Energy and Entropy Balances in a Combustion Chamber: Analytical Solution

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Abstract—An analytical solution of the energy and entropy balance equations for a combustible gas mixture contained in an open combustion chamber, for example of an internal combustion engine, is presented. The solution is free of major assumptions and is in a form suitable for incorporating any detailed models for the effects of wall heat transfer, wall thermal boundary layer, non-uniform temperature distributions in the burnt mixture, crevice regions, mass exchange through the boundaries of the chosen control volume and other similar effects. Explicit expressions for the instantaneous mass of burnt mixture and for the entropy generated by irreversibility are presented as functions of pressure and volume history of the combustion chamber and properties of the gas mixtures.

1 INTRODUCTION

The purpose of this article is to present a general analytical solution of the energy and entropy balance equations for a combustible gas mixture confined in a combustion chamber.

The problem involves no major conceptual difficulties. However, a number of major assumptions are often made in order to simplify the equations and obtain simple analytical solutions (cf., *e.g.*, Krieger and Borman, 1966; Lavoie, Heywood, and Keck, 1970; Harrington, 1975; Danieli, Keck, and Heywood, 1977; McCuiston, Lavoie, and Kauffman, 1977). When accuracy is a requirement, then numerical techniques are adopted (cf., *e.g.*, Patterson and Van Wylen, 1964; Tabaczynski, Ferguson, and Radhakrishnan, 1977).

In this article, we present an analytical approach to the problem, which is at the same time general, flexible and immediately applicable. The resulting general solution of the balance equations involves no major assumptions. Any modeling assumption concerning temperature and composition distributions within the gas mixture may be incorporated, including all the approximations that have been considered in the literature. The flexibility of the solution is obtained by an especially efficacious method for labeling different gas elements in the mixture. Incorporating more detailed modeling assumptions will require only minor modifications, none of which is in the general equations.

The solution can be directly implemented to develop efficient and accurate computer codes for both modeling and diagnostic purposes. As an example, a particular approach to the problem of estimating from the typical pressure measurements, the instantaneous mass fraction of burnt gases in a combustion chamber is discussed. An advantage of the analytical solution of the problem is that it displays explicitly the dependence of the mass fraction burnt on the various physical effects involved in a typical engine operating cycle, and can therefore be used also to obtain order of magnitude estimates of the contributions of each effect under different operating conditions.

The importance of the entropy balance equation stems from its usefulness to availability (or second-law) analyses of internal combustion engines. An explicit analytical expression for the rate of entropy production by irreversibility in a combustion chamber is given. Irreversibility is the physical phenomenon responsible for any loss of useful work (cf., e.g., Keenan, 1941). Thus, identification of the sources of irreversibility in an engine operating cycle and their association with the responsible physical effects is an important piece of information required to evaluate the theoretical potential for improving the thermodynamic efficiency of an internal combustion engine. This major engineering problem is not addressed in the present article; however, an indispensable theoretical background and a useful analytical tool for a correct approach to the problem are presented.

2 SYSTEM DEFINITION AND ASSUMPTIONS

The object of study is an open system composed of a combustible gas mixture inside a variable control volume. For example, the control volume could coincide with a combustion chamber of an internal combustion engine. However, for more detailed descriptions, it could coincide with a subregion of the combustion chamber.

As combustion takes place, the gas mixture of reactants (referred to as the "unburnt" mixture, subscript u) is transformed into a gas mixture of products of combustion (referred to as the "burnt" mixture, subscript b).

The first assumption of the present analysis is to neglect the mass fraction of gases which are at any instant of time in the process of burning. This hypothesis is justified by the fact that the principal exothermic reactions involved in the combustion process are faster than any other major rate process occurring in the combustion chamber. Of course, this hypothesis does not hold if the reactions of interest involve, for example, the formation of nitric oxide; however, such reactions have a minor influence on the bulk thermodynamic properties of the burnt mixture.

