

General Thermodynamic Analysis for Engine Combustion Modeling

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ABSTRACT

The energy and entropy balance equations in an open control volume are treated analytically by a method that can be applied to any level of modeling (zero-dimensional, quasi-dimensional, and multi-dimensional) of any internal combustion engine (homogeneous-charge, stratified-charge, direct-injection, Diesel, adiabatic, ...). The method involves no major assumptions and is, therefore, compatible with any detailed model for physical effects such as liquid fuel atomization and vaporization, heat transfer within the combustion chamber and through its walls, mass transfer (convective and diffusive) within the combustion chamber, with crevice regions, with prechambers, and through the inlet and exhaust ports, temperature, composition, and pressure nonuniformities, and so on. The result is in the form of differential equations for the instantaneous mass fraction of burnt gas mixture and for the entropy generated by irreversibility within the chosen control volume, in terms of the pressure and volume histories and appropriately defined mean variables. The choice of control volume may range from the entire combustion chamber (zero-dimensional approach) to a single mesh point in a numerical solution scheme of the differential local balance equations of mass, chemical species, energy and entropy, coupled with some closure scheme to model diffusion, viscosity, heat conduction and chemical kinetics (multi-dimensional approach). Irrespective of the level of detail of the chosen modeling approach, the entropy balance equation provides an interesting and useful, though very seldom exploited, independent relation to check the consistency of any set of additional modeling assumptions or closure scheme with the second law requirement of nonnegativity of the local and global rate of entropy production by irreversibility.

1. INTRODUCTION

The purpose of this paper is to present a general method for the thermodynamic analysis of a combustible mixture contained in an open control volume, with applications in engine combustion modeling. The method is an extension of that discussed by Beretta and Keck [1] for homogeneous charge internal combustion engines, and has similar characteristic features of generality, flexibility and immediate applicability. Depending on the choice of the control volume, it displays explicitly the local or global dependence of the mass fraction burnt, and the rate of entropy generation by irreversibility, on the various physical effects occurring locally or globally in an engine combustion chamber.

By defining appropriate mean variables, the energy and entropy balance equations are manipulated analytically without making major assumptions. Thus, any additional modeling assumption concerning temperature and composition distributions of the combustible two-phase mixture, including all the approximations that have been considered in the literature [2-18], may be incorporated with only minor modifications, none of which is in the general equations. The flexibility of the method is obtained by an especially efficacious scheme used to label different gas or liquid elements in the chosen control volume at every instant in time.

For either modeling (zero-dimensional, quasi-dimensional, or multi-dimensional) or diagnostic purposes, the problem of interrelating the instantaneous mass fraction of burnt gases

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and the combustion chamber pressure and volume histories, is the typical application of the energy balance equation. To this end, the latter must be complemented by a set of modeling assumptions to account for such effects as fuel distribution after injection and vaporization, wall heat transfer, mass exchange with crevice volumes or through the boundaries of the chosen control volume, nonuniform distributions in temperature and composition, and so on.

The additional independent condition that the rate of entropy production by irreversibility must be nonnegative at every instant in time, is an interesting, useful and seldom exploited practical application of the entropy balance equation. It provides an independent check for the consistency of a given set of modeling assumptions adopted as a closure scheme.

The paper is organized as follows. Definitions and assumptions are discussed in Section 2, the thermodynamic-state method of description in Section 3, the energy and entropy balance equations and the resulting differential equations for the fraction of burnt gases and the entropy generated by irreversibility in Section 4, details of a possible multi-zone quasi-dimensional application of the analysis in Section 5, details of a multi-dimensional modeling application in Section 6, and conclusions in Section 7.

2. SYSTEM DEFINITION AND ASSUMPTIONS

The object of study is an open system composed of a combustible mixture inside a variable control volume. For example, the control volume could coincide with the combustion chamber of an internal combustion engine. Again, for more detailed descriptions, it could coincide with a subregion of the combustion chamber. As combustion takes place, the mixture of reactants is transformed into a gas mixture of products of combustion (referred to as the "burnt mixture," subscript b). The mixture of reactants is composed of an unburnt gas mixture (subscript u) and a liquid phase (subscript l).

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.

The second assumption is that the pressure p is uniform throughout the chosen control volume. As pressure waves travel at the speed of sound in the mixture, local pressure nonuniformities last a negligible time when compared to the characteristic time of the other rate processes. If pressure nonuniformities cannot be neglected (strong permanent swirl inside the combustion chamber, oscillating pressure waves due to the "knock" phenomenon), the present analysis can still be applied provided the combustion chamber

The third assumption is that the burnt and unburnt gas mixtures behave as Gibbs-Dalton mixtures of ideal semi-perfect gases (i.e., with temperature dependent specific heats). The composition of both the unburnt and the burnt gas mixtures will not be assumed to remain either fixed or uniform, whereas the composition of the liquid phase will be assumed to remain fixed at all times. The assumption made in Reference 1 of fixed unburnt gas mixture composition, which restricted the applicability of that analysis to homogeneous charge engines, has been dropped so as to include effects such as charge stratification and unburnt gas mixture nonuniformities that are important in a broader class of applications, e.g., stratified charge, multichamber and Diesel engines, and are essential for the application to multi-dimensional models.

Our last assumption is that the liquid fuel inside the combustion chamber behaves as an incompressible fluid so that specific volume, energy and entropy depend on temperature only.

