2 Zones Thermodynamic Diagnosis model

NOMENCLATURE

ICE Ignition Combustion Engine
c specific heat (J/kgK)
f function
h specific enthalpy (J/kg)
m mass (kg)
p pressure (Pa)
q incoming heat per mass unit (J/kg)
$\dot{q}$ incoming heat flow per mass unite (J/kgs)
Q incoming heat to the system (J)
$\dot{Q}$ incoming heat flow to the system (J/s)
R gas ideal constant (J/kgK)
t time (s)
T temperature (K)
u internal específic energy (J/kg)
U internal energy (J)
v specific volume (m^3/kg)
V volume (m^3)
Y mass fraction (-)
Z number of species

Greek letters
α crankshaft angle (rd)
γ specific heats ratio (-)

Subscripts
b burned
bb blow by
i number of one burned specie
in incoming to the system
out outgoing from the system
u unburned

Superscripts
* correction considering the species dissociation

The 2 zones thermodynamic model distinguishes two differentiated zones, one zone of the unburned mass m_u, and another zone corresponding to the burned mass m_b.

The hypotheses used to propose the diagnostic model are the following:

- Uniform pressure in all the combustion chamber, p.
- Uniform temperature in each zone, T_u y T_b.
- Ideal gas behavior depending on the composition of each zone is assumed, so the equation $pv = RT$ in each zone is applied.
- The unburned mass zone composition does not vary with temperature, however, in the burned mass zone, the composition change is considered because of the displacement of the CO2 dissociation reaction:

$$CO + \frac{1}{2}O_2 \Leftrightarrow CO_2$$

It is considered that the reaction is in equilibrium since in the moments in which there is combustion the temperature of the burned mass is high. The appearance of CO in the burned mass zone makes the chemical energy released in heat is lower.

- The heat transfer between the two zones does not exist, but there are heat transfer between the walls and each zones, q_u and q_b.
- Only the closed valves process is taken account and without leakages.

The model is formulated starting from the energy conservation equation for open systems with uniform properties, so that we have:

$$\frac{dU}{dt} = -p\frac{dV}{dt} + \dot{Q} - \dot{m}_{out}\, h_{out} + \dot{m}_{in}\, h_{in}$$

The internal energies and the enthalpies include the terms of formation and therefore the heat flow corresponds exclusively to the heat transfer.

Expressing the above equation as a function of the intensive magnitudes, we arrive at the following equation:

$$\frac{du}{dt}m + \frac{dm}{dt}u = -p\left(\frac{dm}{dt}v + \frac{dv}{dt}m\right) + \dot{Q} - \dot{m}_{out}\, h_{out} + \dot{m}_{in}\, h_{in}$$

$$\frac{du}{dt}m = -p\frac{dv}{dt}m + \dot{Q} - \frac{dm}{dt}(u + pv) - \dot{m}_{out}\, h_{out} + \dot{m}_{in}\, h_{in}$$

$$\frac{du}{dt}m = -p\frac{dv}{dt}m + \dot{Q} - \frac{dm}{dt}h - \dot{m}_{out}\, h_{out} + \dot{m}_{in}\, h_{in}$$

The specific enthalpy of the mass leaving the system is the same as that of the system, $h = h_{out}$.

In a system where only mass comes out: $dm/dt = -\dot{m}_{out}$ y $\dot{m}_{in} = 0$, so that:

$$\frac{du}{dt}m = -p\frac{dv}{dt}m + \dot{Q} \qquad (1)$$

In a system where only mass enters: $dm/dt = \dot{m}_{in}$ y $\dot{m}_{out} = 0$:

$$\frac{du}{dt}m = -p\frac{dv}{dt}m + \dot{Q} + \frac{dm}{dt}(h_{in} - h)$$

$$\frac{du}{dt}m = -p\frac{dv}{dt}m + \dot{Q} + \dot{m}_{in}(h_{in} - h)$$

$$\frac{du}{dt} = -p\frac{dv}{dt} + \dot{q} + \frac{\dot{m}_{in}}{m}(h_{in} - h) \qquad (2)$$

In this case, the heat flow $\dot{q}$ is per unit mass that enters the system. The Eq. (1) and Eq. (2) will apply to the unburned and burned areas respectively. The additional equations used to close the problem are: the ideal gas state equation Eq. (3), which can be applied to each zone:

$$pv = RT \qquad (3)$$

The volume conservation equation, in the case of an ICE, the volume is variable and depends on the angle rotated by the crankshaft α:

$$\frac{dV}{dt} = f(\alpha) \qquad (4)$$

The conservation equation of the total mass:

$$\frac{dm}{dt} = \frac{dm_u}{dt} + \frac{dm_b}{dt} = -\dot{m}_{bb} \tag{5}$$

where $\dot{m}_{bb}$ is the "blow by" flow, i.e. the unburned mass lost from the combustion chamber through the piston contour.

