Appendix B

Riemann solver for combustion waves

Riemann solver for combustion waves

Thin flame RH exact Riemann solver

This Riemann solver for combustion waves is based on the solver by Teng et.al [1]. The main difference is that two different values for γ can be used, one for the unburned state and one for the burned state. This solver needs a known burning velocity and it does not allow combustion fronts faster than CJ-deflagrations. Figure 1 shows the characteristics of the wave structures with a combustion wave. A Riemann solver relates the states behind the waves, here U_0 and U_I, to the known right and left states U_R and U_L. These states are connected by the eigenvectors and eigenvalues of the system. From the general Riemann solver a right wave connects the U_0 and U_R states if:

$$\psi(p_0; p_R, \rho_R) = \begin{cases} (p_0 - p_R)\sqrt{\frac{A_R}{p_0 - B_R}} & for \quad p_0 > p_R \\ \frac{2c_R}{\gamma_R - 1}\left(\frac{p_0}{p_R}\right)^{\left(\frac{\gamma_R - 1}{2\gamma} - 1\right)} & for \quad p_0 \leq p_R \end{cases} \tag{1}$$

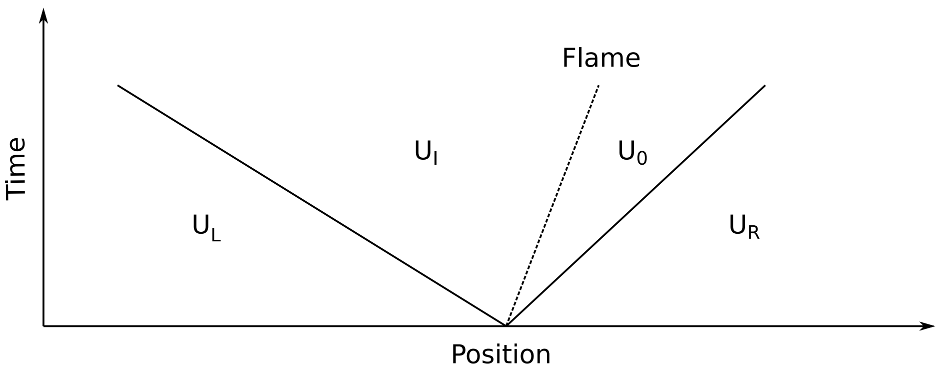

Figure 1:

$A_R = \frac{2}{\rho_R(\gamma_R+1)}$
$B_R = p_R\frac{\gamma_R-1}{\gamma_R+1}$
The U_L and U_I states are connected by left wave if

$$\psi(p_I;p_L,\rho_L) = \begin{cases} (p_I - p_L)\sqrt{\frac{A_L}{p_I-B_L}} & for \quad p_I > p_L \\ \frac{2c_L}{\gamma_L-1}\left(\frac{p_I}{pL}\right)^{\left(\frac{\gamma_L-1}{2\gamma}-1\right)} & for \quad p_I \leq p_L \end{cases} \tag{2}$$

where
$A_L = \frac{2}{\rho_L(\gamma_L+1)}$
$B_L = p_L\frac{\gamma_L-1}{\gamma_L+1}$
For a deflagration wave U_I and U_0 are connected by the deflagration solution in the Rankine-Hugoniot relations. Conservation of mass, momentum and energy equations 3, 4 and 5 express the relations between the two states. Either by expressing U_I as a function of U_0 or U_0 as a function of U_I and solving for U_0 or U_I respectively, the solution is obtained. The process of solving the exact general Riemann problem is described in detail in many text books, for example Toro [2].

$$\rho_I u_I = \rho_0 S \tag{3}$$

$$\rho_I u_I^2 + p_I = \rho_0 u_0^2 + p_0 \tag{4}$$

$$\frac{\gamma_I}{\gamma_I - 1}\frac{p_I}{\rho_I} + \frac{1}{2}u_I^2 = \frac{\gamma_0}{\gamma_0 - 1}\frac{p_0}{\rho_0} + \frac{1}{2}u_0^2 + q \tag{5}$$

Comments on the thin flame Riemann solver by Teng et.al.

In this chapter the Riemann solver for reactive gas by Teng et.al [1] will be discussed with corrections. The discussion of the wave patterns in the phase plane in turbulent combustion in Teng et.al. is further discussed here as the waves in the deflagration solution is calculated incorrectly. The paper reports that this model might produce two or zero solutions. The derivation of the Riemann solver is written here for this discussion. The stationary conservation equations of mass, momentum and energy are basis for the Riemann solver, the reaction zone is assumed to be infinitely thin and all the heat from the reaction is released instantaneously. If we let V be the flame speed, the velocity of the reaction zone relative to a fixed referance frame, then

$$w_0 = u_0 - V, \quad w_1 = u_1 - V \tag{6}$$

Where subscript 0 referes to the unburned state and 1 to the burned state. Conservation of mass and momentum is then expressed as

