EOS 352 Continuum Dynamics
More on the heat equation

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Overview

These notes cover the following

- An extended version of the heat equation: conservation of kinetic and thermal energy

An improved heat equation

We previously derived the heat equation on the basis that heat is supplied to a Lagrangian volume $V(t)$ at a rate

$$\int_{V(t)} a \, \mathrm{d}V,$$

and hence that conservation of internal energy ('heat' — but note that we will come back to the interpretation as heat later) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} \int e \, \mathrm{d}V = -\int_{S(t)} q_i n_i \, \mathrm{d}S + \int_{V(t)} a \, \mathrm{d}V$$

where $q_i = -k\partial T/\partial x_i$ is heat flux, e is internal energy density, and the rate of heat production per unit volume a has to account for conversion of various forms of potential energy. We can now be a little more differentiated about the different forms of heat supply, by considering explicitly the effect of mechanical work. To do this, we separate the effect of converting what we may term mechanical potential energy (gravitational, electrostatic) associated with work done by body forces and the effect of converting other forms of potential energy (e.g. chemical). Specifically, let a_0 be the rate of heat production per unit volume due to conversion of non-mechanical potential energy, so that $a - a_0$ represents the rate of conversion of mechanical potential energy per unit volume.

Recall that the kinetic energy of a point particle of mass m and velocity $\mathbf{u}$ is $m|\mathbf{u}|^2/2$, so the kinetic energy in a Lagrangian volume $V(t)$ in a continuum is $\int_{V(t)} \rho u_i u_i/2 \, \mathrm{d}V$. Consider the sum of thermal and kinetic energy in the volume $V(t)$,

$$\int_{V(t)} \left(e + \frac{1}{2}\rho u_i u_i \right) \mathrm{d}V.$$

This changes over time due to four effects: conduction of heat through the boundary $S(t)$, mechanical work done on the boundary by surface forces, mechanical work done in the interior of the volume by body forces, and the conversion of chemical and other non-mechanical potential energies.

Consider the rates at which work is done on the surface and the volume. The surface force on a small surface element δS is $\delta F_i = \sigma_{ij} n_j \delta S$, and the rate at which work is done by a force δF_i is given by $\delta F_i u_i = u_i \sigma_{ij} n_j \delta S$. Hence the rate at which work is done by surface forces is

$$\int_{S(t)} u_i \sigma_{ij} n_j \, \mathrm{d}S.$$

Similarly, we can show that the rate of work done by body forces is

$$\int_{V(t)} u_i f_i \, \mathrm{d}V.$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V(t)} e + \frac{1}{2}\rho u_i u_i \, \mathrm{d}V = -\int_{S(t)} q_i n_i \, \mathrm{d}S + \int_{S(t)} u_i \sigma_{ij} n_j \, \mathrm{d}S + \int_{V(t)} u_i f_i \, \mathrm{d}V + \int_{V(t)} a_0 \, \mathrm{d}V.$$

Application of Reynolds' transport theorem gives

$$\int_{V(t)} \frac{\partial e}{\partial t} + \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i u_i \right) \mathrm{d}V + \int_{S(t)} h u_i n_i + \frac{1}{2}\rho u_i u_i u_j n_j \, \mathrm{d}S =$$

$$-\int_{S(t)} q_i n_i \, \mathrm{d}S + \int_{S(t)} u_i \sigma_{ij} n_j \, \mathrm{d}S + \int_{V(t)} u_i f_i \, \mathrm{d}V + \int_{V(t)} a_0 \, \mathrm{d}V.$$

and, using the divergence theorem,

$$\int_{V(t)} \frac{\partial e}{\partial t} + \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i u_i \right) + \frac{\partial (e u_i)}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\frac{1}{2}\rho u_i u_i u_j \right) + \frac{\partial q_i}{\partial x_i} - \frac{\partial (u_i \sigma_{ij})}{\partial x_j} - u_i f_i - a_0 \, \mathrm{d}V = 0.$$

As the volume $V(t)$ is arbitrary, this leaves us with

$$\frac{\partial e}{\partial t}+\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i u_i\right)+\frac{\partial(eu_i)}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\frac{1}{2}\rho u_i u_i u_j\right)+\frac{\partial q_i}{\partial x_i}-\frac{\partial(u_i\sigma_{ij})}{\partial x_j}-u_i f_i-a_0=0. \quad (1)$$

