"Affine" ideal gas (Notes for Mila)

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1 Limitations of the ideal-gas model in graduate-physics teaching

The ideal gas of graduate-physics curricula, modelled with (V,T) or equivalent states and the equation of state pV = nRt, targets simplified problems of (Gibbsian) thermostatics, involving comparisons of equilibria. Many students find difficulties when questions involving motion and rates of change are involved, for example "how long will it take for the volume of the gas to change from V_0 to V_1 ?" (given particular conditions). Yet, experiments involving such changes can be readily thought and taught; for example the Assmann-Rüchardt experiment¹, in which a massive piston closes a cylinder containing an ideal gas, and various questions can be asked about the motion of the piston and the changes in volume, pressure, temperature of the gas.

Answers to such questions can for example be given² using the thermo*dynamic* model with (V,T) state as presented in Pekař & Samohýl (2014 § 2.1 model A). But this kind of analysis has some interrelated singular points and limitations: \checkmark Make the following statements more precise; concrete examples

- 1. If we assume the piston to have negligible mass, some evolution equations degenerate, and the gas shows infinitely fast responses
- There is no dissipation and no differences in pressure between compression and expansion, as instead expected in irreversible processes.

Owing to these peculiarities there's often an increased difficulty for the students to move to a continuum ideal gas later on.

The limitations above are connected to the fact that, from a continuum point of view, the gas can be seen as always having uniform pressure and temperature, and negligible mass. Make more precise.

¹ Assmann 1852; Rüchardt 1929. ² See e.g. Porta Mana 2011.

It is possible to model the ideal gas in a slightly more realistic way, having these useful features:

- the state variables are still finite, so we don't need to use continuum mechanics;
- the gas shows different pressures in compression and expansion, viscosity and dissipation;
- dynamical questions can be asked even with massless pistons;
- it's possible to make clearer connections with the continuum model of the gas, and in particular to the question of the boundary conditions necessary to study an continuum model.

Such model is very similar to *model* C in § 2.1 of Pekař & Samohýl (2014). The state of the gas is determined by four quantities: volume v, rate of change of volume \dot{v} , temperature θ at the boundary, and temperature gradient $\nabla \theta$ at the boundary or equivalently heating flux Q at the boundary \mathcal{F} I must check whether it's possible to replace the latter with $\dot{\theta}$.

This model can be introduced as a special class of solutions of the continuum equations. I start from there.

2 Special continuum solution

Some notation: constants are denoted by capital letters, spatially dependent quantities with lowercase letters, and quantities that depend only on time have an overbar.

Let n be the volumic amount of substance, v the velocity, p the (tensorial) pressure, θ the temperature, u the molar internal energy, q the heat flux, and N the total amount of substance in this body of gas. Also,

$$\nabla v^+ \coloneqq \frac{1}{2} (\nabla v + \nabla v^\intercal), \qquad \nabla v^\perp \coloneqq \nabla v^+ - \frac{1}{3} \nabla \cdot v \boldsymbol{I}.$$
 (1)

The independent fields, defining the state of the body, are taken to be (n, v, θ) . Pressure, internal energy, heat flux are local functions of state.

The fields satisfy the balance laws of matter, force, internal energy (the balance of torque is automatically satisfied owing to the symmetry of p):

$$\partial_t n + \nabla \cdot (n v) = 0 \tag{2}$$

$$M \ \partial_t(nv) + M \ \nabla \cdot (nv \otimes v) + \nabla \cdot \boldsymbol{p} = 0 \tag{3}$$

$$\partial_t(nu) + \nabla \cdot (nuv) + \nabla \cdot q + \operatorname{tr}(\mathbf{p}\nabla v^+) = 0 \tag{4}$$

where *M* is the molar mass.

We define the continuum ideal gas by the following constitutive equations:

$$q = -K \nabla \theta \tag{5}$$

$$\mathbf{p} = (Rn\theta - Z\,\nabla \cdot v)\,\mathbf{I} - 2\,H\,\nabla v^{\perp} \tag{6}$$

$$u = C\theta \tag{7}$$

$$R, K, C, H, Z \geqslant 0 \tag{8}$$

K is the thermal conductivity, H the shear viscosity, Z the bulk or volume viscosity. The shear viscosity H should depend on temperature³, but here we consider it constant for simplicity.

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.

Let's now look for a specific class of solutions. Consider a coordinate system (x, y, z) where the centre of mass of the gas is at rest with coordinate x = 0, and assume that the fields have no (y, z) dependence. The problem becomes one-dimensional. The gas can be imagined to be in a cylindrical container of given cross section A, within two pistons movable in the direction x. Let's identify the matter elements of the gas with the coordinate $X \in [-1,1]$ in the reference configuration, the centre of mass being at X = 0.

We require the volumic amount of matter n to be uniform at all times (so it's a constant). The balance of matter (2) then requires that the

³ Sutherland 1893.

motion of a matter element of gas at the reference position *X* can only have a motion of the form

$$x(X,t) = \frac{1}{2A}\bar{v}(t)X. \tag{9}$$

The boundary points of the body of gas – that is, the positions of the two pistons – are $x = \pm \frac{1}{2A} \bar{v}(t)$.