3. THERMODYNAMIC STATE OF THE MIXTURE

To characterize the thermodynamic state of the mixture inside the control volume at every instant in time t , let $x(t)$ be the instantaneous mass fraction of the burnt gas mixture, $f(t)$ the instantaneous mass fraction of liquid fuel, $m(t)$ the total instantaneous mass of the gas and liquid elements in the control volume and $p(t)$ the instantaneous (locally) uniform pressure.

An important role is played in our analysis by the method adopted to label and account for gas or liquid elements that differ in temperature and/or chemical composition. At each instant in time, a continuous variable x' labels all the elements in the control volume. Values of x' between 0 and $x(t)$ correspond to gas elements with a burnt composition. Values of x' between $x(t)$ and $1-f(t)$ correspond to gas elements with an unburnt composition. Values of x' between $1-f(t)$ and 1 correspond to liquid fuel elements. The fraction of total mass in the control volume contributed by gas or liquid elements between x' and $x'+dx'$ is dx' .

It is noteworthy that the labeling scheme and the following analysis and results require no assumptions regarding the spatial distribution of burnt, unburnt and liquid fuel particles within the control volume. Therefore, our results are compatible with any measured, computed, or assumed spatial distribution.

No assumptions are made regarding the composition and temperature distributions of the burnt and unburnt gas elements, and the temperature distribution of the liquid fuel elements. Thus, our results are compatible with any measurement, computation, or assumption regarding such distributions, as exemplified in Sections 5 and 6.

INSTANTANEOUS VOLUME

The mean specific volume is

$$\bar{v}(t) = \frac{V(t)}{m(t)} = \frac{V_b(t) + V_u(t) + V_l(t)}{m(t)} \quad (1)$$

where V represents the total volume (of the chosen control volume). Denoting the specific volumes by v , we have

$$\begin{aligned} \bar{v}(t) = & \int_0^{x(t)} v_b(x',t) dx' + \int_{x(t)}^{1-f(t)} v_u(x',t) dx' \\ & + \int_{1-f(t)}^1 v_l(x',t) dx' \quad (2) \end{aligned}$$

We now define the following mean variables

$$\bar{R}_b(t) = \frac{1}{x(t)} \int_0^{x(t)} R_b(x',t) dx' \quad (3)$$

$$\bar{R}_u(t) = \frac{1}{1-f(t)-x(t)} \int_{x(t)}^{1-f(t)} R_u(x',t) dx' \quad (4)$$

$$\bar{v}_l(t) = \frac{1}{f(t)} \int_{1-f(t)}^1 v_l(x',t) dx' \quad (5)$$

where $R_b = R/M_b$, $R_u = R/M_u$, M_b and M_u are the molecular weights and R is the universal gas constant. Let $\alpha(T) = (1/v)(dv/dT)$ be the coefficient of thermal expansion of the liquid fuel (cf., e.g., Reference 19). Denoting by T_{l0} a reference temperature and by v_{l0} the corresponding reference specific volume, we have

$$\bar{v}_l(t) = \frac{v_{l0}}{f(t)} \int_{1-f(t)}^1 [\exp \int_{T_{l0}}^{T_l(x',t)} \alpha(T) dT] dx' \quad (6)$$

We now define

$$\bar{R}(t) = x(t)\bar{R}_b(t) + [1-f(t)-x(t)]\bar{R}_u(t) \quad (7)$$

$$\bar{T}_b(t) = \frac{1}{x(t)\bar{R}_b(t)} \int_0^{x(t)} R_b(x',t) T_b(x',t) dx' \quad (8)$$

$$\bar{T}_u(t) = \frac{1}{[1-f(t)-x(t)]\bar{R}_u(t)} \int_{x(t)}^{1-f(t)} R_u(x',t) T_u(x',t) dx' \quad (9)$$

$$\bar{T}_l(t) = \frac{1}{f(t)} \int_{1-f(t)}^1 T_l(x',t) dx' \quad (10)$$

$$\bar{T}_g(t) = \frac{x(t)\bar{R}_b(t)\bar{T}_b(t) + [1-f(t)-x(t)]\bar{R}_u(t)\bar{T}_u(t)}{[1-f(t)]\bar{R}(t)} \quad (11)$$

$$\bar{T}(t) = \frac{[1-f(t)]\bar{R}(t)\bar{T}_g(t) + f(t)p(t)\bar{v}_l(t)}{\bar{R}(t)} \quad (12)$$

With the definitions above, Equation 1 becomes

$$\bar{v}(t) = \frac{V(t)}{m(t)} = \frac{\bar{R}(t)\bar{T}(t)}{p(t)} \quad (13)$$

INSTANTANEOUS ENERGY

The mean specific energy is

$$\bar{e}(t) = \frac{E(t)}{m(t)} = \frac{E_b(t) + E_u(t) + E_l(t)}{m(t)} \quad (14)$$

where E represents the total energy in the chosen control volume. Denoting the specific energy by e , we have

$$\begin{aligned} \bar{e}(t) = & \int_0^{x(t)} e_b(x',t) dx' + \int_{x(t)}^{1-f(t)} e_u(x',t) dx' \\ & + \int_{1-f(t)}^1 e_l(x',t) dx' \quad (15) \end{aligned}$$

where

$$e_b(x',t) = e_{b0}(x',t) + \int_{T_{b0}}^{T_b(x',t)} c_{vb}(T,x',t) dT \quad (16)$$

$$e_u(x',t) = e_{u0}(x',t) + \int_{T_{u0}}^{T_u(x',t)} c_{vu}(T,x',t) dT \quad (17)$$