The second assumption is that the pressure p is uniform throughout the chosen control volume. If pressure nonuniformities cannot be neglected, the present analysis can still be applied, provided the combustion chamber is subdivided into smaller regions of uniform pressure.

The third assumption is that the burnt and unburnt gas mixtures behave as Gibbs–Dalton mixtures of ideal semiperfect gases (i.e., the temperature dependence of the specific heats is not neglected). The composition of the unburnt mixture will be assumed to remain fixed ("frozen") and uniform at all times, while that of the burnt mixture will not be assumed to be either fixed or uniform. Thus, the present analysis will include and be directly compatible with most typical assumptions about the chemical composition distribution of the gas elements in the burnt mixture. For example, one might assume that the local composition is that of chemical equilibrium at the local value of temperature and pressure or one might even assume a local constrained equilibrium rate – controlled by the slowest chemical reactions (cf., Keck and Gillespie, 1971; Keck, 1978).

3 THERMODYNAMIC STATE OF THE GAS MIXTURE

To characterize the thermodynamic state of the gas mixture inside the control volume just defined at every instant of time t, let $x(t)$ be the instantaneous mass fraction of

burnt mixture, $m(t)$ the total instantaneous mass in the control volume and $p(t)$ the instantaneous pressure.

An important role is played in this analysis by the method adopted to label and account for gas elements that differ in their temperature and/or chemical composition. At each instant of time, a continuous variable x' will label the gas elements in the combustion chamber. Values of x' between $x(t)$ and 1 will correspond to gas elements with the fixed unburnt composition. Values of x' between 0 and $x(t)$ will correspond to gas elements with a burnt composition, which may differ from element to element. The fraction of total mass contributed by gas elements between x' and $x'+dx'$ will be dx'.

In this section and the next, arbitrary distributions will be assumed for the composition of burnt gas elements and for the temperature of the burnt and unburnt elements. Thus, the general results will be applicable to any particular assumption regarding these distributions as exemplified in Section 5.

The instantaneous volume $V(t)$, total energy $E(t)$ and total entropy $S(t)$ of the gas mixture in the control volume at time t are

$$\bar{v}(t) = \frac{V(t)}{m(t)} = \int_0^{x(t)} v_b(x', t)dx' + \int_{x(t)}^1 v_u(x', t)dx' \equiv \frac{\bar{R}(t)\bar{T}(t)}{p(t)} \tag{1}$$

$$\bar{e}(t) = \frac{E(t)}{m(t)} = \int_0^{x(t)} e_b(x', t)dx' + \int_{x(t)}^1 e_u(x', t)dx'$$
$$\equiv \bar{e}_0(t) + \bar{c}_v(t)(\bar{T}(t) - T_0) \tag{2}$$

$$\bar{s}(t) = \frac{S(t)}{m(t)} = \int_0^{x(t)} s_b(x', t)dx' + \int_{x(t)}^1 s_u(x', t)dx'$$
$$\equiv \bar{s}_0(t) + \bar{c}_p(t)\ln(\bar{T}(t)/T_0) - \bar{R}(t)\ln(p(t)/p_0) \tag{3}$$

where v_b, v_u, e_b, e_u and s_b, s_u are specific volume, specific energy and specific entropy of the gas elements in the burnt and unburnt mixtures and T_0, p_0 are arbitrary reference temperature and pressure. Equations (1)–(3) together with the following Eqs. (4)–(6) define the variables $\bar{R}, \bar{T}, \bar{c}_v, \bar{c}_p, \Delta\bar{e}_0$ and $\Delta\bar{s}_0$

$$\bar{R}(t) = \int_0^{x(t)} R_b(x', t)dx' + (1-x(t))R_u \tag{4}$$

$$\bar{e}_0(t) = \int_0^{x(t)} e_{b0}(x', t)dx' + (1-x(t))e_{u0}$$
$$= e_{u0} - \int_0^{x(t)} \Delta e_0(x', t)dx' \equiv e_{u0} - x(t)\Delta\bar{e}_0(t) \tag{5}$$