It turns out that the class of motions (9) and the balance laws of force and energy lead to a parabolic spatial dependence of pressure, temperature, internal energy, and a linear spatial dependence of the heat flux. We are also assuming this parabolic spatial dependence to be symmetric with respect to the mass centre; this requires the pressures on the two pistons to be equal (to keep the mass centre at rest), and the heat fluxes at the two boundaries to be opposite and equal in magnitude. These last symmetric restrictions can be easily lifted, however.

The solutions for the fields of velocity, matter density, temperature, pressure internal energy, heat flux are found to be

$$v(x,t) = \dot{\bar{v}} \, \frac{x}{\bar{v}} \tag{10}$$

$$n(x,t) = \frac{N}{\bar{v}} \tag{11}$$

$$\theta(x,t) = \bar{\theta} - \frac{1}{2} \frac{M}{R} \frac{\ddot{\bar{v}}}{\bar{v}} \left(x^2 - \frac{\bar{v}^2}{4A^2} \right) \tag{12}$$

$$p(x,t) = NR\frac{\bar{\theta}}{\bar{v}} - \frac{2}{3}H\frac{\dot{\bar{v}}}{\bar{v}} - \frac{1}{2}MN\frac{\ddot{\bar{v}}}{\bar{v}^2} \left(x^2 - \frac{\bar{v}^2}{4A^2}\right)$$
 (13)

$$u(x,t) = C\bar{\theta} - \frac{1}{2} \frac{CM}{R} \frac{\ddot{\overline{v}}}{\bar{v}} \left(x^2 - \frac{\bar{v}^2}{4A^2} \right) \tag{14}$$

$$q(x,t) = \frac{KM}{R} \frac{\ddot{\bar{v}}}{\bar{v}} x \tag{15}$$

where the time dependence of the barred quantities $\bar{\theta}(t)$, $\bar{v}(t)$ has been omitted for brevity. $\bar{\theta}(t)$ is the temperature at the boundaries.

By integration we also find the *average* pressure, total internal energy, heating, and work (found integrating the tr($p\nabla v^+$) term):

$$\bar{p}_{\text{average}}(t) = NR\frac{\bar{\theta}}{\bar{v}} - \frac{2}{3}H\frac{\dot{\bar{v}}}{\bar{v}} + \frac{MN}{12A^2}\ddot{\bar{v}}$$
 (16)

$$\bar{u}_{\text{total}}(t) = CN\bar{\theta} + \frac{1}{3} \frac{CMN}{4RA^2} \bar{v} \ddot{\bar{v}}$$
 (17)

$$\bar{q}_{\text{total}}(t) = \frac{KM}{R} \ddot{\bar{v}} \tag{18}$$

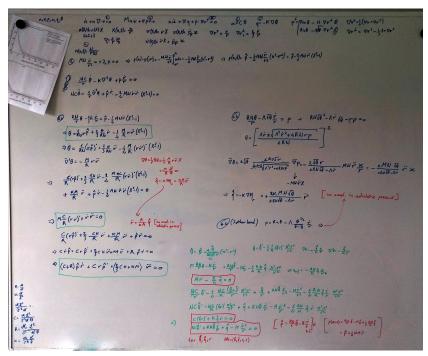
$$\bar{w}_{\text{total}} = \dot{\bar{v}} \; \bar{p}_{\text{average}}$$
 (19)

We see that in this specific class of solutions the state of the ideal gas at time t is completely determined by the variables $(\bar{\theta}, \bar{v}, \dot{\bar{v}}, \ddot{\bar{v}})$, similarly to model model C of Pekař & Samohýl. It is possible to associate to this model the average pressure \bar{p}_{average} above, which is given by an equation of state. Such a pressure shows different values at equilibrium ($\ddot{\bar{v}} = \dot{\bar{v}} = 0$) and during compression or expansion, leading to dissipation.

A result at variance with model C is that the total energy does depend on the state variable $\ddot{\bar{v}}$, whereas it is found in Pekař & Samohýl that it shouldn't have such dependence. \checkmark this can be a computation error on my part. All these calculations have to be rechecked. Also, the equation of balance for the energy hasn't been used yet. It's possible that with some change in the equations above and using the balance of energy, the variable $\ddot{\bar{v}}$ might be replaced by $\dot{\bar{\theta}}$.

The point of the calculations above is to see whether a connection could be made between one of the higher-order models in Pekař & Samohýl and a special state of a continuum ideal gas – just like model A can be interpreted, in one specific case, as describing a continuum ideal gas in a uniform state.

As already mentioned, I believe that such an association could be pedagogically useful, allowing thermodynamics students to study a finite-dimensional system showing dissipation and irreversibility, and at the same time showing them a first connection with its continuum description.



(Some old calculations before I left Trondheim)

Bibliography

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

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