Open Science Framework DOI:10.31219/osf.io/***

Affine ideal gas [draft]

P.G.L. Porta Mana
Kavli Institute, Trondheim <pgl@portamana.org>

23 July 2020; updated 3 August 2020

***

1 Ideal gas in continuum thermomechanics and in thermostatics

Let n be the volumic amount of substance, $\boldsymbol{v}$ the velocity, $\boldsymbol{p}$ the (tensorial) pressure, θ the temperature, u the molar internal energy, $\boldsymbol{q}$ the heat flux. They are space-time-dependent fields. Also,

$$\nabla\boldsymbol{v}^{+} := \tfrac{1}{2}(\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^{\intercal}), \quad \nabla\boldsymbol{v}^{\perp} := \nabla\boldsymbol{v}^{+} - \tfrac{1}{3}\nabla\cdot\boldsymbol{v}\,\boldsymbol{I} \tag{1}$$

In continuum thermomechanics an ideal gas is usually defined by the following constitutive equations:

$$\boldsymbol{q} = -K\,\nabla\theta \tag{2}$$

$$\boldsymbol{p} = (Rn\theta - Z\,\nabla\cdot\boldsymbol{v})\,\boldsymbol{I} - 2\,H\,\nabla\boldsymbol{v}^{\perp} \tag{3}$$

$$u = C\theta \tag{4}$$

$$R, K, C, H, Z \geqslant 0 \tag{5}$$

K is the thermal conductivity, H the shear viscosity, Z the bulk or volume viscosity. These are field equations. The independent fields, defining the state of the body, are taken to be $(n, \boldsymbol{v}, \theta)$. Then pressure, internal energy, heat flux are local functions of state. The fields satisfy the balance laws of matter, force, internal energy:

$$\partial_t n + \nabla\cdot(n\boldsymbol{v}) = 0 \tag{6}$$

$$M\,\partial_t(n\boldsymbol{v}) + M\,\nabla\cdot(n\boldsymbol{v}\otimes\boldsymbol{v}) + \nabla\cdot\boldsymbol{p} = 0 \tag{7}$$

$$\partial_t(nu) + \nabla\cdot(nu\boldsymbol{v}) + \nabla\cdot\boldsymbol{q} + \boldsymbol{p} : \nabla\boldsymbol{v}^{+} = 0 \tag{8}$$

where M is the molar mass.

The thermomechanic processes of the system are determined by the system of partial differential equations above together with appropriate initial and boundary conditions. The latter, for example, may consist in the specification of the pressure and heat flux on the boundary of the body.

In introductory thermostatics courses the ideal gas is usually intended in a much more restrictive way: a body for which matter density, temperature, pressure are uniform at all times, with $p = Rn\theta$ and $u = C\theta$. The state of the system is taken to be given by the spatially-independent quantities (n, θ) or (V, θ), where V is the volume. It is possible to model thermomechanic processes for such a body; see for example Samohýl & Pekař[1].

This uniform model has some singular features, however. In passing from a state of rest in an inertial frame to a compression process, for example, parts of the body will be accelerated. This is only possible if the divergence of the pressure is not zero at some times, owing to the balance law for the force. And the thermal conductivity must be infinite, in order to keep a uniform temperature when there is a heating flux at the boundary. The introduction of additional state variables such as the rate of change of volume $\partial_t V$[2] allows us to model interesting non-equilibrium phenomena, such as non-equilibrium pressures. But the singular features remain.

These singular features also lead the boundary conditions to eliminate some state quantities. For example, the specification of the pressure at the boundary is equivalent to its specification through the whole body. This places a constraint between n and T (and $\partial_t V$) for example, from the constitutive equation of the pressure.

I present here a slightly less simplified model. The idea is to allow a non-constant spatial dependence of some fields, but of a fixed mathematical kind. This idea can be seen as a simple generalization of the spatially constant dependence of the uniform model.

If we require the volumic amount of matter n to be uniform at all times, then the body can only undergo affine motions, that is, motions of the form

$$\boldsymbol{x}(\boldsymbol{X}, t) = \boldsymbol{L}(t)\,\boldsymbol{X} + \boldsymbol{c}(t) \,, \tag{9}$$

where $\boldsymbol{X}$ are its points in a reference configuration.

