Dynamics of Combustion Systems
A. K. Oppenheim

Dynamics of Combustion Systems

With 224 Figures and 39 Tables

Springer
To Min, the great companion of my life for over sixty years,
to Terry, our magnificent daughter of over fifty years,
and to Jessica and Zachary, our marvelous grandchildren of
over twenty years, and wonderful JoAnn of over forty years.
Preface

Of prime concern in this book are combustion systems – confined fields of compressible fluids where exothermic processes of combustion take place. Their purpose is to generate motive power. In their course, exothermic energy* is created by chemical reaction and deposited in the field, both actions carried out concomitantly and referred to popularly as ‘heat release.’ Particular examples of such systems are cylinders in internal combustion engines, combustors of gas turbines and rockets, as well as explosions engendering blast waves - non-steady flow fields bounded by incident shock fronts that impose on them the constraints of confinement.

The process of combustion is carried out, as a rule, at a high rate, the life time of chemically reacting component being of an order of microseconds, while the exothermic reaction of the whole system is accomplished in few milliseconds. For that reason, its execution has been considered so far to be beyond the intervention of interactive controls – a hindrance that, in our age of microelectronics for which a millisecond is a relatively long time, can be eliminated.

The technological objective of the book is to pave the way towards this end by bringing forth the dynamic features of combustion systems. Their properties are expressed therefore as those of dynamic objects – entities amenable to management by modern tools of control technology.

Sensible properties of combustion systems are displayed in a three-dimensional physical space, while their processes are disclosed in a multi-dimensional thermophysical phase space, where the states of components of the working substance are identified and the transformations of its constituents are disclosed. The dimension of the latter is equal to the degrees of freedom - the number of reaction constituents plus two, as specified by the Gibbs phase rule.

* potential energy of thermal kind known as ‘heat of reaction’ and measured in terms of ‘heating value’ determined by the change in internal energy taking place at NTP (normal pressure and temperature)
Equilibrium states of the working substance and its components are specified in the *thermodynamic phase space* – a three-dimensional subset of the thermophysical space, provided that the internal energy, \(e\), is one of its coordinates, as pointed out by Gibbs\(^1\) and Poincaré\(^2\). If \(e\) is expressed in units of energy per mole, it is compatible with temperature, \(T\), as its concomitant coordinate. If \(e\) is expressed in units of energy per unit mass, as appropriate for mass conserving chemical reactions, its dimensionally compatible coordinate is the *dynamic potential*, \(w \equiv pv\) - a parameter providing principal service of liaison between the physical space, where it is established, and the thermodynamic space, where it is employed as a fundamental coordinate of state. The concept of \(pv\) is well known in the literature as ‘flow work’, without realizing its pivotal role in thermodynamics.

The subject matter of the book is exposed in three parts, each consisting of four chapters, Part 1 - *Exothermicity* – considering the thermodynamic effects due to evolution of exothermic energy in a combustion system; Part 2 – *Field* – exposing the dynamic properties of flow fields where the exothermic energy is deposited; Part 3 - *Explosion* – revealing the dynamic features of fields and fronts due to rapid deposition of exothermic energy.

In Part 1,

Chapter 1 - *Thermodynamic Aspects* - presents the evolution of the combustion system by a model consisting of two parts: (1) the *dynamic aspects*, dealing with the properties of combustion in the physical space, and (2) the *thermodynamic aspects*, treating the processes of combustion in the phase space.

Chapter 2 - *Evolutionary Aspects* – elucidates the fundamental features of evolution.

Chapter 3 - *Heat Transfer Aspects* – describes experimental and analytical studies of energy loss incurred in a combustion system by heat transfer to its surroundings.

Chapter 4 - *Chemical Kinetic Aspects* – furnishes a résumé of analytical technique for resolution of chemical kinetic processes of combustion.

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In Part 2,

Chapter 5 - *Aerodynamic Aspects* – provides a fundamental background for fluid dynamic analysis of flow fields at the limit of infinite Peclet and Damköhler numbers commensurate with inadequacy of molecular diffusivity and thermal conductivity to affect the rapid process of combustion taking place in *exothermic centers* – sites referred to in the literature as ‘hot spots.’

Chapter 6 - *Random Vortex Method* – presents the analytical technique, introduced by Chorin\(^3\)\(^4\), that provides an insight into the mechanism of turbulent flow fields in terms of random vortex motion, mimicking the physical nature of turbulence as a phenomenon due to random walk of vortex elements called blobs.

