Shock tube model for real gases

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1. Introduction

Shock tubes are used to study blast waves or to briefly obtain high pressure and temperature for studying combustion or other reactions. A simplified, one dimensional model neglecting gas viscosity is described by Glass et al. (Glass I.I. 1953) for the case of perfect gases (i.e. ideal gases with constant heat capacity). Below, this model is generalised to non-ideal gases.

Initially the shock tube consists of two sections: The high pressure (or driver) section and the low pressure (or driven) sections. A diaphragm separates the two sections. At time zero the diaphragm bursts and gas flows from the driver to the driven side. Figure 1 shows the wave trajectories and a sample pressure profile after a few milliseconds.

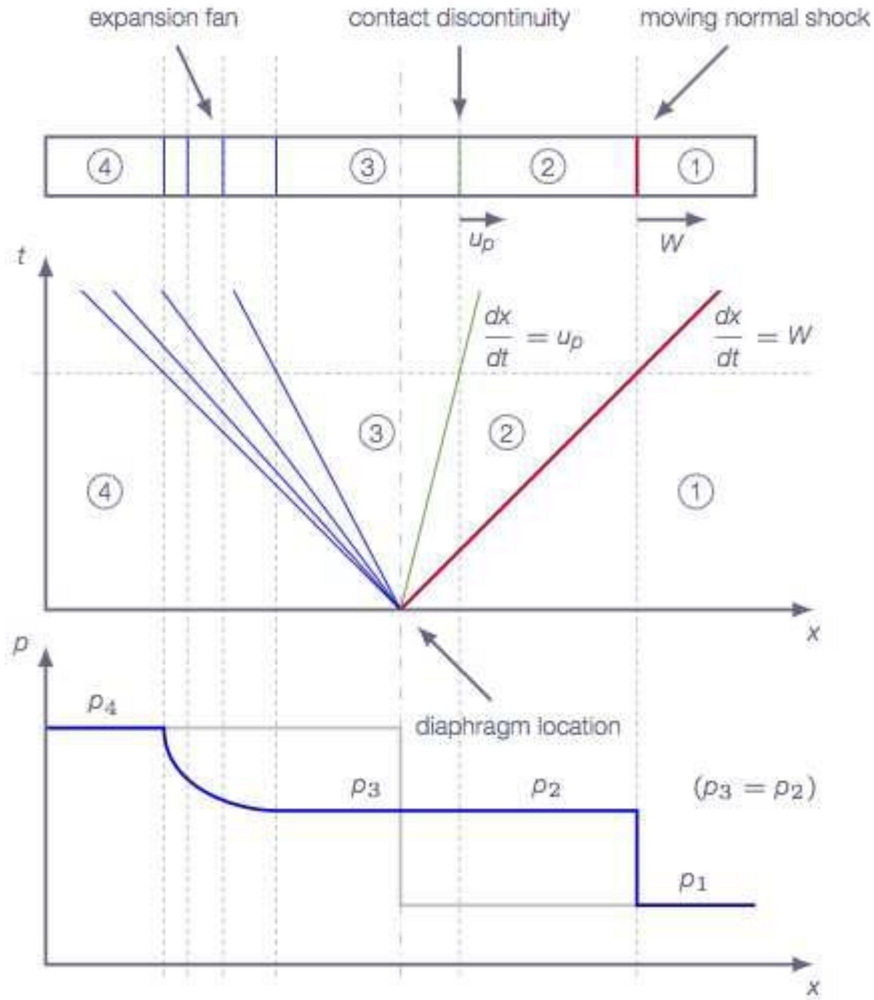

Figure 1: Shock tube waves and pressure profile. Source: (Anderson n.d.)

A rarefaction wave moves into the driver gas on the left at the local speed of sound. This is denoted "expansion fan" in the figure. At the same time a shock wave moves into the driven gas on the right. Since we neglect viscosity and thus friction, the pressure and the flow velocity are constant between the right-hand end of the rarefaction wave and the shock. We disregard any mixing at the contact surface between diver and driven gas, so this contact surface moves with the gas flow velocity. In Figure 1 four regions are indicated:

1) Undisturbed driven gas
2) Driven gas behind shock wave
3) Fully expanded driver gas
4) Undisturbed driver gas

If the tube has a rigid end wall to the right, the shock wave will hit this wall and be reflected, defining another region:

5) Gas behind (to the right of) the reflected wave.

The expansion wave will hit the end of the driver section and a reflected wave will move to the right. A pattern of interacting waves with increasing complexity will appear as time increases. This is not included in the model.