$$\bar{s}_0(t) = \int_0^{x(t)} s_{b0}(x', t)dx' + (1-x(t))s_{u0}$$

$$= s_{u0} + \int_0^{x(t)} \Delta s_0(x',t)dx' \equiv s_{u0} + x(t)\Delta\bar{s}_0(t) \tag{6}$$

where R_b, R_u, e_{b0}, e_{u0} and s_{b0}, s_{u0} are specific gas constant ($R_b=R/M_b$, $R_u=R/M_u$, with M_b, M_u the molecular weights), specific reference energy and specific reference entropy of the burnt and unburnt Gibbs–Dalton mixtures with the composition of the gas element labeled by x' at time t and the reference temperature T_0 and pressure p_0. Moreover, $\Delta e_0=e_{u0}-e_{b0}$ and $\Delta s_0=s_{b0}-s_{u0}$ are the energy and the entropy of reaction (defined in such a way that they assume positive values for most exothermic reactions), corresponding to the change from the fixed unburnt composition to the burnt composition associated with x' at time t. Their values are related to the values of the enthalpy of reaction $\Delta h_0=h_{u0}-h_{b0}$ and the Gibbs free energy of reaction $\Delta g_0=g_{u0}-g_{b0}$ via the relations

$$\Delta e_0(x', t) = \Delta h_0(x', t) + T_0(R_b(x', t)-R_u) \tag{7}$$

$$T_0\Delta s_0(x', t) = \Delta g_0(x', t)-\Delta h_0(x', t) \tag{8}$$

For a Gibbs–Dalton mixture of ideal gases, the following relations hold

$$v_b(x', t) = \frac{R_b(x', t)T_b(x', t)}{p(t)} \tag{9}$$

$$v_u(x', t) = \frac{R_u T_u(x', t)}{p(t)} \tag{10}$$

$$e_b(x', t) = e_{b0}(x', t) + \int_{T_0}^{T_b(x',t)} c_{vb}(T, x', t)dT \tag{11}$$

$$e_u(x', t) = e_{u0} + \int_{T_0}^{T_u(x',t)} c_{vu}(T, x', t)dT \tag{12}$$

$$s_b(x', t) = s_{b0}(x', t) + \int_{T_0}^{T_b(x',t)} c_{pb}(T, x', t)\frac{dT}{T} - R_b(x', t)\ln\frac{p(t)}{p_0} \tag{13}$$

$$s_u(x', t) = s_{u0} + \int_{T_0}^{T_b(x',t)} c_{pu}(T, x', t)\frac{dT}{T} - R_u\ln\frac{p(t)}{p_0} \tag{14}$$

It is noteworthy that the specific heats c_{vb}, c_{vu}, c_{pb} and c_{pu} in Eqs. (11)–(14) are those of a Gibbs–Dalton mixture with the composition of the gas element labeled by x' at time t and temperature T. As already noted, the values of the specific heats may vary from element to element not only because of differences in their temperature but also because of differences in their chemical composition.

The expressions defining the variables $\bar{T}$, $\bar{c}_v$ and $\bar{c}_p$ at each instant in time become

$$\frac{p(t)V(t)}{m(t)} = \bar{R}(t)\bar{T}(t) = x(t)\bar{R}_b(t)\bar{T}_b(t) + (1-x(t))R_u\bar{T}_u(t) \tag{15}$$

$$\bar{c}_v(t)(\bar{T}(t)-T_0) = x(t)\bar{c}_{vb}(t)(\bar{T}_b(t)-T_0)+(1-x(t))\bar{c}_{vu}(t)(\bar{T}_u(t)-T_0) \tag{16}$$

$$\bar{c}_p(t) \ln \frac{\bar{T}(t)}{T_0} = x(t)\bar{c}_{pb}(t) \ln \frac{\bar{T}_b(t)}{T_0} + (1-x(t))\bar{c}_{pu}(t) \ln \frac{\bar{T}_u(t)}{T_0} \tag{17}$$