We now have a rather lengthy and complicated-looking equation. But we can use the product rule and some of the other conservation laws to simplify this. For instance, we have

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i u_i\right)&=\frac{1}{2}u_i u_i\frac{\partial \rho}{\partial t}+\rho\frac{\partial u_i}{\partial t}u_i\\ \frac{\partial}{\partial x_j}\left(\frac{1}{2}\rho u_i u_i u_j\right)&=\frac{1}{2}u_i u_i\frac{\partial(\rho u_j)}{\partial x_j}+\rho u_j\frac{\partial u_i}{\partial x_j}u_i\\ \frac{\partial(u_i\sigma_{ij})}{\partial x_j}&=\frac{\partial \sigma_{ij}}{\partial x_j}u_i+\sigma_{ij}\frac{\partial u_i}{\partial x_j}\end{aligned}$$

Substituting in (1),

$$\begin{aligned}0=&\frac{\partial e}{\partial t}+\frac{1}{2}u_i u_i\frac{\partial \rho}{\partial t}+\rho\frac{\partial u_i}{\partial t}u_i+\frac{\partial(eu_i)}{\partial x_i}+\frac{1}{2}u_i u_i\frac{\partial(\rho u_j)}{\partial x_j}+\rho u_j\frac{\partial u_i}{\partial x_j}u_i\\ &+\frac{\partial q_i}{\partial x_i}-\frac{\partial \sigma_{ij}}{\partial x_j}u_i-\sigma_{ij}\frac{\partial u_i}{\partial x_j}-u_i f_i-a_0\\ =&\frac{1}{2}u_i u_i\left(\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_j)}{\partial x_j}\right)\\ &+\left(\rho\frac{\partial u_i}{\partial t}+\rho u_j\frac{\partial u_i}{\partial x_j}-\frac{\partial \sigma_{ij}}{\partial x_j}-f_i\right)u_i\\ &+\frac{\partial e}{\partial t}+\frac{\partial(eu_i)}{\partial x_i}+\frac{\partial q_i}{\partial x_i}-\sigma_{ij}\frac{\partial u_i}{\partial x_j}-a_0\end{aligned}$$

But the first two bracketed expressions after the last equality sign are zero by conservation of mass and momentum, respectively. In particular, the second bracketed term being zero accounts for the portion of work done that simply goes towards changing kinetic energy.

This leaves us only with

$$\frac{\partial e}{\partial t}+\frac{\partial(eu_i)}{\partial x_i}+\frac{\partial q_i}{\partial x_i}-\sigma_{ij}\frac{\partial u_i}{\partial x_j}-a_0=0$$

or

$$\frac{\partial e}{\partial t}+\frac{\partial(eu_i)}{\partial x_i}+\frac{\partial q_i}{\partial x_i}=a_0+\sigma_{ij}\frac{\partial u_i}{\partial x_j}. \quad (2)$$

The terms on the left-hand side are the usual terms we expect in a conservation law: rate of change of density, advection and conduction. The terms on the right-hand side represent the production rate density, which is now split between a term a_0 representing the conversion of chemical and other non-mechanical potential energies, and a second term representing the effect of forces. Essentially $\sigma_{ij}\frac{\partial u_i}{\partial x_j}$ is mechanical work done that is not accounted for by changing kinetic energy.

This term is often re-written in slightly different form. Note that $\sigma_{ij} = \sigma_{ji}$

$$\begin{aligned}\sigma_{ij}\frac{\partial u_i}{\partial x_j} &= \frac{1}{2}(\sigma_{ij} + \sigma_{ij})\frac{\partial u_i}{\partial x_j}\\ &= \frac{1}{2}(\sigma_{ij} + \sigma_{ji})\frac{\partial u_i}{\partial x_j}\\ &= \frac{1}{2}\sigma_{ij}\frac{\partial u_i}{\partial x_j} + \frac{1}{2}\sigma_{ji}\frac{\partial u_i}{\partial x_j}\\ &= \frac{1}{2}\sigma_{ij}\frac{\partial u_i}{\partial x_j} + \frac{1}{2}\sigma_{ij}\frac{\partial u_j}{\partial x_i},\end{aligned}$$

where the last line holds because i and j are dummy indices that are summed over and can therefore be changed into different indices, and hence be swapped. It follows that

$$\sigma_{ij}\frac{\partial u_i}{\partial x_j} = \sigma_{ij}\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right).$$