$$e_l(x',t) = e_{l0} + \int_{T_{l0}}^{T_l(x',t)} c_l(T) dT \quad (18)$$

c_{vu} and c_{vb} are the specific heats at constant volume of the gases, c_l is the specific heat of the liquid fuel and e_{b0} , e_{u0} and e_{l0} are the reference specific energies corresponding to the reference temperatures T_{b0} , T_{u0} and T_{l0} . The choice of three different reference temperatures can be useful in the calculation of the integrals in Equations 16, 17 and 18. We note that c_{vb} and c_{vu} depend on T which is the variable of integration, on x' because of differences in chemical composition between elements, and on

time, whereas c_l depends only on T because all liquid elements are assumed to have the same composition which is independent of time. We now define

$$\bar{e}_{bo}(t) = \frac{1}{x(t)} \int_0^{x(t)} e_{bo}(x',t) dx' \quad (19)$$

$$\bar{e}_{uo}(t) = \frac{1}{1-f(t)-x(t)} \int_{x(t)}^{1-f(t)} e_{uo}(x',t) dx' \quad (20)$$

$$\begin{aligned} \bar{e}_o(t) &= x(t)\bar{e}_{bo}(t) + f(t)e_{lo} \\ &+ [1-f(t)-x(t)]\bar{e}_{uo}(t) \end{aligned} \quad (21)$$

$$\bar{c}_{vb}(t) = \frac{\int_0^{x(t)} \int_{T_{bo}}^{T_b(x',t)} c_{vb}(T,x',t) dT dx'}{x(t)[\bar{T}_b(t) - T_{bo}]} \quad (22)$$

$$\bar{c}_{vu}(t) = \frac{\int_{x(t)}^{1-f(t)} \int_{T_{uo}}^{T_u(x',t)} c_{vu}(T,x',t) dT dx'}{[1-f(t)-x(t)][\bar{T}_u(t) - T_{uo}]} \quad (23)$$

$$\bar{c}_{vl}(t) = \frac{\int_{1-f(t)}^1 \int_{T_{lo}}^{T_l(x',t)} c_l(T) dT dx'}{f(t)[\bar{T}_l(t) - T_{lo}]} \quad (24)$$

$$\begin{aligned} \bar{c}_v(t)[\bar{T}(t)-T_o] &= x(t)\bar{c}_{vb}(t)[\bar{T}_b(t)-T_{bo}] \\ &+ [1-f(t)-x(t)]\bar{c}_{vu}(t)[\bar{T}_u(t)-T_{uo}] \\ &+ f(t)\bar{c}_{vl}(t)[\bar{T}_l(t)-T_{lo}] \end{aligned} \quad (25)$$

where T_o is another arbitrary reference temperature. Equation 14 then becomes

$$\bar{e}(t) = \bar{e}_o(t) + \bar{c}_v(t)[\bar{T}(t) - T_o] \quad (26)$$

INSTANTANEOUS ENTROPY

The mean specific entropy is

$$\bar{s}(t) = \frac{S(t)}{m(t)} = \frac{S_b(t) + S_u(t) + S_l(t)}{m(t)} \quad (27)$$

where S represents the total entropy in the chosen control volume. Denoting the specific entropy by s we have

$$\begin{aligned} \bar{s}(t) &= \int_0^{x(t)} s_b(x',t) dx' + \int_{x(t)}^{1-f(t)} s_u(x',t) dx' \\ &+ \int_{1-f(t)}^1 s_l(x',t) dx' \end{aligned} \quad (28)$$

where

$$\begin{aligned} s_b(x',t) &= s_{bo}(x',t) + \int_{T_{bo}}^{T_b(x',t)} c_{pb}(T,x',t) \frac{dT}{T} \\ &- R_b(x',t) \ln \frac{p(t)}{p_o} \end{aligned} \quad (29)$$

$$\begin{aligned} s_u(x',t) &= s_{uo}(x',t) + \int_{T_{uo}}^{T_u(x',t)} c_{pu}(T,x',t) \frac{dT}{T} \\ &- R_u(x',t) \ln \frac{p(t)}{p_o} \end{aligned} \quad (30)$$

$$s_l(x',t) = s_{lo} + \int_{T_{lo}}^{T_l(x',t)} c_l(T) \frac{dT}{T} \quad (31)$$

p_o is an arbitrary reference pressure and c_p denotes the specific heat at constant pressure. As already noted, the values of the specific heats vary from element to element because of differences in their chemical composition. We now define

$$\bar{s}_{bo}(t) = \frac{1}{x(t)} \int_0^{x(t)} s_{bo}(x',t) dx' \quad (32)$$

$$\bar{s}_{uo}(t) = \frac{1}{1-f(t)-x(t)} \int_{x(t)}^{1-f(t)} s_{uo}(x',t) dx' \quad (33)$$

$$\begin{aligned} \bar{s}_o(t) &= x(t)\bar{s}_{bo}(t) + f(t)s_{lo} \\ &+ [1-f(t)-x(t)]\bar{s}_{uo}(t) \end{aligned} \quad (34)$$

$$\bar{c}_{pb}(t) = \frac{\int_0^{x(t)} \int_{T_{bo}}^{T_b(x',t)} c_{pb}(T,x',t) \frac{dT}{T} dx'}{x(t) \ln[\bar{T}_b(t)/T_{bo}]} \quad (35)$$

$$\bar{c}_{pu}(t) = \frac{\int_{x(t)}^{1-f(t)} \int_{T_{uo}}^{T_u(x',t)} c_{pu}(T,x',t) \frac{dT}{T} dx'}{[1-f(t)-x(t)] \ln[\bar{T}_u(t)/T_{uo}]} \quad (36)$$

$$\bar{c}_{p\ell}(t) = \frac{\int_{1-f(t)}^1 \int_{T_{\ell o}}^{T_{\ell}(x',t)} c_{\ell}(T) \frac{dT}{T} dx'}{f(t) \ln[\bar{T}_{\ell}(t)/T_{\ell o}]} \quad (37)$$

$$\begin{aligned} \bar{c}_p(t) \ln \frac{\bar{T}(t)}{T_o} &= x(t) \bar{c}_{pb}(t) \ln \frac{\bar{T}_b(t)}{T_{bo}} \\ &+ [1-f(t)-x(t)] \bar{c}_{pu}(t) \ln \frac{\bar{T}_u(t)}{T_{uo}} \\ &+ f(t) \bar{c}_{p\ell}(t) \ln \frac{\bar{T}_{\ell}(t)}{T_{\ell o}} \end{aligned} \quad (38)$$