The specific variables internal energies and enthalpies are related to the temperature through the thermal equations of the state of each zone, so for each zone, the specific volume, the mass and the temperature (or in this case the specific internal energy) are unknowns.

This system of 6 equations can be reduced to a system of only three differential equations of the form

$$\frac{dy_i}{dt} = f(y_1, y_2, y_3)$$

in which the rest of the unknowns can be determined algebraically from the variables y_i. In this way the system can be integrated by numerical methods.

The derivatives of the unknowns to be cleared are: the temporal variation of the burned mass, dm_b/dt, the internal energy of the burned, du_b/dt, and the internal energy of the unburned, du_u/dt.

Calculation of dm_b/dt

Applying equations to each system Eq. (1) and Eq. (2)

For the area of unburned products:

$$\frac{du_u}{dt} = -p\frac{dv_u}{dt} + \dot{q}_u \tag{6}$$

For the area of burned products, the incoming mass $\dot{m}_e = dm_b/dt$:

$$\frac{du_b}{dt} = -p\frac{dv_b}{dt} + \dot{q}_b + \frac{dm_b}{dt}\frac{(h_u - h_b)}{m_b} \tag{7}$$

Applying to each system the Eq. (3) and deriving with respect to time

$$\frac{dP}{dt}v_u + \frac{dv_u}{dt}p = R_u\frac{dT_u}{dt} \tag{8}$$

$$\frac{dP}{dt}v_b + \frac{dv_b}{dt}p = R_b\frac{dT_b}{dt} \tag{9}$$

The derivatives of the temperature must be replaced by derivatives of the internal energy, for which the ideal gas hypothesis is used. The application in the area without burning is immediate as the composition does not change, and therefore:

$$\frac{du_u}{dt} = \frac{du_u}{dT}\frac{dT_u}{dt} = c_{vu}\frac{dT_u}{dt}$$

However, in the burned area it is necessary to take into account the possibility of variation of the composition. To obtain an expression of dT_b/dt as a function of the internal energy, where Z is the number of species and Y_i the mass fraction of species i, the internal energy must be expressed as a function of that of each species and each one of them treat it with an ideal gas:

$$u_b = \sum_{i=1}^{i=Z_b} u_{bi}\, Y_{bi}$$

$$\frac{du_b}{dt} = \sum_{i=1}^{i=Z_b}\left(\frac{du_{bi}}{dt}Y_{bi} + \frac{dY_{bi}}{dt}u_{bi}\right)$$

$$\frac{du_b}{dt} = \sum_{i=1}^{i=Z_b}\left(\frac{du_{bi}}{dT_b}\frac{dT_b}{dt}Y_{bi} + \frac{\partial Y_{bi}}{\partial T_b}\frac{dT_b}{dt}u_{bi} + \frac{\partial Y_{bi}}{\partial p}\frac{dp}{dt}u_{bi}\right)$$

$$\frac{du_b}{dt} = \sum_{i=1}^{i=Z_b}\frac{dT_b}{dt}\left(\frac{du_{bi}}{dT_b}Y_i + \frac{\partial Y_{bi}}{\partial T_b}u_{bi}\right) + \sum_{i=1}^{i=Z_b}\frac{\partial Y_{bi}}{\partial p}\frac{dp}{dt}u_{bi}$$

$$\frac{du_b}{dt} = \frac{dT_b}{dt}\sum_{i=1}^{i=Z_b}\left(\frac{du_{bi}}{dT_b}Y_{bi} + \frac{\partial Y_{bi}}{\partial T_b}u_{bi}\right) + \frac{dp}{dt}\sum_{i=1}^{i=Z_b}\frac{\partial Y_{bi}}{\partial p}u_{bi}$$