The combination of velocity derivatives on the right-hand side is simply the strain rate tensor D_{ij}:

$$D_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right).$$

so the mechanical work term can be written as

$$\sigma_{ij}\frac{\partial u_i}{\partial x_j} = \sigma_{ij}D_{ij}.$$

With the usual definition of pressure $p = -\sigma_{ii}/3$ and deviatoric stress $\tau_{ij} = \sigma_{ij} + p\delta_{ij}$, we can also write this in the form

$$\sigma_{ij}\frac{\partial u_i}{\partial x_j} = \tau_{ij}D_{ij} - p\frac{\partial u_i}{\partial x_i}. \tag{3}$$

These terms can be understood as follows: the second involves the divergence of the velocity field $\nabla \cdot \mathbf{u} = \partial u_i/\partial x_i$ and is associated with the compression or expansion of the material. From conservation of mass,

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0. \tag{4}$$

it is easy to see that for an incompressible material (with constant ρ), we have zero divergence $\partial u_i/\partial x_i$, and the divergence of the velocity field is in fact the rate expansion of material. $-p\partial u_i/\partial x_i$ is therefore work done in expanding the material, which leads to a loss of internal energy.[1] The second term $\tau_{ij}D_{ij}$ is work done that is not associated with expansion or compression of the material, but instead with sideways deformation or *shearing* of the material.

To turn (2) into a more recognizable heat equation requires additional information about how the internal energy density e depends on the state of the material, and this depends on the material in question. For instance, for an elastic material, internal energy e includes potential energy stored in the recoverable deformation of the material — so work done in compressing or shearing the material does not make it hotter, as should be obvious from stretching a piece of rubber. This is different from fluids, where compression or expansion may be partly or fully recoverable but shearing is not. More specifically, if you hold the valve on a bicycle pump shut and push the plunger down slowly, the work done does heat up the gas inside, but if you slowly let go of the plunger again before the gas has cooled down, the gas will do work in pushing the plunger out and in the process will return to its original temperature, so the work done in pushing the plunger in slowly is recoverable. By contrast, vigorous stirring of the air inside the pump simply heats the gas up, and this cannot be fully reversed.

Incompressible fluids

There is therefore no universal heat equation that is more specific than (2), and constitutive assumptions are required to make further headway. For an incompressible fluid like water, internal energy often depends only on temperature T, $e = e(T)$. In fact, this is often written as $e = \rho h(T)$, where h is then *specific internal energy*, meaning internal energy per unit mass of material. Heat capacity is then defined as

$$c = \frac{\mathrm{d}h}{\mathrm{d}T} \tag{5}$$

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[1] This is basically the $-p\delta V$ term in the first law of thermodynamics, here merely stated in continuum form in both space and time. For an everyday example of loss of internal energy due to work done in expanding a material, open the valve on a gas cylinder (maybe don't try this at home, especially if the gas is flammable!). The cylinder will get cold.

With this and using conservation of mass (4), we get

$$\begin{aligned}\frac{\partial e}{\partial t} + \frac{\partial (e u_i)}{\partial x_i} &= \frac{\partial \rho}{\partial t} h + \rho \frac{\partial h}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} h + \rho u_i \frac{\partial h}{\partial x_i} \\ &= \rho \left(\frac{\partial h}{\partial t} + u_i \frac{\partial h}{\partial x_i} \right) \\ &= \rho \left(\frac{\mathrm{d}h}{\mathrm{d}T} \frac{\partial T}{\partial t} + u_i \frac{\mathrm{d}h}{\mathrm{d}T} \frac{\partial T}{\partial x_i} \right) \\ &= \rho c \frac{\partial T}{\partial t} + \rho c u_i \frac{\partial T}{\partial x_i}.\end{aligned}$$

Substituting this into (2), and using Fourier's law $q_i = -k \partial T / \partial x_i$, we get

$$\rho c \frac{\partial T}{\partial t} + \rho c u_i \frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i} \left(k \frac{\partial T}{\partial x_i} \right) = a_0 + \tau_{ij} D_{ij}. \tag{6}$$

where we have used the fact that $\partial u_i / \partial x_i = 0$ for an incompressible material to get rid of the compression term in (3). The term $\tau_{ij} D_{ij}$ is then usually called the *dissipation rate*. For a viscous incompressible fluid, we have

$$\tau_{ij} = 2 \mu D_{ij}$$

and so

$$\tau_{ij} D_{ij} = 2 \mu D_{ij} D_{ij}.$$

Compressible gases and adiabatic processes

For a compressible gas, e will typically depend on *thermodynamic* pressure $\bar{p}$ as well as temperature. For instance, for an ideal gas, we have

$$e = \frac{\rho a R T}{m}, \qquad \rho = \frac{m \bar{p}}{R T} \tag{7}$$

where $R = 8.314$ J kg^{-1} mol^{-1} is the ideal gas constant, m is the molar mass of the gas and a is a constant that depends on the number motions (linear motion, rotations, vibrations) that can a molecule of the gas can undergo. T is absolute temperature.