where the following mean quantities have been defined

$$\bar{R}_b(t) \equiv \frac{1}{x(t)} \int_0^{x(t)} R_b(x', t)dx' \tag{18}$$

$$\bar{T}_b(t) \equiv \frac{1}{x(t)\bar{R}_b(t)} \int_0^{x(t)} R_b(x', t)T_b(x', t)dx' \tag{19}$$

$$\bar{T}_u(t) \equiv \frac{1}{1-x(t)} \int_{x(t)}^1 T_u(x', t)dx' \tag{20}$$

$$\bar{c}_{vb}(t) \equiv \frac{1}{x(t)(\bar{T}_b(t)-T_0)} \int_0^{x(t)} \int_{T_0}^{T_b(x',t)} c_{vb}(T, x', t)dT\, dx' \tag{21}$$

$$\bar{c}_{vu}(t) \equiv \frac{1}{(1-x(t))(\bar{T}_u(t)-T_0)} \int_{x(t)}^1 \int_{T_0}^{T_u(x',t)} c_{vu}(T, x', t)dT\, dx' \tag{22}$$

$$\bar{c}_{pb}(t) \equiv \frac{1}{x(t) \ln(\bar{T}_b(t)/T_0)} \int_0^{x(t)} \int_{T_0}^{T_b(x',t)} c_{pb}(T, x', t)\frac{dT}{T} dx' \tag{23}$$

$$\bar{c}_{pu}(t) \equiv \frac{1}{(1-x(t))\ln(\bar{T}_u(t)/T_0)} \int_{x(t)}^1 \int_{T_0}^{T_u(x',t)} c_{pu}(T, x', t)\frac{dT}{T} dx' \tag{24}$$

The definitions given in this section allow the representation of the gas mixture in the control volume by means of an equivalent "quasi-ideal gas" at pressure p, temperature $\bar{T}$ and with specific gas constant $\bar{R}$. In fact the equation of state $pV = m\bar{R}\bar{T}$ holds by virtue of such definitions (Eq. 15). The artifice is however only mathematical and no physical significance should be attached to this representation. It is in fact noteworthy that the Mayer relation for ideal gases is not satisfied by the specific heats $\bar{c}_v$ and $\bar{c}_p$, since $\bar{c}_p - \bar{c}_v \neq \bar{R}$. In what follows the dependence on t will be dropped, unless its explicit appearance is required for clarity.

The energy and entropy balance equations will be solved explicitly in terms of the mean quantities just defined. The quantities $\bar{R}_b$, $\bar{T}_b$, $\bar{T}_u$, $\bar{c}_{vb}$, $\bar{c}_{vu}$, $\bar{c}_{pb}$, $\bar{c}_{pu}$, $\Delta\bar{e}_0$ and $\Delta\bar{s}_0$ will depend upon the particular distributions assumed for temperature and composition. The dependence of the specific heats with temperature, needed to perform the integrations with respect to T in Eqs. (21)-(24), has been studied in the

literature for several particular conditions especially relevant to internal combustion engine technology. We refer for this matter to the JANAF *Thermochemical Tables* (1971) and the works of Gordon and McBride (1971), Olikara and Borman (1975), Hires *et al.* (1976), Way (1976) and Martin and Heywood (1977).

4 ENERGY AND ENTROPY BALANCE EQUATIONS

In this section, the energy and entropy balance equations are derived and solved analytically in terms of the quantities just defined. Let the control volume under study be open to a net mass flux $\dot{m}$ (positive if inward) of mean specific enthalpy h_m and mean specific entropy s_m. For example, in the study of a combustion chamber of an internal combustion engine, depending on the choice of the control volume, the mass influx should take into account exchanges of mass through the inlet and exhaust valves, with the crevice regions between piston, piston-ring and cylinder wall (if not included in the control volume) and prechambers.