Equation 27 then becomes

$$\bar{s}(t) = \bar{s}_o(t) + \bar{c}_p(t) \ln \frac{\bar{T}(t)}{T_o} - \bar{R}(t) \ln \frac{p(t)}{p_o} \quad (39)$$

Next, we define

$$\Delta \bar{e}_{go}(t) = \bar{e}_{uo}(t) - \bar{e}_{bo}(t) \quad (40)$$

$$\Delta \bar{e}_{\ell o}(t) = e_{\ell o} - \bar{e}_{uo}(t) \quad (41)$$

$$\Delta \bar{s}_{go}(t) = \bar{s}_{bo}(t) - \bar{s}_{uo}(t) \quad (42)$$

$$\Delta \bar{s}_{\ell o}(t) = \bar{s}_{uo}(t) - s_{\ell o} \quad (43)$$

so that Equations 21 and 34 become

$$\bar{e}_o(t) = \bar{e}_{uo}(t) - x(t) \Delta \bar{e}_{go}(t) + f(t) \Delta \bar{e}_{\ell o}(t) \quad (44)$$

$$\bar{s}_o(t) = \bar{s}_{uo}(t) + x(t) \Delta \bar{s}_{go}(t) - f(t) \Delta \bar{s}_{\ell o}(t) \quad (45)$$

The definitions in this section allow the representation of the mixture in the control volume by means of an equivalent "quasi-ideal gas" at pressure $p(t)$, temperature $\bar{T}(t)$ and specific gas constant $\bar{R}(t)$. In fact, the equation of state $p(t)V(t) = m(t)\bar{R}(t)\bar{T}(t)$ holds by virtue of such definitions. However, the artifice is 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}_p and \bar{c}_v since $\bar{c}_p - \bar{c}_v \neq \bar{R}$.

The "quasi-ideal gas" representation appears to be convenient despite the presence of the

liquid phase. In fact, under Diesel operating conditions, the effect of the liquid phase is not dominating, so much that it is often assumed in the literature that liquid fuel vaporizes immediately after injection, i.e., with our notation, that $f(t) = 0$ (cf., e.g., Reference [13]).

The values of the thermophysical properties can be found, for example, in References 19 and 21 to 24. These include properties of liquid and gaseous fuels, air, combustion products and correlations for these properties. Reference 25 describes a useful methodology to obtain approximate relationships for combustion products. It has been applied in the context of the present approach in Reference 26.

In what follows, the dependence on t will be dropped unless its explicit appearance is required for clarity.

4. ENERGY AND ENTROPY BALANCE EQUATIONS

In this section the energy and entropy balance equations are manipulated analytically in terms of the quantities just defined. Let the control volume under study be open to a mass flux \dot{m} (positive if inward) of mean specific enthalpy h_m and mean specific entropy s_m . For example, in zero-dimensional studies 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 prechambers and the crevice regions between piston, piston-ring and cylinder wall (if not included in the control volume), and due to injected fuel entering the volume. Again, for multi-dimensional models, the control volume may correspond to a mesh point in a numerical approximation scheme. Detailed expressions for h_m and s_m in this case are given in Section 6.

The energy and entropy balance equations are

$$\dot{E} = \dot{m}h_m - \dot{Q}_w - p\dot{V} \quad (46)$$

$$\dot{S} = \dot{m}s_m - \frac{\dot{Q}_w}{T_w} + \dot{S}_{irr} \quad (47)$$

where \dot{Q}_w is the rate of heat loss through the surface of the control volume, T_w is a properly defined mean temperature of the surface of the control volume (cf. Section 6), 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 use the balance equations, the explicit expressions of \dot{E} and \dot{S} are needed. From the definitions of the last section, we obtain

$$\dot{E} = \dot{m}\bar{e} + m\dot{\bar{e}} \quad (48)$$

$$\dot{S} = \dot{m}\bar{s} + m\dot{\bar{s}} \quad (49)$$

where \bar{e} and \bar{s} are given by Equations 26 and 39. Taking the time derivative of Equations 13, 26 and 39, yields

$$\frac{\dot{T}}{T} = \frac{\dot{p}}{p} + \frac{\dot{V}}{V} - \frac{\dot{m}}{m} - \frac{\dot{R}}{R} \quad (50)$$

$$\dot{e} = \dot{e}_o + \bar{c}_v \frac{pV}{mR} \frac{\dot{T}}{T} + \bar{c}_v \left(\frac{pV}{mR} - T_o \right) \quad (51)$$

$$\dot{s} = \dot{s}_o + \bar{c}_p \frac{\dot{T}}{T} + \bar{c}_p \ln \frac{pV}{mRT_o} - \bar{R} \frac{\dot{p}}{p} - \bar{R} \ln \frac{p}{p_o} \quad (52)$$