Defining

$$c_{vb}^{*} = \sum_{i=1}^{i=Z_b}\left(\frac{du_{bi}}{dT_b}Y_{bi} + \frac{\partial Y_{bi}}{\partial T_b}u_{bi}\right) = c_{vb} + \sum_{i=1}^{i=Z_b}\frac{\partial Y_{bi}}{\partial T_b}u_{bi}$$

Due to specific internal energies of each species are independent on pressure:

$$\frac{\partial u_b}{\partial p} = \sum_{i=1}^{i=Z_b}\frac{\partial Y_{bi}}{\partial p}u_{bi}$$

$$\frac{du_b}{dt} = c_{vb}^{*}\frac{dT_b}{dt} + \frac{\partial u_b}{\partial p}\frac{dp}{dt}$$

Then:

$$\frac{dT_b}{dt} = \frac{1}{c_{vb}^{*}}\frac{du_b}{dt} - \frac{\frac{\partial u_b}{\partial p}}{c_{vb}^{*}}\frac{dp}{dt}$$

Substituting dT/dt in Eq. (8) and Eq. (9):

$$\frac{dp}{dt}v_u + \frac{dv_u}{dt}p = \frac{R_u}{c_{vu}}\frac{du_u}{dt} \qquad (10)$$

$$\frac{dp}{dt}v_b + \frac{dv_b}{dt}p = \frac{R_b}{c_{vb}^*}\frac{du_b}{dt} - \frac{R_b\frac{\partial u_b}{\partial p}}{c_{vb}^*}\frac{dp}{dt} \qquad (11)$$

Calling:

$$\gamma_b^* = \frac{c_{vb}^* + R_b}{c_{vb}^*}$$

Then:

$$\frac{dp}{dt}\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right) + \frac{dv_b}{dt}p = (\gamma_b^* - 1)\frac{du_b}{dt}$$

From the Eq. (4), separating the total volume $V = V_u + V_b$, and using the specific volume $v = V/m$:

$$\frac{dm_b}{dt}v_b + \frac{dv_b}{dt}m_b + \frac{dm_u}{dt}v_u + \frac{dv_u}{dt}m_u = f(\alpha) \qquad (12)$$

Doing the same for Eq. (5), $m = m_u + m_b - m_{bb}$:

$$\frac{dm_b}{dt} = -\frac{dm_u}{dt} - \dot{m}_{bb} \qquad (13)$$

Substituting Eq. (6) in Eq (*8*):

$$\frac{dp}{dt}v_u + \frac{dv_u}{dt}p = \frac{R_u}{c_{vu}}\left(-p\frac{dv_u}{dt} + \dot{q}_u\right)$$

$$\frac{dv_u}{dt}p\left(1 + \frac{R_u}{c_{vu}}\right) = \frac{dv_u}{dt}p\gamma_u = -\frac{dp}{dt}v_u + \frac{R_u}{c_{vu}}\dot{q}_u \qquad (14)$$

Substituting Eq. (7) in Eq. (11):

$$\frac{dp}{dt}\left(v_b + K_p\right) + \frac{dv_b}{dt}p = \frac{R_b}{c_{vb}^*}\left(-p\frac{dv_b}{dt} + \dot{q}_b + \frac{dm_b}{dt}\frac{h_u - h_b}{m_b}\right)$$

$$\frac{dv_b}{dt}p\gamma_b^* - \frac{dm_b}{dt}\frac{R_b}{c_{vb}^* m_b}(h_u - h_b) = -\frac{dp}{dt}\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right) + \frac{R_b}{c_{vb}^*}\dot{q}_b$$

$$\frac{dv_b}{dt}m_b p\gamma_b^* - \frac{dm_b}{dt}\frac{R_b}{c_{vb}^*}(h_u - h_b) = -\frac{dp}{dt}m_b\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right) + \frac{R_b}{c_{vb}^*}\dot{Q}_b \qquad (15)$$

Substituting Eq. (14) in Eq. (12):

$$\frac{dm_b}{dt}v_b + \frac{dv_b}{dt}m_b + \frac{dm_u}{dt}v_u + m_u\left(-\frac{dp}{dt}\frac{v_u}{p\,\gamma_u} + \frac{R_u}{c_{vu}\,p\,\gamma_u}\dot{q}_u\right) = f(\alpha)$$