$$\rho_1 w_1 = \rho_0 w_0 = -M \tag{7}$$

$$\rho_1 w_1^2 + p_1 = \rho_0 w_0^2 + p_0 \tag{8}$$

For simplicity the heat capacity ratio γ is assumed identical for the burned and unburned gas and the energy conservation equation is expressed by

$$p_0(\tau_0 - \mu^2\tau_1) - p_1(\tau_1 - \mu^2\tau_0) - 2\mu^2\Delta = 0 \tag{9}$$

$$\tau = \frac{1}{\rho} \tag{10}$$

$$\mu = \frac{\gamma - 1}{\gamma + 1} \tag{11}$$

Δ is the specific energy released by the reaction and is defined with a negative value for an exothermal reaction. From the conservation equations of mass and momentum we can derive the pressure-velocity relations

$$M = \frac{p_1 - p_0}{u_1 - u_0}, \quad M^2 = \frac{p_0 - p_1}{\tau_1 - \tau_0} \tag{12}$$

With the energy equation and the two pressure-velocity relations we can eliminate the mass flow and the density of the burned gas.

$$\frac{p_1 - p_0}{u_1 - u_0} = \sqrt{\frac{p_0\rho_0\left(\frac{\gamma-1}{2} + \frac{(\gamma+1)p_1}{2p_0}\right)}{1 + \frac{(\gamma-1)\rho_0\Delta}{p_1 - p_0}}} \tag{13}$$

An expression for the velocity in the burned state as a function of only the unburned state and the pressure in the burned state can be derived.

$$u_1 = u_0 + (p_1 - p_0)\sqrt{\frac{(1-\mu^2)\tau_0 - \frac{2\mu^2\Delta}{p_0 - p_1}}{\mu^2 p_0 + p_1}} \tag{14}$$

Chapman-Jouguet waves

A CJ-wave moves with the speed of sound with respect to the burned gas. With this information a pressure/density relation for the states on both sides of the CJ wave can be derived.

$$-(\rho_1 c_1)^2 = \frac{p_1 - p_0}{\tau_1 - \tau_0} \tag{15}$$

the soundspeed is defined as $c_1 = \sqrt{\gamma \frac{p_1}{\rho_1}}$

$$\frac{p_1 - p_0}{\tau_1 - \tau_0} = -\rho_1 \gamma \frac{p_1}{\rho_1} = -\frac{\gamma p_1}{\rho_1} \tag{16}$$

or, by solving for τ_1

$$\tau_1 = \frac{\gamma \tau_0 p_1}{p_1(1+\gamma) - p_0} \tag{17}$$

Changing the subscript 1 to CJ we get an expression for p_{CJ} from the energy equation and the expression for τ_{CJ}

$$p_{CJ}^2 + 2ap_{CJ} + b = 0 \tag{18}$$

$$a = -p_0 + \Delta(\gamma - 1)\rho_0 \tag{19}$$

$$b = p_0^2 - 2\mu^2 \rho_0 p_0 \Delta \tag{20}$$

solving this second order equation yields

$$p_{CJ} = p_0 - (\gamma - 1)\rho_0 \Delta \left(1 \pm \sqrt{1 - \frac{2\gamma p_0}{(\gamma^2 - 1)\rho_0 \Delta}} \right) \tag{21}$$

the pluss sign corresponds to the CJ-detonation and the minus sign corresponds to the CJ-deflagration.

$$u_{CJ} = u_0 + (p_{CJ} - p_0) \sqrt{\frac{(1-\mu^2)\tau_0 - \frac{2\mu^2 \Delta}{p_0 - p_{CJ}}}{\mu^2 p_0 + p_{CJ}}} \tag{22}$$

$$\tau_{CJ} = \frac{\gamma \tau_0 p_{CJ}}{p_{CJ}(1+\gamma) - p_0} \tag{23}$$

The speed of the CJ-wave is determined from the conservation of mass and the equations for the CJ state.

$$V_{CJ} = u_0 + \frac{c_0^2}{\sqrt{-\frac{(\gamma^2-1)\Delta}{2} + c_0^2} \pm \sqrt{-\frac{(\gamma^2-1)\Delta}{2}}} \tag{24}$$

Here the pluss sign corresponds to the deflagration state and the minus sign corresponds to the detonation state.