the time derivatives of \bar{e}_o and \bar{s}_o are obtained by taking the time derivative of Equations 44 and 45. Substituting into the energy and entropy balance Equations 46 and 47 and solving for the mass fraction burning rate \dot{x} and the rate of entropy generation by irreversibility \dot{S}_{irr} , yields

$$\begin{aligned} \dot{x} = & \frac{pV}{m\Delta\bar{e}_{go}} \frac{\bar{c}_v}{\bar{R}} \left[\frac{\dot{p}}{p} + \frac{\bar{c}_v + \bar{R}}{\bar{c}_v} \frac{\dot{V}}{V} - \frac{\dot{R}}{R} + \frac{\bar{c}_v}{\bar{c}_v} \left(1 - \frac{mRT_o}{pV} \right) \right] \\ & + \frac{\dot{Q}_w}{m\Delta\bar{e}_{go}} - \frac{\dot{m}}{m} \left[x + \frac{h_m \bar{e}_{uo} + \bar{c}_v T_o}{\Delta\bar{e}_{go}} - f \frac{\Delta\bar{e}_{\ell o}}{\Delta\bar{e}_{go}} \right] \\ & - x \frac{\dot{\Delta\bar{e}_{go}}}{\Delta\bar{e}_{go}} + (1-f) \frac{\dot{\bar{e}_{uo}}}{\Delta\bar{e}_{go}} + f \frac{\dot{\Delta\bar{e}_{\ell o}}}{\Delta\bar{e}_{go}} \quad (53) \end{aligned}$$

$$\begin{aligned} \dot{S}_{irr} = & m\bar{c}_p \left[\frac{\bar{c}_p - \bar{R}}{\bar{c}_p} \frac{\dot{p}}{p} + \frac{\dot{V}}{V} - \frac{\dot{R}}{R} \left(1 + \frac{\bar{R}}{\bar{c}_p} \ln \frac{p}{p_o} \right) + \frac{\bar{c}_p}{\bar{c}_p} \ln \frac{pV}{mRT_o} \right] \\ & + m\dot{x}\Delta\bar{s}_{go} + \frac{\dot{Q}_w}{T_w} + m \left[x\dot{\Delta\bar{s}}_{go} + (1-f)\dot{\bar{s}}_{uo} - f\dot{\Delta\bar{s}}_{\ell o} \right] \\ & + m \left[x\dot{\Delta\bar{s}}_{go} + \dot{\bar{s}}_{uo} - \dot{s}_m + \bar{c}_p \left(\ln \frac{pV}{mRT_o} - 1 \right) \right. \\ & \left. - \bar{R} \ln \frac{p}{p_o} - f\Delta\bar{s}_{\ell o} \right] \quad (54) \end{aligned}$$

It is noteworthy that the time derivatives of \bar{R} , \bar{c}_v , $\Delta\bar{e}_{go}$ and $\Delta\bar{e}_{\ell o}$ depend on the value of \dot{x} . Therefore, differential Equation 53 is not in its normal form (a similar comment holds for differential Equation 54). However, the terms in which the time derivatives of \bar{R} and \bar{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 to evaluate \bar{c}_v , \bar{c}_p , their time derivatives, and \dot{Q}_w , T_w , \dot{m} , h_m , s_m as discussed in the example of Section 5.

As a consequence of the second law of thermodynamics, \dot{S}_{irr} must be nonnegative at every instant in time. This requirement provides a useful independent check of the consistency of any particular set of additional modeling assumptions adopted to close the problem.

An alternative more useful analytical rearrangement of the energy and entropy balance equations is obtained by integrating Equations 46 and 47 from time t' to time t

$$E - E' = H_m - Q_w - W \quad (55)$$

$$S - S' = S_m - S_w + \Delta S_{irr} \quad (56)$$

where

$$H_m = \int_{t'}^t \dot{m} h_m dt \quad (57)$$

$$Q_w = \int_{t'}^t \dot{Q}_w dt \quad (58)$$

$$W = \int_{t'}^t pV dt \quad (59)$$

$$S_m = \int_{t'}^t \dot{m} s_m dt \quad (60)$$

$$S_w = \int_{t'}^t \frac{\dot{Q}_w}{T_w} dt \quad (61)$$

$$\Delta S_{irr} = \int_{t'}^t \dot{S}_{irr} dt \quad (62)$$

Equation 55, combined with our definitions in Section 3, can be solved for the instantaneous mass fraction of burnt mixture, to yield

$$x(t) = \frac{Q_w + W - H_m + A(t) - A(t') + x(t')B(t')}{B(t)} \quad (63a)$$

where

$$A = \frac{\bar{c}_{vb}}{\bar{R}_b} [pV - m(1-f)\bar{R}_u\bar{T}_u - mf\bar{p}v_\ell] + m(\bar{e}_{uo} + f\Delta\bar{e}_{\ell o}) + m[(1-f)\bar{c}_{vu}(\bar{T}_u - T_{uo}) + f\bar{c}_{v\ell}(\bar{T}_\ell - T_{\ell o})] \quad (63b)$$

$$B = m[\Delta\bar{e}_{go} + \bar{c}_{vb}T_{bo} - \bar{c}_{vu}T_{uo} + (1 - \frac{\bar{R}_u\bar{c}_{vb}}{\bar{R}_b\bar{c}_{vu}})\bar{c}_{vu}\bar{T}_u]. \quad (63c)$$

