\dot{Q}_{uv}$, the rate of heat transfer, per unit volume, to the differential control volume $d\mathcal{V}$. The heat flux vector $\mathbf{q}$ is introduced, which gives the magnitude and direction of the heat flux. For a differential surface area $d\mathcal{A}$ with an outward normal $\mathbf{n}$ to the underlining control volume, the rate of increase in internal energy due to the heat flux across $d\mathcal{A}$ is (see Figure 1):

$$-\mathbf{n}\cdot\mathbf{q}\,d\mathcal{A}\,.$$

The heat flux (heat transfer) can be due to conduction or to radiation. Only conduction will be addressed in these notes. Summing up the rate of heat transfer across the entire control surface, the rate of heat transfer $\dot{Q}$ to a control volume is given by

$$\dot{Q} = -\iint\limits_{CS} \mathbf{n}\cdot\mathbf{q}\,d\mathcal{A}\,. \tag{9}$$

Applying this to a differential control volume (see Figure 2), Equation (8) becomes, after multiplying through by $d\mathcal{V}$:

$$\rho\frac{D\hat{u}}{Dt}d\mathcal{V} = -\iint\limits_{CS} \mathbf{n}\cdot\mathbf{q}\,d\mathcal{A} - p\nabla\cdot\mathbf{V}d\mathcal{V}\,. \tag{10}$$

In order to evaluate the surface integral for the differential volume element with sides of length dx, dy, and dz, consider the evaluation of the integral for the left and right faces, respectively. With $\mathbf{q} = (q_x, q_y, q_z)$, for the left face:

$$-\iint\limits_{CS_L} \mathbf{n}\cdot\mathbf{q}\,d\mathcal{A} = -(-q_x)\Big|_x dydz = +q_x\Big|_x dydz\,, \tag{11}$$

since $\mathbf{n}\cdot\mathbf{q} = -\mathbf{i}\cdot\mathbf{q} = -q_x$ at the left face. Similarly, for the right face:

$$-\iint\limits_{CS_R} \mathbf{n}\cdot\mathbf{q}\,d\mathcal{A} = -(+q_x)\Big|_{x+dx} dydz = -(q_x + \frac{\partial q_x}{\partial x}dx)\Big|_x dydz\,, \tag{12}$$

since $\mathbf{n}\cdot\mathbf{q} = +\mathbf{i}\cdot\mathbf{q} = +q_x$ at the right face. Summing Equations (11) and (12) gives $-\dfrac{\partial q_x}{\partial x}dxdydz$. Similar arguments from the top and bottom, and front and back, faces results in $-\dfrac{\partial q_y}{\partial y}dxdydz$ and

$-\dfrac{\partial q_z}{\partial z}dxdydz$, respectively. Finally, summing up these three results, with $d\mathcal{V} = dxdydz$,

$$-\iint\limits_{CS} \mathbf{n}\cdot\mathbf{q}\,d\mathcal{A} = -\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right)d\mathcal{V} = -\nabla\cdot\mathbf{q}\,d\mathcal{V}\,. \tag{13}$$

When the result from Equation (13) is plugged into Equation (10), the result is, dividing out $d\mathcal{V}$:

$$\rho\frac{D\hat{u}}{Dt} = -\nabla\cdot\mathbf{q} - p\nabla\cdot\mathbf{V}\,. \tag{14}$$

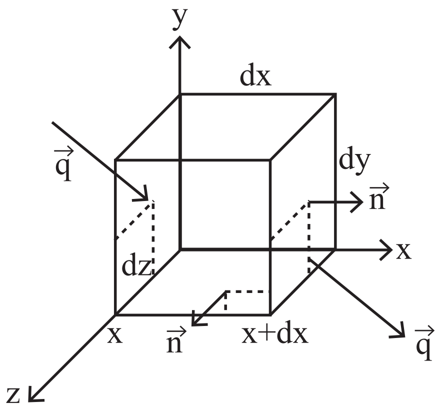

Figure 2: Differential control volume.

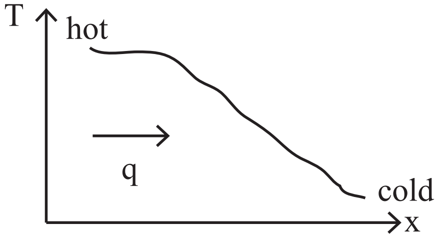

Figure 3: Heat flux from higher to lower temperature.