Deflagrations

If we look at the deflagration wave and use a model for the flame speed

$$V = u_0 + K\left(\frac{p_0}{\rho_0}\right)^Q, \quad K, Q \ constants \tag{25}$$

Q=$\frac{1}{2}$ for the laminar burning velocity and Q>$\frac{1}{2}$ for turbulent burning velocity. The burning velocity $(V - u_0)$ must be less than or equal to the CJ-deflagration velocity.

$$K\left(\frac{p_0}{\rho_0}\right)^Q \leq \frac{c_0^2}{\sqrt{-\frac{(\gamma^2-1)\Delta}{2} + c_0^2} + \sqrt{-\frac{(\gamma^2-1)\Delta}{2}}} \tag{26}$$

The speed, w of the unburned state 0 is then written as

$$w_0 = -K\left(\frac{p_0}{\rho_0}\right)^Q \tag{27}$$

From the general Riemann solver the U_0 and U_R states are connected by a right wave if

$$\phi(p_0; p_R, \rho_R) = \begin{cases} (p_0 - p_R)\sqrt{\frac{(1-\mu^2)\tau_R}{p_0+\mu^2 p_R}} & p_0 \geq p_R \\ \frac{\sqrt{(1-\mu^2)\tau_R p_R}}{\mu^2}\left(p_0^{\frac{\gamma-1}{2\gamma}} - p_R^{\frac{\gamma-1}{2\gamma}}\right) & p_0 < p_R \end{cases} \tag{28}$$

$$u_0 = u_R + \phi(p_0; p_R, \rho_R) \tag{29}$$

We now need an expression that connect unburned and the burned state by a deflagration wave, eleminating w_1 and ρ_1 form the conservation equations we get an expression for massflow.

$$\rho_0 w_0 = -\sqrt{\frac{\mu^2 p_0 + p_1}{(1-\mu^2)\tau_0 - \frac{2\mu^2\Delta}{p_0 - p_1}}} \tag{30}$$

solving for p_1 with $M_0 = -\frac{w_0}{c_0} = \frac{K\left(\frac{p_0}{\rho_0}\right)^Q}{\left(\gamma\frac{p_0}{\rho_0}\right)^{0.5}} = \frac{K}{\gamma^{0.5}}\left(\frac{p_0}{\rho_0}\right)^{Q-0.5}$ being the Mach number of the reaction zone relative to the unburned state.

$$p_1 = p_0\left(\frac{1}{2}(1-\mu^2)(1+\gamma M_0^2) + \frac{1}{2}\sqrt{(1+\mu^2)(1-M_0^2) + 8\mu^2\gamma^2 M_0^2\frac{\Delta}{c_0^2}}\right) \tag{31}$$

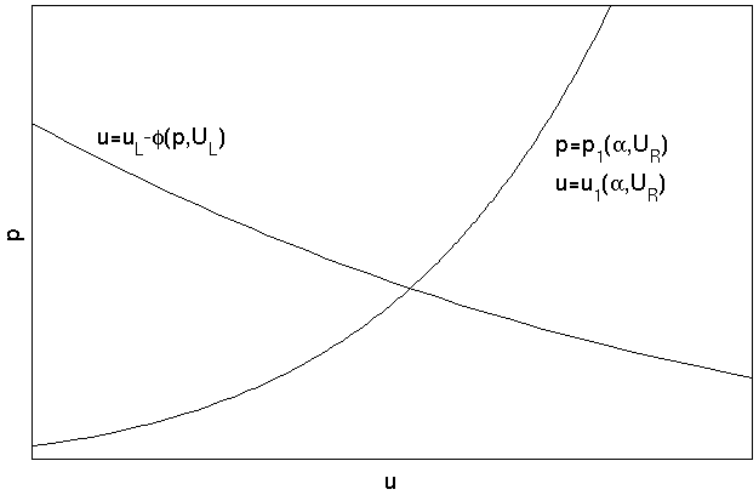

Figure 2: Hugoniot locus with Q=2.

The states U_L and U_1 are connected by a left wave in the same manner as U_0 and U_R. The intersection of the curves $U = U(U_L)$ and $U = U(U_R)$ in state space, called a Hugoniot locus, is the solution of the Riemann problem. Figure 2 shows the Hugoniot locus with an example of a turbulent flame with Q=2.

One way of getting several solutions, or none, is to use a positve Δ in the CJ deflagration velocity expression. The Mach number of the flame with respect to the unburned gas will then become imaginary while the square of the Mach number becomes real. This can be the reason for the non monotonic behaviour of the waves in the p,u plane presented in the article. An example of a solution in state space with turbulent deflagration and a positive Δ is shown in figure 3. When the CJ deflagration velocity is reached, the curve becomes non-monotonic and two solutions are obtained.

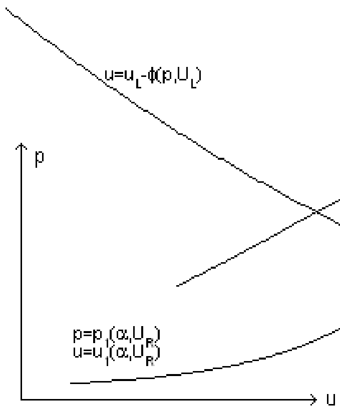

Figure 3: Hugoniot locus with Q=2 and Δ is positive.

Bibliography

[1] Teng, T. H., Chorin, A. J., Liu, T. P. *Riemann problems for reacting gas, with applications to transition* SIAM J. Appl. Math. 42 (5), 1982.

[2] Toro, E. F., *Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction, Berlin, Heidelberg, Germany, Springer-Verlag, 1999.*