The energy and entropy balance equations are

$$\dot{E} = \dot{m}h_m - \dot{Q}_w - p\dot{V} \tag{25}$$

$$\dot{S} = \dot{m}s_m - \dot{Q}_w/T_w + \dot{S}_{irr} \tag{26}$$

where $\dot{Q}_w$ is the heat loss to the surface of the control volume which is assumed to be isothermal at temperature T_w (typically, the surface coincides with the wall of the combustion chamber and the piston head) and $\dot{S}_{irr}$ (always non-negative by the second law of thermodynamics) is the rate of entropy generation by irreversibility inside the control volume.

To solve the balance equations, the explicit expressions of $\dot{E}$ and $\dot{S}$ are needed. From the definitions of the last section, the following relations are obtained

$$\dot{E} = \dot{m}\bar{e} + m\dot{e} \tag{27}$$

$$\dot{S} = \dot{m}\bar{s} + m\dot{s} \tag{28}$$

with $\bar{e}$ and $\bar{s}$ given by Eqs. (2) and (3). Taking the time derivative of Eqs. (1), (2) and (3), yields

$$\frac{\dot{T}}{T} = \frac{\dot{p}}{p} + \frac{\dot{V}}{V} - \frac{\dot{m}}{m} - \frac{\dot{R}}{R} \tag{29}$$

$$\dot{e} = -\dot{x}\Delta\bar{e}_0 - x\Delta\dot{e}_0 + \bar{c}_v \frac{pV}{m\bar{R}} \frac{\dot{T}}{T} + \bar{c}_v\left(\frac{pV}{m\bar{R}} - T_0\right) \tag{30}$$

$$\dot{s} = \dot{x}\Delta\bar{s}_0 + x\Delta\dot{s}_0 + \bar{c}_p \frac{\dot{T}}{T} + \bar{c}_p \ln\frac{pV}{m\bar{R}T_0} - \bar{R}\frac{\dot{p}}{p} - \bar{R}\ln\frac{p}{p_0} \tag{31}$$

Substituting into the energy and entropy balance Equations (25) and (26) and solving for the mass fraction burning rate $\dot{x}$ and the rate of entropy generation by irreversibility $\dot{S}_{irr}$, yields

$$\dot{x} = \frac{pV}{m\Delta\bar{e}_0} \frac{\bar{c}_v}{\bar{R}} \left[\frac{\dot{p}}{p} + \frac{\bar{c}_v + \bar{R}}{\bar{c}_v} \frac{\dot{V}}{V} - \frac{\hat{R}}{\bar{R}} + \frac{\dot{c}_v}{\bar{c}_v}\left(1 - \frac{m\bar{R}T_0}{pV}\right) \right]$$

$$+ \frac{\dot{Q}_w}{m\Delta\bar{e}_0} - \frac{\dot{m}}{m}\left(x + \frac{h_m - e_{u0} + \bar{c}_v T_0}{\Delta\bar{e}_0}\right) - x \frac{\Delta\dot{e}_0}{\Delta\bar{e}_0} \qquad (32)$$

$$\dot{S}_{\text{irr}} = m\dot{x}\Delta\bar{s}_0 + m\bar{c}_p\left[\frac{\bar{c}_p - \bar{R}}{\bar{c}_p} \frac{\dot{p}}{p} + \frac{\dot{V}}{V} - \frac{\hat{R}}{\bar{R}}\left(1 + \frac{\bar{R}}{\bar{c}_p}\ln\frac{p}{p_0}\right) + \frac{\dot{c}_p}{\bar{c}_p}\ln\frac{pV}{m\bar{R}T_0}\right]$$

$$+ \frac{\dot{Q}_w}{T_w} + m x\Delta\dot{s}_0 + \dot{m}\left[x\Delta\bar{s}_0 + s_{u0} - s_m + \bar{c}_p\left(\ln\frac{pV}{m\bar{R}T_0} - 1\right) - \bar{R}\ln\frac{p}{p_0}\right] \qquad (33)$$

If, for example, we assume $\dot{m}=0$ and assume a uniform temperature distribution for the burnt mixture, then Eq. (32) can be shown to be equivalent to the solution of Kreiger and Borman (1966).