2. Isentropic gas flow

We assume that we have access to a thermodynamic model giving the Helmholtz free energy and its partial derivatives up to order three. This lets us calculate all thermodynamic variables and their derivatives as functions of temperature T and molar volume v. A Matlab version of such a model for a number of gases is available at GitHub (Mjaavatten 2020).

Viscosity and friction are ignored in this simple model. Then molar entropy is conserved everywhere except at the shock front. In this paragraph we derive some expressions for isentropic gas processes.

Notation: $\left(\frac{\partial x}{\partial y}\right)_z$ is the partial derivative of variable x with respect to y, with y and z as the free variables, meaning that z is kept constant in the differentiation.

For constant entropy s the entropy differential ds is zero:

$$ds = \left(\frac{\partial s}{\partial T}\right)_v dT + \left(\frac{\partial s}{\partial v}\right)_T dv = 0 \tag{1}$$

It follows that:

$$\left(\frac{\partial T}{\partial v}\right)_s = -\frac{\left(\frac{\partial s}{\partial v}\right)_T}{\left(\frac{\partial s}{\partial T}\right)_v} \tag{2}$$

The speed of sound, c is given by:

$$c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} \tag{3}$$

The differential dc for the speed of sound c may be written:

$$
\begin{aligned}
dc &= \left(\frac{\partial c}{\partial T}\right)_v dT + \left(\frac{\partial c}{\partial v}\right)_T dv \\
&= \left\{\left(\frac{\partial c}{\partial T}\right)_v \left(\frac{\partial T}{\partial v}\right)_s + \left(\frac{\partial c}{\partial v}\right)_T\right\} dv + \left(\frac{\partial c}{\partial T}\right)_v \left(\frac{\partial T}{\partial s}\right)_v ds
\end{aligned}
\tag{4}
$$

Setting $ds = 0$ we see that

$$
\left(\frac{\partial c}{\partial v}\right)_s = \left(\frac{\partial c}{\partial T}\right)_v \left(\frac{\partial T}{\partial v}\right)_s + \left(\frac{\partial c}{\partial v}\right)_T dv \tag{5}
$$

For the pressure:

$$
\begin{aligned}
dp &= \left(\frac{\partial p}{\partial T}\right)_v dT + \left(\frac{\partial p}{\partial v}\right)_T dv \\
&= \left\{\left(\frac{\partial p}{\partial T}\right)_v \left(\frac{\partial T}{\partial v}\right)_s + \left(\frac{\partial p}{\partial v}\right)_T\right\} dv + \left(\frac{\partial p}{\partial T}\right)_v \left(\frac{\partial T}{\partial s}\right)_v ds
\end{aligned}
\tag{6}
$$

Setting $ds = 0$ and inserting for dv from (43):

$$
\left(\frac{\partial p}{\partial c}\right)_s = \frac{\left(\frac{\partial p}{\partial T}\right)_v \left(\frac{\partial T}{\partial v}\right)_s + \left(\frac{\partial p}{\partial v}\right)_T}{\left(\frac{\partial c}{\partial T}\right)_v \left(\frac{\partial T}{\partial v}\right)_s + \left(\frac{\partial c}{\partial v}\right)_T} \tag{7}
$$

3. Wave motion

In the following I follow the report by Glass et al. (Glass I.I. 1953), but generalise to use rigorous thermodynamic models instead of perfect gas. Let M_w denote the molar mass of the gas in question and define the density ρ as

$$
\rho = \frac{M_w}{v} \tag{8}
$$

Let t denote time and x position along the pipe. The continuity equation for constant flow area is

$$
\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial x} = 0 \tag{9}
$$

Newton's second law gives:

$$
\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0 \tag{10}
$$

In addition, we stipulate that the flow is isentropic for all x and t except at the shock front:

$$
s = const. \tag{11}
$$

We write (9) as:

$$
\frac{c}{\rho}\left(\frac{\partial \rho}{\partial c}\right)_s \left(\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x}\right) + c\frac{\partial u}{\partial x} = 0 \tag{12}
$$

and (10) as

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+\frac{1}{\rho c}\left(\frac{\partial p}{\partial c}\right)_s c\frac{\partial c}{\partial x}=0 \tag{13}$$

Rarefication waves

This follows (Glass I.I. 1953), but see also (Morawretz 1981).