Similarly, Equation 56 yields

$$\Delta S_{irr} = S_w - S_m + C(t) - C(t') \quad (64a)$$

where

$$C = m\bar{x}\bar{c}_{pb} \ln\left[\frac{pV}{m\bar{R}_bT_{bo}} - (1-f-x)\frac{\bar{R}_u\bar{T}_u}{\bar{R}_bT_{bo}} - f\frac{\bar{p}v_\ell}{\bar{R}_bT_{bo}}\right] + m(\bar{s}_{uo} + x\Delta\bar{s}_{go} - f\Delta\bar{s}_{\ell o} - \bar{c}_{pb}x\ln x) + m(1-f-x)\bar{c}_{pu} \ln\frac{\bar{T}_u}{T_{uo}} + mf\bar{c}_{p\ell} \ln\frac{\bar{T}_\ell}{T_{\ell o}} - m[x\bar{R}_b + (1-f-x)\bar{R}_u] \ln\frac{p}{p_o} \quad (64b)$$

We see that when f goes to zero and the unburnt mixture has a uniform fixed composition (i.e., \bar{e}_{uo} and \bar{s}_{uo} are constant in time), Equations 63 and 64 reduce to Equations 42 and 44 of Reference 1.

5. MULTI-ZONE QUASI-DIMENSIONAL APPLICATION: MASS FRACTION BURNT FROM PRESSURE MEASUREMENTS

The results of Section 4 hold for any distribution of temperature and composition within the burnt and unburnt mixtures. Moreover, even the definition of the mixtures is relatively unspecified. For example, we are free to consider the case of liquid fuel injection or of premixed gaseous fuel and air, to include the residual burnt gases in either the burnt or the unburnt mixture, or even to distribute them among the two, according to some modeling scheme.

As an application of the analysis, we will 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 Diesel combustion chamber with no residual burnt fraction (a similar application for the case of a homogeneous-charge spark-ignition engine is discussed in Reference 1).

We let the control volume coincide with the walls of the combustion chamber and assume that it can be subdivided into several zones within which 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 assume the following subdivision.

Burnt Mixture (2 zones):

a. Fresh charge burnt, at a core temperature T_b^O , composition of equilibrium at T_b^O and p , fraction of total mass x_b^O .

b. 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_b^C .

Unburnt Mixture (N+2 zones):

c. Liquid fuel at temperature T_ℓ^O , specific volume v_ℓ^O , fraction of total mass f .

d. N gaseous zones with increasing fuel concentrations, each with uniform composition and temperature. For the i -th zone, the gaseous fuel concentration will be denoted by C_i , the uniform temperature by T_i and the mass fraction by x_i .

e. Fresh charge unburnt, at crevice temperature T_u^C , fraction of total mass x_u^C . The fuel concentration in this zone is assumed to be equal to $(\sum_i x_i C_i) / (\sum_i x_i)$.

We have

$$x = x_b^O + x_b^C \quad (65)$$

$$1 - f - x = \sum_i x_i + x_u^C \quad (66)$$

Moreover, the definitions of the mean variables given in Section 3 become

$$\bar{R}_b = \frac{x_b^O R_b^O + x_b^C R_b^C}{x_b^O + x_b^C} \quad (67)$$

$$\bar{R}_u = \frac{\sum_i x_i R_u^i + x_u^C R_u^C}{\sum_i x_i + x_u^C} \quad (68)$$

$$\bar{T}_b = \frac{x_b^O R_b^O T_b^O + x_b^C R_b^C T_b^C}{x_b^O R_b^O + x_b^C R_b^C} \quad (69)$$

$$\bar{T}_u = \frac{\sum_i x_i R_u^i T_i + x_u^c R_u^c T_u^c}{\sum_i x_i R_u^i + x_u^c R_u^c} \quad (70)$$

$$\bar{T}_l = T_l^o \quad \text{and} \quad \bar{v}_l = v_l^o \quad (71)$$

$$\bar{e}_{bo} = \frac{x_b^o e_{bo}^o + x_b^c e_{bo}^c}{x_b^o + x_b^c} \quad (72)$$

$$\bar{e}_{uo} = \frac{\sum_i x_i e_{uo}^i + x_u^c e_{uo}^c}{\sum_i x_i + x_u^c} \quad (73)$$

$$\bar{c}_{vb} = \frac{x_b^o \int_{T_{bo}}^{T_{bo}^o} c_{vb}^o(T) dT + x_b^c \int_{T_{bo}}^{T_{bo}^c} c_{vb}^c(T) dT}{(x_b^o + x_b^c)(\bar{T}_b - T_{bo})} \quad (74)$$

$$\bar{c}_{vu} = \frac{\sum_i x_i \int_{T_{uo}}^{T_{uo}^i} c_{vu}^i(T) dT + x_u^c \int_{T_{uo}}^{T_{uo}^c} c_{vu}^c(T) dT}{(\sum_i x_i + x_u^c)(\bar{T}_u - T_{uo})} \quad (75)$$

$$\bar{c}_{vl} = \frac{\int_{T_{lo}}^{T_{lo}^o} c_l(T) dT}{T_{lo}^o - T_{lo}} \quad (76)$$

As a possible iterative step by step solution scheme, we consider the following. We first define the set $\underline{\alpha}$ of variables

$$\underline{\alpha} = \{x_b^c, R_b^c, T_b^c, T_y^c, p_y^c; T_l^o, v_l^o, f; x_i, R_u^i, T_i; R_u^c, T_u^c; m; Q_w\}.$$

To close the problem, enough additional independent models are needed so that $\underline{\alpha}$ can be evaluated whenever the values of all the variables of the problem (not only those in $\underline{\alpha}$) are known. The problem of estimating the liquid fuel fraction f and the rate of liquid fuel vaporization is discussed, e.g., in References 20 and 27 to 31. The heat loss \dot{Q}_w to the combustion chamber walls can be estimated using the correlation proposed by Woschni [32] or by more sophisticated methods (cf., e.g., Keck [33]).