And applying Eq. (13):

$$\frac{dm_b}{dt}v_b + \frac{dv_b}{dt}m_b - \frac{dm_b}{dt}v_u - \dot{m}_{bb} + m_u\left(-\frac{dp}{dt}\frac{v_u}{p\,\gamma_u} + \frac{R_u}{c_{vu}\,p\,\gamma_u}\dot{q}_u\right) = f(\alpha)$$

$$\frac{dm_b}{dt}(v_b - v_u) + \frac{dv_b}{dt}m_b - \dot{m}_{bb} = m_u\left(\frac{dp}{dt}\frac{v_u}{p\,\gamma_u} - \frac{R_u}{c_{pu}\,p}\dot{q}_u\right) + f(\alpha)$$

$$\frac{dv_b}{dt}m_b = m_u\frac{dp}{dt}\frac{v_u}{p\,\gamma_u} - \frac{R_u}{c_{pu}\,p}\dot{Q}_u - \frac{dm_b}{dt}(v_b - v_u) + f(\alpha) + \dot{m}_{bb} \qquad (16)$$

Substituting Eq. (16) in Eq. (15):

$$p\gamma_b^*\left(m_u\frac{dp}{dt}\frac{v_u}{p\,\gamma_u} - \frac{R_u}{c_{pu}\,p}\dot{Q}_u - \frac{dm_b}{dt}(v_b - v_u) + f(\alpha) + \dot{m}_{bb}\right)$$
$$= \frac{dm_b}{dt}\frac{R_b}{c_{vb}^*}(h_u - h_b) - \frac{dp}{dt}m_b\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right) + \frac{R_b}{c_{vb}^*}\dot{Q}_b$$

Clearing dm_b/dt :

$$\frac{dm_b}{dt}\left(\frac{R_b}{c_{vb}^*}(h_u - h_b) + p\gamma_b^*(v_b - v_u)\right)$$
$$= m_u v_u\frac{\gamma_b^*}{\gamma_u}\frac{dp}{dt} - \frac{R_u}{c_{vu}}\frac{\gamma_b^*}{\gamma_u}\dot{Q}_u + p\gamma_b^*(f(\alpha) + \dot{m}_{bb}) + \frac{dp}{dt}m_b\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right)$$
$$- \frac{R_b}{c_{vb}^*}\dot{Q}_b$$

$$\frac{dm_b}{dt} = \frac{m_u v_u\frac{\gamma_b^*}{\gamma_u}\frac{dp}{dt} - \frac{R_u}{c_{vu}}\frac{\gamma_b^*}{\gamma_u}\dot{Q}_u + p\gamma_b^*(f(\alpha) + \dot{m}_{bb}) + \frac{dp}{dt}m_b\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right) - \frac{R_b}{c_{vb}^*}\dot{Q}_b}{\frac{R_b}{c_{vb}^*}(h_s - h_b) + p\gamma_b(v_b - v_u)}$$

$$\frac{dm_b}{dt} = \frac{\frac{dp}{dt}\left(m_u v_u\frac{\gamma_b^*}{\gamma_u} + m_b\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right)\right) - \left(\frac{R_u}{c_{pu}}\frac{\gamma_b^*}{\gamma_u}\dot{Q}_u + \frac{R_b}{c_{vb}^*}\dot{Q}_b\right) + p\gamma_b^*(f(\alpha) + \dot{m}_{bb})}{\frac{R_b}{c_{vb}^*}(h_u - h_b) + p\gamma_b^*(v_b - v_u)}$$

$$\frac{dm_b}{dt} = \frac{\frac{dp}{dt}\left(m_u v_u\frac{\gamma_b^*}{\gamma_u} + m_b\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right)\right) - \left(\frac{\gamma_u - 1}{\gamma_u}\gamma_b^*\dot{Q}_u + \frac{R_b}{c_{vb}^*}\dot{Q}_b\right) + p\gamma_b^*(f(\alpha) + \dot{m}_{bb})}{\frac{R_b}{c_{vb}^*}(h_u - h_b) + p\gamma_b^*(v_b - v_u)} \qquad (17)$$

Using the expression of γ_b^*

$$\frac{dm_b}{dt} = \frac{\frac{dp}{dt}\left(m_u v_u\frac{\gamma_b^*}{\gamma_u} + m_b\left(v_b + (\gamma_b^* - 1)\frac{\partial u_b}{\partial p}\right)\right) - \left(\frac{\gamma_u - 1}{\gamma_u}\gamma_b^*\dot{Q}_u + (\gamma_b^* - 1)\dot{Q}_b\right) + p\gamma_b^*\left(\frac{dV(\alpha)}{dt} + \dot{m}_{bb}\right)}{\gamma_b^*(u_u - u_b) + (h_u - h_b)}$$

The denominator of Eq. (17) does not take values close to zero even if the masses of burned or unburned are small or null. This is a great advantage when integrating the differential equation in the areas where combustion starts or ends.