A disturbance propagates with the local speed of sound c, relative to the moving gas. With gas velocity u the velocity is $u \pm c$. In the expansion fan the flow is to the right, so $u > 0$. The trajectory of a disturbance in the (x,t) plane is called a characteristic. The characteristic with velocity $u-c$ moves to the left and is called a rarefication characteristic, as it represents a rarefication wave. The one with velocity $u+c$ is called a compression characteristic and takes the form of a shock. Let x, t represent a point on a rarefication characteristic and define y as:

$$y \equiv \frac{x}{t} \tag{14}$$

Then

$$dy=\frac{1}{t}dx-\frac{x}{t^2}dt \tag{15}$$

It follows that:

$$\left(\frac{\partial y}{\partial x}\right)_t=\frac{1}{t},\ \left(\frac{\partial y}{\partial t}\right)_x=-\frac{x}{t^2}=-\frac{y}{t} \tag{16}$$

Thus, for any function $z(t,x)$:

$$\frac{\partial z}{\partial t}=\frac{dz}{dy}\left(\frac{\partial y}{\partial t}\right)_x=-\frac{y}{t}\frac{dz}{dy} \tag{17}$$

$$\frac{\partial z}{\partial x}=\frac{dz}{dy}\left(\frac{\partial y}{\partial x}\right)_t=\frac{1}{t}\frac{dz}{dy} \tag{18}$$

Using this, (9) and (10) can be written:

$$\frac{\rho'}{t}(u-y)=\frac{\rho}{t}u' \tag{19}$$

$$\frac{u'}{t}(u-y)=-\frac{c^2\rho'}{\rho t} \tag{20}$$

Here $u'=\frac{du}{dy}$ and $\rho'=\frac{d\rho}{dy}$. Division of (20) by (19) gives:

$$\left(\frac{u'}{\rho'}\right)^2=\left(\frac{c}{\rho}\right)^2 \tag{21}$$

It follows that

$$du=\pm\frac{c}{\rho}d\rho \tag{22}$$

During the expansion u increases and ρ decreases, thus the – sign is relevant-

$$du = -\frac{c}{\rho}d\rho = \frac{c}{v}dv \tag{23}$$

We can find T and v from u by solving

$$\frac{du}{dv} = \frac{c(T,v)}{v} \tag{24}$$

while keeping the entropy constant. From (2):

$$\frac{dT}{dv} = \left(\frac{\partial T}{\partial v}\right)_s = -\frac{\left(\frac{\partial s}{\partial v}\right)_T}{\left(\frac{\partial s}{\partial T}\right)_v} \tag{25}$$

Solving the ODE system consisting of (24) and (25), with initial conditions

$$u(v_4) = 0, \quad T(v_4) = T_4 \tag{26}$$

will give us u and T as functions of v. From v and T we may calculate all thermodynamic variables, most notably the pressure p. This allows us to find p_3 as a function of u_3.

Shock wave

The shock front moves into the undisturbed driven gas at velocity W. In a coordinate system moving with the front, the driven gas moves into the front at velocity $\hat{u}_1 = -W$ and leaves at velocity $\hat{u}_2 = u_2 - W$, where u_2 is the gas velocity relative to a coordinate system at rest. The following conservation equations (often called the Hugoniot relations) must be satisfied across the shock front (Landau and Lifschitz 1959):

Conservation of mass (or moles):

$$\frac{\hat{u}_2}{v_2} - \frac{\hat{u}_1}{v_1} = 0 \tag{27}$$

Conservation of momentum:

$$\frac{\hat{u}_2^2}{v_2} + \frac{p_2}{M_w} - \frac{\hat{u}_1^2}{v_1} - \frac{p_1}{M_w} = 0 \tag{28}$$

Conservation of energy:

$$\tfrac{1}{2}M_w\hat{u}_2^2 + h_2 - \tfrac{1}{2}M_w\hat{u}_1^2 - h_1 = 0 \tag{29}$$

We assume that the pressure and temperature in state 1 are known, as well as the velocity $u_1 = 0$. The thermodynamic model gives us $p_2(T_2, v_2)$ and $h_2(T_2, v_2)$. If the flow velocity u_2 behind the shock is given, we have three equations and tree unknowns T_2, v_2 and W. Solving (27) through (29) then gives us p_2 as a function of u_2.

In the shock tube, the flow velocity and pressure must be continuous over the contact surface between the driver and driven gas, so that we must have:

$$u_2 = u_3 \tag{30}$$

$$p_2(u_2) = p_3(u_3) \tag{31}$$

In practice, we integrate (24) and (25) using (31) as a stop criterion.