It is noteworthy that $\hat{R}$ and $\dot{c}_v$ depend on the value of $\dot{x}$; therefore, Eq. (32) is not "explicitly" solved for $\dot{x}$. Thus, an iterative step by step solution may be required if high accuracy is needed. However, the terms in which $\hat{R}$ and $\dot{c}_v$ appear are generally of at least one order of magnitude smaller than the leading pressure and volume terms. It is also noteworthy that modeling assumptions other than the standard assumptions stated in Section 2 are required only to evaluate $\bar{c}_v$, $\dot{c}_v$, $\bar{c}_p$, $\dot{c}_p$ and $\dot{Q}_w$, T_w, $\dot{m}$, h_m, s_m as discussed in the example of Section 5.

An alternative more useful analytical solution of the energy and entropy balance equations is obtained by integration of Eqs. (25) and (26) from time t' to time t. This yields

$$E - E' = \Delta H_m - \Delta Q_w - \Delta W \qquad (34)$$

$$S - S' = \Delta S_m - \Delta S_w + \Delta S_{\text{irr}} \qquad (35)$$

where

$$\Delta H_m \equiv \int_{t'}^{t} \dot{m}h_m\,dt \qquad (36)$$

$$\Delta Q_w \equiv \int_{t'}^{t} \dot{Q}_w\,dt \qquad (37)$$

$$\Delta W \equiv \int_{t'}^{t} p\dot{V}\,dt \qquad (38)$$

$$\Delta S_m \equiv \int_{t'}^{t} \dot{m}s_m\,dt \qquad (39)$$

$$\Delta S_w \equiv \int_{t'}^{t} \frac{\dot{Q}_w}{T_w}\,dt \qquad (40)$$

$$\Delta S_{\mathrm{irr}} \equiv \int_{t'}^{t} \dot{S}_{\mathrm{irr}}\, dt \tag{41}$$

(note that if T_w is time invariant then $\Delta S_w = \Delta Q_w/T_w$).

Equation (34), combined with Eqs. (2), (15), (16) and corresponding definitions, can be solved for the instantaneous mass fraction of burnt mixture, to yield

$$x(t) = \frac{\Delta Q_w + \Delta W - \Delta H_m + A(t) - A(t') + x(t')B(t')}{B(t)} \tag{42a}$$

where

$$A \equiv \frac{\bar{c}_{vb}}{\bar{R}_b}(pV - mR_u\bar{T}_u) + m\bar{c}_{vu}(\bar{T}_u - T_0) + me_{u0} \tag{42b}$$

and

$$B \equiv m\left[\Delta\bar{e}_0 - (\bar{c}_{vu} - \bar{c}_{vb})T_0 + \left(1 - \frac{R_u\,\bar{c}_{vb}}{\bar{R}_b\,\bar{c}_{vu}}\right)\bar{c}_{vu}\,\bar{T}_u\right] \tag{42c}$$

If, for example, we assume that m, $\bar{R}_b$, $\bar{c}_{vb}$, $\bar{c}_{vu}$ are constant in time, define $\gamma_u \equiv (\bar{c}_{vu} + R_u)/\bar{c}_{vu}$ and $\gamma_b \equiv (\bar{c}_{vb} + \bar{R}_b)/\bar{c}_{vb}$, include the residual burnt gases in the "unburnt" mixture, choose t' such that $x(t') = 0$ and let $p' = p(t')$, $V' = V(t')$ and $\bar{T}_u' = \bar{T}_u(t')$ then we obtain

$$x = \frac{pV - p'V' + (\gamma_b - 1)(W + Q_w) + (\gamma_b - \gamma_u)m\bar{c}_{vu}(\bar{T}_u - \bar{T}_u')}{m\{(\gamma_b - 1)[\Delta\bar{e}_0 - (\bar{c}_{vu} - \bar{c}_{vb})T_0] + (\gamma_b - \gamma_u)\bar{c}_{vu}\bar{T}_u\}} \tag{43}$$

which is Eq. (11) of Lavoie, Heywood, and Keck (1970).