Assuming that enough such models are available, a step by step solution scheme starting from an instant in time, t , at which all the variables of the problem have known values (and $x \neq 0$), would be to first evaluate $\underline{\alpha}(t+dt) = \underline{\alpha}(t) + \dot{\underline{\alpha}}(t)dt$ and then use Equation 53 to find a first estimate of $x(t+dt)$, namely, $x(t+dt) = x(t)$

+ $\dot{x}(t)dt$. With these estimates at time $t+dt$, we would estimate the following variables (the sequence in which equations are used is important): x_b^o and x_u^c (Equations 65 and 66), \bar{R}_b and \bar{R}_u (Equations 67 and 68), \bar{T}_u (Equation 70), \bar{T}_b (Equations 11 to 13, using the instantaneous measured values of p and V), T_b^o (Equation 69) and \bar{e}_{bo} , \bar{e}_{uo} , \bar{c}_{vb} , \bar{c}_{vu} and \bar{c}_{vl} (Equations 72 to 76). With these estimates we can finally use Equation 63 to find an improved estimate for $x(t+dt)$. The sequence above could then be repeated to refine the estimate. Before proceeding to the next step in time, we must use the data at times t and $t+dt$ to estimate the values of \bar{c}_v , \bar{R} , \bar{e}_{uo} , Δe_{go} and their time derivatives for subsequent use in Equation 53.

When $x = 0$ or $x \ll 1$, the estimate of T_b^o through the direct use of Equations 11 to 13 is critical and could be substituted with an estimate based on setting T_b^o approximately equal to the adiabatic flame temperature corresponding to a mean unburnt temperature and composition. It is noteworthy that the value of T_b^o enters the final Equation 63 only through the value of \bar{c}_{vb} given by Equation 74.

6. MULTI-DIMENSIONAL MODELING APPLICATION

As repeatedly stated, our thermodynamic analysis, method and results are applicable not only to zero-dimensional or quasi-dimensional engine combustion models but to multi-dimensional models as well [34-35]. In this section, we give explicit expressions for h_m and s_m (cf. Section 4) for a control volume represented, for example, by a mesh point in a numerical solution scheme of the general differential equations expressing the local balances of mass, chemical species, momentum, energy and entropy.

Using the notation in Reference 34, the instantaneous local balance equations are

$$\partial \rho / \partial t + \nabla \cdot (\rho \underline{u}) = 0 \quad (77)$$

$$\partial (\rho Y_i) / \partial t + \nabla \cdot [\rho Y_i (\underline{u} + \underline{u}_i)] = w_i \quad (78)$$

$$\partial (\rho \underline{u}) / \partial t + \nabla \cdot (\rho \underline{u} \underline{u}) + \nabla p + \nabla \cdot \underline{\sigma} = 0 \quad (79)$$

$$\begin{aligned} \partial (\rho e + \rho u^2 / 2) / \partial t + \nabla \cdot [(\rho e + \rho u^2 / 2) \underline{u} + p \underline{u} + \underline{u} \cdot \underline{\sigma}] \\ + \sum_i \nabla \cdot (\rho Y_i h_i \underline{u}_i) + \nabla \cdot (-\lambda \nabla T) = 0 \end{aligned} \quad (80)$$

$$\begin{aligned} \partial (\rho s) / \partial t + \nabla \cdot (\rho s \underline{u}) + \sum_i \nabla \cdot (\rho Y_i s_i \underline{u}_i) \\ + \nabla \cdot [-(\lambda \nabla T) / T] = \dot{s}_{irr} \geq 0 \end{aligned} \quad (81)$$

Equation 80, combined with Equations 77 and 79, may be rearranged to yield

$$\partial(\rho e)/\partial t + \nabla \cdot (\rho h \underline{u}) + \sum_i \nabla \cdot (\rho Y_i h_i \underline{u}_i) - \underline{u} \cdot \nabla p - \phi + \nabla \cdot (-\lambda \nabla T) = 0 \quad (82)$$

In Equations 77 to 82, ρ is the local bulk density, \underline{u} is the local bulk velocity vector, Y_i is the local mass fraction of species i ($\sum_i Y_i = 1$), \underline{u}_i is the local diffusion velocity vector of species i superimposed to the bulk velocity \underline{u} ($\sum_i Y_i \underline{u}_i = 0$), w_i is the local chemical rate of production of mass of species i per unit volume ($\sum_i w_i = 0$), p is the local static pressure, \underline{g} is the deviatoric or viscosity shear tensor including second viscosity, e is the local bulk specific internal energy ($e = \sum_i Y_i e_i$), e_i is the local specific internal energy of species i , h is the local bulk specific enthalpy ($h = \sum_i Y_i h_i$, $h = e + p/\rho$), h_i is the local specific enthalpy of species i ($h_i = e_i + p/\rho Y_i$), s is the local bulk specific entropy ($s = \sum_i Y_i s_i$), s_i is the specific entropy of species i , T is the local bulk temperature, λ is the local Fourier bulk conductivity, and \dot{s}_{irr} is the local rate of entropy production by irreversibility per unit volume. The term $\phi = \underline{u} \cdot (\nabla \cdot \underline{g}) - \nabla \cdot (\underline{u} \cdot \underline{g}) = -\sigma_{ij} u_{i,j}$ is the rate of internal energy generation by viscous dissipation per unit volume. The condition that $\dot{s}_{irr} \geq 0$ in Equation 81 is required by the second law of thermodynamics.