The next step is to determine $\mathbf{q}$, considering here heat transfer only due to conduction. One would expect that the direction of heat transfer will be from hotter to colder regions (see Figure 3). So with T as the temperature, then if $\dfrac{\partial T}{\partial x} < 0$, say, then one would expect $q_x > 0$, and vice-versa. Furthermore, one would expect that as $\left|\dfrac{\partial T}{\partial x}\right|$ increases, then so would $|q_x|$, and vice-versa. In general, if the temperature differences are not too large, it is found that

$$q_x = -\kappa\frac{\partial T}{\partial x}\,, \tag{15}$$

where $\kappa = \kappa(T)$, the thermal conductivity. Equation (15) is called Fourier's law of Heat Conduction. In three dimensions it is

$$(q_x, q_y, q_z) = -\kappa\left(\frac{\partial T}{\partial x}, \frac{\partial T}{\partial y}, \frac{\partial T}{\partial z}\right), \text{ or} \tag{16}$$

$$\mathbf{q} = -\kappa \nabla T$$

in vector notation. Plugging Equation (16) into Equation (14), the result is:

$$\rho \frac{D\hat{u}}{Dt} = \nabla \cdot (\kappa \nabla T) - p \nabla \cdot \mathbf{V} \, . \tag{17}$$

From here forward, it will be assumed that the temperature fluctuations are small. This implies that

$$\kappa(T) = \kappa(T_0) + \left.\frac{d\kappa}{dT}\right|_{T_0} (T - T_0) + \ldots \approx \kappa(T_0) = \kappa_0 \, , \text{ say} \tag{18}$$

using a Taylor series expansion of κ, where T_0 is a reference temperature, κ_0 is the constant value of κ at T_0, and assuming $(T - T_0)$ is 'small'. With this, Equation (17) becomes:

$$\rho \frac{D\hat{u}}{Dt} = \kappa_0 \nabla^2 T - p \nabla \cdot \mathbf{V} \, . \tag{19}$$

The final step is to determine the internal energy per unit mass, $\hat{u}$, in terms of the temperature, T. From thermodynamics, for many systems, when a system evolves incrementally from one state to a nearby state, the change in internal energy per unit mass is given by

$$d\hat{u} = c \, dT \, , \tag{20}$$

where c is a specific heat, and usually $c = c(T)$. For an ideal gas, c in Equation (20) is given by the specific heat at constant volume, c_v. Therefore, considering the system to be a small volume of fluid in motion, where the substantial derivative gives the rate of change of $\hat{u}$ for this system:

$$\frac{D\hat{u}}{Dt} = c_v \frac{DT}{Dt} \tag{21}$$

Again from thermodynamics, since for an ideal gas $\rho = p/RT$, where R is the gas constant, then

$$d\rho(p, T) = \left.\frac{\partial \rho}{\partial p}\right|_T dp + \left.\frac{\partial \rho}{\partial T}\right|_p dT = \frac{1}{RT} dp - \frac{p}{RT^2} dT \approx -\frac{\rho}{T} dT \, , \tag{22}$$

using the expression for the ideal gas law several times. The latter approximation holds since ρ is more sensitive to changes in T rather than p. Therefore,

$$\frac{D\rho}{Dt} = -\frac{\rho}{T}\frac{DT}{Dt} \, . \tag{23}$$

Therefore, note that, from Equation (23) and using the continuity equation,

$$-p \nabla \cdot \mathbf{V} = \frac{p}{\rho}\frac{D\rho}{Dt} = \frac{p}{\rho}\left(-\frac{\rho}{T}\right)\frac{DT}{Dt} = -\frac{\rho R T}{T}\frac{DT}{Dt} = -\rho(c_p - c_v)\frac{DT}{Dt} \tag{24}$$

using the fact that $R = c_p - c_v$. Using Equations (21) and (24) in Equation (19) gives:

$$\rho c_v \frac{DT}{Dt} = -\rho(c_p - c_v)\frac{DT}{Dt} + \kappa_0 \nabla^2 T$$

or, canceling the terms with c_v, and moving the substantial derivative term to the LHS of the equation:

$$\rho c_p \frac{DT}{Dt} = \kappa_0 \nabla^2 T\,. \tag{25}$$

For liquids and for solids, $c_p \approx c_v \approx c$, and $\nabla \cdot \mathbf{V} = 0$ usually, so Equation (25) can be obtained from Equation (19) more generally. For small temperature changes, c_p is approximately constant as well, which will be assumed to be the case henceforth. Therefore, Equation (25) can be written as

$$\frac{DT}{Dt} = k\nabla^2 T\,, \tag{26}$$

where $k = \kappa/\rho c_p$ is the thermal diffusivity.