Similarly, Eq. (35), combined with Eqs. (3), (15), (16) and corresponding definitions, can be solved for the total entropy produced by irreversibility between t' and t, to yield

$$\Delta S_{\mathrm{irr}} = \Delta S_w - \Delta S_m + C(t) - C(t') \tag{44a}$$

where

$$C \equiv ms_{u0} + mx\Delta\bar{s}_0 + mx\bar{c}_{pb}\ln\left[\frac{pV}{m\bar{R}_bT_0} - (1 - x)\frac{R_u\bar{T}_u}{\bar{R}_bT_0}\right]$$

$$+ m(1 - x)\bar{c}_{pu}\ln\frac{\bar{T}_u}{T_0} - m(x\bar{R}_b + (1 - x)R_u)\ln\frac{p}{p_0} - m\bar{c}_{pb}x\ln x \tag{44b}$$

5 MASS FRACTION BURNT FROM PRESSURE MEASUREMENTS

The results of Sections 3 and 4 hold for any distribution of temperature and composition within the burnt and unburnt mixtures. Moreover, even the definition of the two mixtures are relatively unspecified. For example, we are free to include the residual burnt gases in either the "unburnt" mixture (thus considering their com-

position as frozen) or in the "burnt" mixture, or even to distribute them among the two mixtures according to some modeling assumption.

As an application of the analysis, we will divide each of the two mixtures into several "zones" and assume that, within each zone, temperature and composition are uniform. Thus, the integrals $\int dx'$ will transform into weighted summations, the weights being the mass fractions of the different zones.

We consider the problem of estimating from measurements of pressure and volume history, the mass fraction of burnt gases as a function of time in a homogeneously charged combustion chamber with no residual burnt fraction.

As an example, we subdivide the gas mixture into the following four zones.

Burnt mixture (2 zones):

1) Fresh charge burnt, at a "core" temperature $T_b{}^0$, composition of equilibrium at $T_b{}^0$ and p, fraction of total mass x_{b0};

2) Fresh charge burnt, at crevice temperature $T_b{}^c$, frozen composition corresponding to equilibrium at $T_y{}^c$ and $p_y{}^c$, fraction of total mass x_{bc}.

Unburnt mixture (2 zones):

3) Fresh charge unburnt, at an "adiabatic core" temperature $T_u{}^0$, composition fixed, fraction of total mass x_{u0};

4) Fresh charge unburnt, at crevice temperature $T_u{}^c$, composition fixed, fraction x_{uc}.

We have clearly assumed that some independent model provides an estimate of the mass fractions x_{bc} and x_{uc}, the temperatures $T_b{}^c$ and $T_u{}^c$, and the composition ($T_y{}^c$, $p_y{}^c$) of gases that are instantaneously present in the crevice regions of the combustion chamber, such as those between piston, piston-ring and cylinder wall.

In this case, Eqs. (18)–(22) become

$$\bar{R}_b = \frac{x_{b0}R_b{}^0 + x_{bc}R_b{}^c}{x_{b0} + x_{bc}} \tag{45}$$

$$\bar{T}_b = \frac{x_{b0}R_b{}^0 T_b{}^0 + x_{bc}R_b{}^c T_b{}^c}{x_{b0}R_b{}^0 + x_{bc}R_b{}^c} \tag{46}$$

$$\bar{T}_u = \frac{x_{u0}T_u{}^0 + x_{uc}T_u{}^c}{x_{u0} + x_{uc}} \tag{47}$$

$$\bar{c}_{vb} = \frac{x_{b0}\displaystyle\int_{T_0}^{T_b{}^0} c_{vb}{}^0(T)\,dT + x_{bc}\displaystyle\int_{T_0}^{T_b{}^U} c_{vb}{}^c(T)\,dT}{(x_{b0} + x_{bc})(\bar{T}_b - T_0)} \tag{48}$$

$$\bar{c}_{vu} = \frac{x_{u0}\displaystyle\int_{T_0}^{T_u{}^0} c_{vu}(T)\,dT + x_{uc}\displaystyle\int_{T_0}^{T_u{}^c} c_{vu}(T)\,dT}{(x_{u0} + x_{uc})(\bar{T}_u - T_0)} \tag{49}$$

where the superscripts 0 and c of $c_{vb}{}^c$ and $c_{vb}{}^c$ refer to the different compositions of zones 1 and 2. Clearly, $x=x_{b0}+x_{bc}$ and $1-x=x_{u0}+x_{uc}$.