Reflected shock

When the shock wave hits the end of the tube it is reflected. The reflected shock moves to the right. In front of the shock the velocity is u_2. Behind (to the right of) the shock the gas velocity is $u_5 = 0$. The unknowns are the shock velocity W and the state behind the shock, given T_5 and v_5. The equations to be solved are (27) through (29), with index 5 substituted for index 1.

4. Perfect gas

For completeness we develop the shock tube equations for the special case of a perfect gas.

Rarefaction wave

A perfect gas is an ideal gas with constant heat capacities. Let γ be the heat capacity ratio $\gamma \equiv \frac{c_p}{c_v}$. For an isentropic process starting at $(T_4,\ v_4)$ we have that:

$$\frac{T}{T_4} = \left(\frac{p}{p_4}\right)^{\frac{\gamma-1}{\gamma}} \tag{32}$$

$$\frac{v}{v_4} = \left(\frac{p_4}{p}\right)^{\frac{1}{\gamma}} \tag{33}$$

It follows that:

$$\left(\frac{\partial v}{\partial p}\right)_s = \frac{1}{\gamma} v_4 p_4^{-\frac{1}{\gamma}} p^{\frac{1}{\gamma}-1} \tag{34}$$

The speed of sound is

$$c = \sqrt{\frac{\gamma RT}{M_w}} \tag{35}$$

(23) takes the form

$$du = \frac{c}{v} dv = \frac{c}{v}\left(\frac{\partial v}{\partial p}\right)_s dp \tag{36}$$

Inserting from expressions (43) to (35) and using the ideal gas equation of state, we get:

$$du = -\mathrm{c}_4 p_4^{-\frac{\gamma-1}{2\gamma}} p^{-\frac{\gamma+1}{2\gamma}} dp \tag{37}$$

We integrate from p_4 to p_3, remembering that $u_4 = 0$:

$$u_3 = u_4 - \mathrm{c}_4 p_4^{-\frac{\gamma-1}{2\gamma}} \int_{p_4}^{p_3} p^{-\frac{\gamma+1}{2\gamma}} dp = \frac{2}{\gamma-1}\mathrm{c}_4\left(1-\left(\frac{p_3}{p_4}\right)^{\frac{\gamma-1}{2\gamma}}\right) \tag{38}$$

Shock wave

From the ideal gas shock equations, e.g. (Landau and Lifschitz 1959) we get that the flow velocity behind the shock is:

$$u_2 = \frac{2c_1}{\gamma + 1}\left(M_1 - \frac{1}{M_1}\right) \tag{39}$$

where c_1 is the speed of sound in the undisturbed driven gas and M_1 is the shock Mach number, given by:

$$M_1 = \sqrt{\frac{\frac{p_2}{p_1}(\gamma_1 + 1) + \gamma_1 - 1}{2\gamma_1}} \tag{40}$$

u_2 can be written as

$$u_2 = 2c_1 \frac{\frac{p_2}{p_1} - 1}{\sqrt{2\gamma_1}\sqrt{\gamma 2_1 + (\gamma_1 + 1)\left(\frac{p_2}{p_1} - 1\right)}} \tag{41}$$

Combining (30), (31), (38) and (43):

$$\frac{2}{\gamma_4 - 1} \mathrm{c}_4 \left(1 - \left(\frac{p_3}{p_4}\right)^{\frac{\gamma_4 - 1}{2\gamma_4}}\right) = \frac{2c_1}{\gamma_1 + 1} \frac{\frac{p_2}{p_1}(\gamma_1 + 1) - \gamma_1 - 1}{\sqrt{2\gamma_1}\sqrt{\frac{p_2}{p_1}(\gamma_1 + 1) + \gamma_1 - 1}} \tag{42}$$

This can be simplified to

$$\frac{p_4}{p_1} = \frac{p_2}{p_1} \frac{(\gamma_4 - 1)\frac{c_1}{c_4}\left(\frac{p_2}{p_1} - 1\right)}{\sqrt{2\gamma_1}\sqrt{2\gamma_1 + (\gamma_1 + 1)\left(\frac{p_2}{p_1} - 1\right)}} \tag{43}$$

This can be solved numerically for p_2. M_1 follows from (40) and u_2 from (39). T_2 is given by

$$T_2 = T_1 \frac{\left(2\gamma M_1^2 - (\gamma - 1)\right)\left((\gamma - 1)M_1^2 + 2\right)}{(\gamma - 1)^2 M_1^2} \tag{44}$$

Matlab functions for calculating both real gas and perfect gas shock tube equations are given by (Mjaavatten 2020).

5. Bibliography

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