Equation 81 is very seldom considered in the fluid mechanics literature. It is independent of the other equations and should be used to calculate \dot{s}_{irr} . The nonnegativity requirement yields an independent consistency check on the additional modeling equations used to close the problem, and on the numerical results.

For a general control volume (including, e.g., that represented by a mesh point in a numerical solution scheme) with volume V , surface area A , surface outward normal versor \underline{n} , and surface outward velocity \underline{a} , the following identifications establish the link with our analysis in Sections 3 and 4.

$$m = \int_V \rho dV \quad (83)$$

$$E = \int_V \rho e dV \quad (84)$$

$$S = \int_V \rho s dV \quad (85)$$

$$\dot{Q}_w = -\int_A \lambda \nabla T \cdot \underline{n} dA = -\int_V \nabla \cdot (\lambda \nabla T) dV \quad (86)$$

$$\dot{V} = \int_A \underline{a} \cdot \underline{n} dA \quad (87)$$

$$\dot{S}_{irr} = \int_V \dot{s}_{irr} dV \quad (88)$$

$$T_w = \frac{\int_A \lambda \nabla T \cdot \underline{n} dA}{\int_A (1/T) \lambda \nabla T \cdot \underline{n} dA} \quad (89)$$

$$p = \frac{\int_A p(\underline{u} - \underline{a}) \cdot \underline{n} dA}{\int_A (\underline{u} - \underline{a}) \cdot \underline{n} dA} \quad (90)$$

$$\dot{m} = -\int_A \rho(\underline{u} - \underline{a}) \cdot \underline{n} dA \quad (91)$$

$$h_m = \frac{\int_A \rho h(\underline{u} - \underline{a}) \cdot \underline{n} dA + \sum_i \int_A \rho Y_i h_i \underline{u}_i \cdot \underline{n} dA}{\int_A \rho(\underline{u} - \underline{a}) \cdot \underline{n} dA} + \frac{\int_V p \nabla \cdot \underline{u} dV - p \int_V \nabla \cdot \underline{u} dV - \int_V \phi dV}{\int_A \rho(\underline{u} - \underline{a}) \cdot \underline{n} dA} \quad (92)$$

$$s_m = \frac{\int_A \rho s(\underline{u} - \underline{a}) \cdot \underline{n} dA + \sum_i \int_A \rho Y_i s_i \underline{u}_i \cdot \underline{n} dA}{\int_A \rho(\underline{u} - \underline{a}) \cdot \underline{n} dA} \quad (93)$$

The second term in the right hand side of Equation 92 represents the contributions of pressure nonuniformities within the control volume and of internal energy generation by viscous dissipation. As discussed in Section 2, the condition of pressure uniformity is a criterion for the selection of the control volume. Within a single mesh point in a numerical computation, both such contributions may be calculated, but it is anticipated that their magnitude is negligible with respect to the convective and diffusion contributions to the value of h_m .

All our expressions in Section 3 are still valid even for a control volume represented by a single mesh point, and can be very useful in interpreting and structuring the numerical model and solution scheme. For example, if the mesh point is assumed to have only two internal zones, e.g., the gas mixture and the liquid fuel, and each zone is represented by a single temperature, then our analysis in Section 3 shows that the two temperatures are \bar{T}_g (Equation 11) for the gas mixture and \bar{T}_l (Equation 10) for the liquid fuel.

Our general analysis suggests that the readability of numerical simulations could be improved by appropriately defined multi-zone internal structure of each mesh point. For example, displaying the numerical results in

terms of the mesh-point mean gas temperature \bar{T}_g is not directly interpretable, especially where the mesh-point composition Y_i is very different from the equilibrium composition corresponding to the mesh-point value of \bar{T}_g . Indeed, to the extent that our first assumption in Section 2 is valid, this would be a clear indication that the internal structure of the mesh point has at least two zones, with different compositions and temperatures.

Thus, an improved numerical scheme based on at least three zones (i.e., burnt gas mixture, unburnt gas mixture, and liquid fuel) within each mesh point, could display the results more readably in terms of the mesh-point mass fraction x of burnt gases. To this end, a simplified version of our multi-zone example in Section 5 could be used within each mesh point. The results of such an improved multi-dimensional numerical simulation could be more readily compared with detailed analyses of experimental results on the structure of turbulent flames (like, e.g., the analysis in Reference 36).

7. CONCLUSIONS

We presented a general analytical treatment of the energy and entropy balance equations in an arbitrary control volume. The results can be applied to any kind of typical internal combustion engine (homogeneous-charge, stratified-charge, direct-injection, Diesel, adiabatic, ...) and any level of combustion modeling detail (zero-dimensional, quasi-dimensional, and multi-dimensional). The general treatment involves no major assumptions and is valid for arbitrary distributions of temperature and composition within the burnt and unburnt mixtures.

The equations presented here may also be useful to estimate the relative importance of the different physical effects occurring during the combustion process (such as combustion, compression and expansion, heat losses, mass losses, temperature dependence of the specific heats, liquid fuel injection and vaporization, crevice volumes, ...).

Equations 54 and 64 give explicitly the entropy generation by irreversibility inside the control volume. These equations are important tools for any internal combustion engine analysis, whether it be for modeling or diagnostic purposes.

The second-law nonnegativity requirement on the local and global rate of entropy production by irreversibility constitutes an important, seldom exploited, independent check of the consistency of any set of additional modeling assumptions selected to close the problem.

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