Calculation of du_u/dt:

From Eq. (6)

$$p\frac{dv_u}{dt} = -\frac{du_u}{dt} + \dot{q_u}$$

And substituting this term in Eq. (*10*):

$$\frac{dp}{dt}v_u - \frac{du_u}{dt} + \dot{q_u} = \frac{R_u}{c_{vu}}\frac{du_u}{dt}$$

Clearing du_u/dt:

$$\frac{du_u}{dt} = \left(\frac{dp}{dt}v_u + \dot{q_u}\right)\frac{1}{\gamma_u} \qquad (18)$$

Calculation of du_b/dt:

Case in which $\dot{m}_b \cong 0$

HYPOTHESIS

When the burned mass is very small, $\dot{m}_b \cong 0$, the burned products are at adiabatic flame temperature is assumed, so that $h_u = h_b$

$$u_u + pv_u = u_b + pv_b$$

$$u_u + R_uT_u = u_b + R_bT_b$$

$$\frac{du_u}{dt} + \frac{R_u}{c_{vu}}\frac{du_u}{dt} = \frac{du_b}{dt} + \frac{R_b}{c_{vb}^*}\frac{du_b}{dt} - K_p\frac{dp}{dt}$$

$$\frac{du_b}{dt} = \frac{\gamma_u\frac{du_u}{dt} + K_p\frac{dp}{dt}}{\gamma_b^*}$$

So, when $\dot{m}_b \cong 0$:

$$\frac{du_b}{dt} = \left(\frac{dp}{dt}v_u + \dot{q_u} + K_p\frac{dp}{dt}\right)\frac{1}{\gamma_b^*} \qquad \dot{m}_b \cong 0$$

$$\frac{du_b}{dt} = \left(\frac{dp}{dt}\left(v_u + K_p\right) + \dot{q_u}\right)\frac{1}{\gamma_b^*} \qquad \dot{m}_b \cong 0 \qquad (19)$$

Case in which $\dot{m}_b > 0$

In Eq. (16) clearing:

$$\frac{dv_b}{dt} = -\frac{1}{m_b}\left[m_u \frac{dp}{dt}\frac{v_u}{p\,\gamma_u} - \frac{R_u}{c_{pu}\,p}\dot{Q}_u - \frac{dm_b}{dt}(v_b - v_u) + f(\alpha) + \dot{m}_{bb}\right]$$

And substituting this term in Eq. (7):

$$\frac{du_b}{dt} = -\frac{p}{m_b}\left[m_u \frac{dp}{dt}\frac{v_u}{p\,\gamma_u} - \frac{R_u}{c_{pu}\,p}\dot{Q}_u - \frac{dm_b}{dt}(v_b - v_u) + f(\alpha) + \dot{m}_{bb}\right] + \dot{q}_b + \frac{dm_b}{dt}\frac{(h_u - h_b)}{m_b}$$

$$\frac{du_b}{dt} = -\frac{1}{m_b}\left[\frac{dp}{dt}\frac{v_u m_u}{\gamma_u} - \frac{R_u}{c_{pu}}\dot{Q}_u - \dot{Q}_b - \frac{dm_b}{dt}\left[p(v_b - v_u) + (h_u - h_b)\right] + p\,(f(\alpha) + \dot{m}_{bb})\right]$$

$$\frac{du_b}{dt} = \frac{dm_b}{dt}\frac{(u_u - u_b)}{m_b} - \frac{dp}{dt}\frac{v_u m_u}{\gamma_{um_b}} + \frac{1}{m_b}\left(\frac{R_u}{c_{pu}}\dot{Q}_u + \dot{Q}_b\right) + \frac{p}{m_b}\left(\frac{dV(\alpha)}{dt} + \dot{m}_{bb}\right) \qquad \dot{m}_b > 0 \qquad (20)$$