We can obtain the "adiabatic core" temperature $T_u{}^0$ by using the isentropic relation

$$d \ln T_u{}^0 = \frac{R_u}{c_{vu}(T_u{}^0)+R_u} \, d \ln p \tag{50}$$

Thus, we can evaluate $\bar{R}_b$ and $\bar{T}_u$ from Eqs. (45) and (47), then use Eq. (15) to find $\bar{T}_b$ (note that Eq. (15) must be always satisfied by any particular assumption that may be adopted), finally obtain $T_b{}^0$ from Eq. (46) and proceed to evaluate $\bar{c}_{vb}$ and $\bar{c}_{vu}$ from Eqs. (48) and (49). At early stages of the combustion process, i.e., for x very close to zero, Eq. (15) cannot be used reliably to estimate $\bar{T}_b$, but $T_b{}^0$ can be assumed to equal the adiabatic flame temperature corresponding to the instantaneous unburnt core temperature $T_u{}^0$.

The instantaneous values of $\bar{R}_b$, $\bar{T}_b$, $\bar{T}_u$, $\bar{c}_{vb}$, $\bar{c}_{vu}$ and $\Delta\bar{e}_0$ may then be used in Eq. (42) to determine the mass fraction burnt x and in Eq. (32) to determine the mass fraction burning rate $\dot{x}$, for the given measurements of pressure and volume history.

Clearly, other modeling assumptions are needed to solve Eqs. (32) and (42). The heat loss $(\dot{Q}_w, T_w)$ at the boundaries of the control volume may be estimated by means of the correlation proposed by Woshni (1967) or by more sophisticated methods, which may include the effect of the cylinder wall thermal boundary layer (cf., Keck, 1981). A model is also needed to determine the instantaneous mass exchange $(\dot{m}, h_m, s_m)$ occurring at the boundaries of the control volume.

6 CONCLUSIONS

A general analytical solution of the energy and entropy balance equations in a combustion chamber has been presented. Among the advantages of this solution, the following are noteworthy:

1) No major approximations were necessary to obtains Eqs. (32), (33), (42) and (44). These equations are valid for arbitrary distributions of temperature and composition within the burnt and unburnt mixtures. Flexibility is a major characteristic of the proposed general solution. A simple set of assumptions has been indicated as a particularly useful example and it has been noted that temperature dependence of the specific heats need not be neglected.

2) The proposed solution is analytical, therefore its implementation requires only trivial numerical techniques. The accuracy and readability of the calculations can be enhanced with respect to conventional methods based on numerical solutions of implicit functional relations. Moreover, the present solution is already in a form suitable for incorporating detailed models of the wall thermal boundary layer, the crevice volumes of the combustion chamber, the mass exchange through the boundaries of the chosen control volume, the nonuniform temperature distribution of the burnt gas mixture, and other similar effects.

3) Equation (32), when solved for the rate of pressure change $\dot{p}$, or Eq. (42), when solved for p, show explicitly the contributions of the different physical effects involved in the combustion process (such as combustion, compression and expansion, heat losses, mass losses, temperature dependence of the specific heats). The equations are

thus useful also as practical and didactical tools to obtain estimates of the relative importance of these effects.

4) Equations (33) and (44) give explicit expressions for the rate of entropy production and the total entropy produced by irreversibility inside the combustion chamber of internal combustion engines. The equations are thus useful also as practical tools for the availability analysis of these important energy conversion devices.

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