2 One-Dimensional Problem

In class and in the discussion of finite-volume numerical methods, the one-dimensional heat equation, with $\mathbf{V} = \mathbf{0}$, will be considered. In this case Equation (26) reduces to

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial y^2}\,. \tag{27}$$

This is a partial differential equation with T as the unknown (dependent) variable, and (y, t) as the independent variables. It is first order in time, so that to solve it usually an initial condition must be given. It is second order in space, so that two boundary conditions are needed.

Consider the temperature $T(y, t)$ defined over the domain $0 \le y \le L$. Then generally the following information is needed to solve for the behavior of T as a function of y and t.

- Initial Conditions: the temperature distribution at a given time t_0, i.e.,

  $$T(y, t_0) = F(y) \quad 0 \le y \le L$$

  where F is a known function of y, and usually $t_0 = 0$.

- Boundary Conditions: the behavior of the temperature at $y = 0$ and $y = L$. This behavior is usually determined by an understanding of the problem. For example,

  - if the temperature at $y = 0$ and $y = L$ is held constant with some type of heating device, then

    $$T(0, y) = T_0\,, \quad T(L, y) = T_L$$

    where T_0 and T_L are constant temperatures (or possibly functions of time). Or

  - the heat flux at $y = 0$ and $y = L$ is specified, e.g.,

    $$-\frac{1}{\rho c_v} q_y\bigg|_0 = k\frac{\partial T}{\partial y}\bigg|_0 = 0 \quad \text{no heat flux, insulated, or}$$

    $$k\frac{\partial T}{\partial y}\bigg|_0 = hA(T|_0 - T_{\text{amb}})$$

    where h is a coefficient of heat transfer, A is the surface area at $y = 0$, and T_{am} is the ambient temperature.

Of course it is also possible to have mixed boundary conditions, with constant temperature boundary conditions at one end and heat flux boundary conditions at the other end.

One important piece of information is the total amount of internal energy in a volume of interest, in our case

$$E_T = \iiint\limits_{CV} \rho \hat{u} d\mathcal{V} = A \int_0^L \rho \hat{u} dy = A\rho c \int_0^L T(y,t) dy \,, \tag{28}$$

where A is the cross-sectional area of the object of interest (in the $x - z$ directions), and c a specific heat. Assuming the ρ, A and c are constants, then the total energy will change with time only if the integral $\displaystyle\int_0^L T(y,t)dy$ changes with time.

Consider the integral of Equation (27) over $0 \leq y \leq L$, i.e.,

$$\int_0^L \frac{\partial T}{\partial t} dy = \int_0^L k \frac{\partial^2 T}{\partial y^2} dy \,. \tag{29}$$

Evaluating the LHS of this equation,

$$\int_0^L \frac{\partial T}{\partial t} dy = \frac{d}{dt} \int_0^L T(y,t) dy = \frac{d}{dt}\left(\frac{E_T}{\rho A c}\right) = \frac{1}{\rho A c} \frac{d}{dt} E_T(t) \tag{30}$$

using Leibniz' rule in commuting the derivative and the integral. Evaluating the RHS of Equation (29),

$$\int_0^L k \frac{\partial^2 T}{\partial y^2} dy = k \int_0^L \frac{\partial}{\partial y}\left(\frac{\partial T}{\partial y}\right) dy = k \left.\frac{\partial T}{\partial y}\right|_0^L = k \left(\left.\frac{\partial T}{\partial y}\right|_L - \left.\frac{\partial T}{\partial y}\right|_0 \right) . \tag{31}$$

Combining Equations (30) and (31) in Equation (29),

$$\frac{1}{\rho A c} \frac{d}{dt} E_T(t) = k \left(\left.\frac{\partial T}{\partial y}\right|_L - \left.\frac{\partial T}{\partial y}\right|_0 \right) . \tag{32}$$

Therefore the change in the total energy with respect to time depends on what happens at the boundaries. In particular, for insulated boundaries, there is no heat transfer at the boundaries, i.e., $\left.\dfrac{\partial T}{\partial y}\right|_{0,L} = 0$, and so

$$\frac{d}{dt} E_T(0) = 0 \,, \text{ or } E_T(t) = \text{constant} = E_T(0) \,,$$

i.e., the total internal energy in the volume is constant in time. Note that later in the course we will find similar conservation properties for jets and wakes.

There are several reasons to compute the value of the total internal energy (or related quantities in jets and wakes):

- it is an important feature of the problem, and
- energy conservation can be an important check on numerical solutions.