[1] Samohýl & Pekař 2014. [2] Samohýl & Pekař 2014.

It turns out that such an "affine" model is consistent with the balance laws if we assume a parabolic spatial dependence of pressure, temperature, and internal energy, and a linear spatial dependence of the heat flux.

If we moreover consider an inertial frame in which the mass centre of the body is at rest, then the pressure must be equal throughout the boundary; its parabolic spatial dependence is therefore symmetric with respect to the mass centre. The same symmetry holds for the parabolic spatial dependence of the temperature if the heating flux at the boundary is also assumed constant with respect to the surface normal.

In the following we shall assume that the body is in a cylindrical container of given cross section, within movable pistons in the direction x, and mass centre at rest at $\boldsymbol{x} = 0$. The motion (9) can be simplified to

$$x(X, t) = r(t)\, X, \qquad X \in [-1, 1] \tag{10}$$

with the y and z coordinates remaining constant. This motion requires the pressures on the two pistons, at positions r and $-r$, to be equal (to keep the mass centre at rest). We also require that the heat fluxes at the two pistons be equal in magnitude and opposite.

Under these conditions the symmetric parabolic profile along x of the temperature field $\theta(x, t)$ can be summarized by two numbers, for example the values of the temperature $\theta[r(t), t] =: \hat{\theta}(t)$ and of the temperature gradient $(\partial_x \theta)[r(t), t] =: \widehat{\nabla\theta}(t)$ at one piston surface. These two values can be considered state quantities. One more state quantity is the uniform $n(t)$ or equivalently the volume occupied by the body, which is in turn equivalent to the specification of the position $r(t) > 0$ of one piston, the other having position $-r(t)$, so that the volume is given by $2r(t) \times$ cross-sectional area.

From the motion (10) we can calculate the simplified space-time dependence of all the fields through the equations (2)–(6):

$$v(x,t) = \dot{r}\,\frac{x}{r} \tag{11}$$

$$n(x,t) = \frac{N}{r} \tag{12}$$

$$\begin{aligned} p(x,t) &= R\,n\,\hat{\theta} + \tfrac{1}{2}\,R\,n\,\widehat{\nabla\theta}\,\frac{x^2-r^2}{r} - r\,\frac{\dot{r}}{r} \\ &= \hat{p} + \tfrac{1}{2}\,R\,n\,\widehat{\nabla\theta}\,\frac{x^2-r^2}{r} \end{aligned} \tag{13}$$

$$\theta(x,t) = \hat{\theta} + \tfrac{1}{2}\,\widehat{\nabla\theta}\,\frac{x^2-r^2}{r} \tag{14}$$

$$u(x,t) = C\,\hat{\theta} + \tfrac{1}{2}\,C\,\widehat{\nabla\theta}\,\frac{x^2-r^2}{r} \tag{15}$$

$$q(x,t) = -K\,\widehat{\nabla\theta}\,\frac{x}{r} \tag{16}$$

where it we have omitted the time-dependence of the quantities $r(t)$, $\hat{p}(t)$, $\dot{r}(t)$, $\hat{\theta}(t)$, $\widehat{\nabla\theta}(t)$

$$\begin{gathered} M = 4\times10^{-3}\ \mathrm{kg/mol} \qquad C = 21\ \mathrm{J/(mol\ K)} \qquad K = 0.15\ \mathrm{W/(m\ K)} \\ R = 8.3\ \mathrm{m^3\ Pa/(mol\ K)} \qquad H = 2\times10^{-5}\ \mathrm{Pa\ s} \qquad N = 1\ \mathrm{mol} \qquad Z = 0\ \mathrm{Pa\ s} \end{gathered} \tag{17}$$

Bibliography

("de *X*" is listed under D, "van *X*" under V, and so on, regardless of national conventions.)

Samohýl, I., Pekař, M. (2014): *The Thermodynamics of Linear Fluids and Fluid Mixtures*. (Springer, Cham). First published as **samohyl1987**.