If we write more generally $e = \rho h(\bar{p}, T)$ and $\rho = \rho(\bar{p}, T)$ for a gas, then by analogy with the incompressible material case above, we have

$$\begin{aligned}\frac{\partial e}{\partial t}+\frac{\partial(eu_i)}{\partial x_i}&=\frac{\partial \rho}{\partial t}h+\rho\frac{\partial h}{\partial t}+\frac{\partial(\rho u_i)}{\partial x_i}h+\rho u_i\frac{\partial h}{\partial x_i}\\&=\rho\left(\frac{\partial h}{\partial t}+u_i\frac{\partial h}{\partial x_i}\right)\\&=\rho\left[\left(\frac{\partial h}{\partial T}\right)_p\frac{\partial T}{\partial t}+u_i\left(\frac{\partial h}{\partial T}\right)_{\bar p}\frac{\partial T}{\partial x_i}+\left(\frac{\partial h}{\partial \bar p}\right)_T\frac{\partial \bar p}{\partial t}+u_i\left(\frac{\partial h}{\partial \bar p}\right)_T\frac{\partial \bar p}{\partial x_i}\right]\\&=\rho c\left(\frac{\partial T}{\partial t}+u_i\frac{\partial T}{\partial x_i}\right)+\rho\left(\frac{\partial h}{\partial \bar p}\right)_T\left(\frac{\partial \bar p}{\partial t}+u_i\frac{\partial \bar p}{\partial x_i}\right)\\&=-\frac{\partial q_i}{\partial x_i}+a_0+\sigma_{ij}D_{ij}\end{aligned}$$

where we use the notation $(\partial h/\partial T)_{\bar p}$ (which is commonly used in thermodynamics) to mean the partial derivative of h taken while $\bar p$ is held constant. Now the stress tensor σ_{ij} can typically be split into a pressure term $-\bar p\delta_{ij}$ and an 'extra stress' τ^e_{ij}. For instance, for a viscous compressible gas, we would typically have

$$\tau^e_{ij}=2\mu\left(D_{ij}-\frac{1}{3}D_{kk}\delta_{ij}\right)+\mu_b D_{kk}\delta_{ij}$$

with μ the dynamic viscosity and μ_b the bulk viscosity. For an inviscid gas, both viscosities are simply zero and $\tau^e_{ij}=0$. The mechanical work term can then be written as

$$\sigma_{ij}=(\tau^e_{ij}-p\delta_{ij})D_{ij}=\tau^e_{ij}D_{ij}-\bar p\frac{\partial u_i}{\partial x_i}$$

But the last term on the right-hand side can be re-written using the mass conservation equation (4) as

$$\begin{aligned}\frac{\partial u_i}{\partial x_i}&=-\frac{1}{\rho}\left(\frac{\partial \rho}{\partial t}+u_i\frac{\partial \rho}{\partial x_i}\right),\\&=-\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{\bar p}\left(\frac{\partial T}{\partial t}+u_i\frac{\partial T}{\partial x_i}\right)-\frac{1}{\rho}\left(\frac{\partial \rho}{\partial \bar p}\right)_T\left(\frac{\partial \bar p}{\partial t}+u_i\frac{\partial \bar p}{\partial x_i}\right)\end{aligned}$$

so

$$\begin{aligned}\rho c\left(\frac{\partial T}{\partial t}+u_i\frac{\partial T}{\partial x_i}\right)+\rho\left(\frac{\partial h}{\partial \bar p}\right)_T\left(\frac{\partial \bar p}{\partial t}+u_i\frac{\partial \bar p}{\partial x_i}\right)&=-\frac{\partial q_i}{\partial x_i}+\tau_{ij}D_{ij}\\&+\frac{\bar p}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{\bar p}\left(\frac{\partial T}{\partial t}+u_i\frac{\partial T}{\partial x_i}\right)+\frac{\bar p}{\rho}\left(\frac{\partial \rho}{\partial \bar p}\right)_T\left(\frac{\partial \bar p}{\partial t}+u_i\frac{\partial \bar p}{\partial x_i}\right)\end{aligned}$$

or

$$\left[\rho c-\frac{\bar p}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{\bar p}\right]\left(\frac{\partial T}{\partial t}+u_i\frac{\partial T}{\partial x_i}\right)+\left[\rho\left(\frac{\partial h}{\partial \bar p}\right)_T-\frac{\bar p}{\rho}\left(\frac{\partial \rho}{\partial \bar p}\right)_T\right]\left(\frac{\partial \bar p}{\partial t}+u_i\frac{\partial \bar p}{\partial x_i}\right)=$$

$$-\frac{\partial q_i}{\partial x_i} + a_0 + \tau^e_{ij} D_{ij} \tag{8}$$

Often, so called *adiabatic processes* in *inviscid* gases are of major interest. An inviscid gas is one in which dynamic viscosity μ and bulk viscosity μ_b are zero, so $p = \bar{p}$ and $\tau^e_{ij} = 0$. An adiabatic process is one in which there is no heat conduction (for instance, thermal conductivity is negligibly small) and no supply of energy from non-mechanical sources. In that case, the right-hand side of (8) is zero. Usually, some of the derivatives of h and ρ above are also re-written in more standard thermodynamic form. For instance, the thermal expansion coefficient α and compressibility β are defined through

$$\alpha = \rho \left(\frac{\partial (1/\rho)}{\partial T} \right)_{\bar{p}} = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_{\bar{p}}, \qquad \beta = -\rho \left(\frac{\partial (1/\rho)}{\partial \bar{p}} \right)_T = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial \bar{p}} \right)_T$$

In addition, we write as a shorthand

$$\nu = \left(\frac{\partial h}{\partial \bar{p}} \right)_T .$$

This allows us to write the adiabatic version of (8) in the form

$$[\rho c + \alpha \bar{p}] \left(\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} \right) + [\rho \nu - \beta \bar{p}] \left(\frac{\partial \bar{p}}{\partial t} + u_i \frac{\partial \bar{p}}{\partial x_i} \right) = 0.$$

Recall that

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = \frac{\mathrm{d}\phi(\mathbf{x}(t), t)}{\mathrm{d}t}$$

is the material derivative of a quantity ϕ — that is, the derivative taken when following a material particle at position $\mathbf{x}(t)$ moving at the local velocity field $\mathbf{u}(t)$. Then we have

$$[\rho c + \alpha \bar{p}] \frac{\mathrm{d}T(\mathbf{x}(t), t)}{\mathrm{d}t} = [\beta \bar{p} - \rho \nu] \frac{\mathrm{d}\bar{p}(\mathbf{x}(t), t)}{\mathrm{d}t}.$$

This can sometimes be integrated to give a relationship between T and $\bar{p}$ along the particle path. In particular, for an ideal gas satisfying (7), we have

$$h = \frac{aRT}{m},$$

and hence

$$\rho c = a\bar{p}/T, \qquad \rho \nu = 0, \qquad \alpha = 1/T, \qquad \beta = 1/\bar{p}$$

so

$$(a+1) \frac{\bar{p}}{T} \frac{\mathrm{d}T(\mathbf{x}(t), t)}{\mathrm{d}t} = \frac{\mathrm{d}\bar{p}(\mathbf{x}(t), t)}{\mathrm{d}t}.$$

Separating variables and integrating with respect to t,

$$(a+1) \log[T(\mathbf{x}(t), t)] = \log(\bar{p}) + C_0$$

where C_0 is a constant for any given particle trajectory. Rearranging,

$$T = C\bar{p}^{1/(a+1)}$$

where C is again constant for any given particle trajectory. Frequently, it is appropriate to assume that C is simply a constant independent of position or time.

Similarly, density is now a function of pressure only, as we have

$$\rho = \frac{m\bar{p}}{RT} = \frac{m}{C}\bar{p}^{a/(a+1)},$$

where $a/(a+1)$ is often denoted by γ, and is often characterized as the ratio of the heat capacity $c_v = c$ 'at constant volume' to the heat capacity $c_p = c(1 + 1/a)$ 'at constant pressure'.