Chapter 7 - *Gasdynamic Aspects* - describes classical analysis of compressible flow fields, featuring the method of characteristics for solution of hyperbolic equations in terms of which their gasdynamic properties are expressed.

Chapter 8 - *Fronts and Interfaces* - furnishes analytical treatment of gasdynamic effects produced by shock and detonation fronts, as well as by interfaces (impermeable fronts) and simple waves that act as borders between different state regimes.

In Part 3,

Chapter 9 - *Blast Wave Theory* – provides a fundamental background for analysis of far fields created by an explosions, with respect to which sizes of their kernels, where the exothermic energy was deposited, is negligibly small.

Chapter 10 - *Self-Similar Solution* - presents salient features of linearly, cylindrically and spherically symmetric fields created by point explosions whose fronts propagate into a vacuum.

Chapter 11 - *Phase Space Method* - ushers in an analytical technique for treating blast waves propagating into atmospheres of finite pressure and density.

Chapter 12 - *Detonation* - displays the dynamic properties of fronts associated with exothermic processes.

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\(^3\) Chorin AJ (1973) Numerical studies of slightly viscous flow. J. Fluid Mech. 57: 785-796

Acknowledgement

I am grateful to my collaborators, Professors Harold Schock, Cornel Stan and Andrew Packard, for helpful comments, to my old friends, Professors George Leitmann, Alexandre Chorin and John Lee for valuable advice and inspiration, to my student and associate, Eilyan Bitar, for congenial companionship and valuable assistance in computations and graphics, and to my former students and associates from whom I learned so much.
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PART 1

EXOTHERMICITY
1. Thermodynamic Aspects

1.1. Combustion System

A combustion system, S, is a confined field of compressible fluid where exothermic process of combustion takes place, subject to restrictions imposed by boundary conditions at its, in general, deformable borders. Presented here are global properties of these systems.

The composition of a combustion system is specified by mass fractions of its initial components, $Y_K$, where $K = F, A$ and $B$, for, respectively, fuel, air and the non-reacting portion of the fluid, like the recirculated exhaust or residual gas. The reactants, $Y_R = Y_F + Y_A$, are formed by a mixture of fuel and air involved in the exothermic chemical reaction of combustion. The composition of a combustible mixture is expressed by the air/fuel ratio, $\sigma_K \equiv Y_{AK}/Y_F$, ($K = R, S$). For the reactants, $\sigma_R$ is identified usually with the measured flow rates of air and fuel, whereas for the system, $\sigma_S$ is deduced from the exhaust gas analysis. The values of these ratios are expressed conventionally in terms of the air-equivalence ratio with respect to the stoichiometric proportion, referred to by subscript “st”, $\lambda_{K} \equiv \sigma_{K}/\sigma_{st}$, reciprocal of the fuel-equivalence ratio, $\phi_K$. Thus,

$$Y_K \equiv (1 + \sigma_K)Y_F \equiv (1 + \sigma_{st}\lambda_K)Y_F \quad (1.1)$$

whence, for the same mass fraction of fuel, $Y_F$,

$$\frac{Y_F}{Y_K} = \frac{1}{1 + \sigma_K} = \frac{1}{1 + \sigma_{st}\lambda_K} \quad (1.2)$$

A phase diagram of the mass fraction of system components is displayed in Fig.1.1 with respect to the mass fraction of products, $y_P$, i.e. those generated by oxidation of fuel and their mixing with the non-reacted portion of the cylinder charge. The variable mass fractions are denoted in it by small letters and the constants defining the system by capital letters.
Fig. 1.1. Phase diagram of component mass fractions with respect to mass fraction of products

As displayed by this figure, in the course of combustion the mass fractions of components, $y_K$ ($K = F, A$), are linear functions of the mass fraction of products, $y_P$, namely

$$y_K = \frac{Y_K}{Y_R} (Y_R - y_P) \quad (1.3)$$

while the mass fraction of fuel

$$x_F = Y_R y_P \quad (1.4)$$

For a system constrained by walls of its enclosure, like a cylinder in a piston engine, the sole purpose of combustion is to generate pressure. With a measured pressure profile, the objective of its thermodynamic analysis is the solution of an inverse problem: the deduction on this basis of data on the evolution of the thermodynamic state parameters of the system components, as well as of the mass fraction of combustion products - a quantity proportional, according to (1.4), to that of fuel.

Mass fractions of fuel, $x_F$, and of products, $y_P$, consist of effective parts, $x_E$ and $y_E$, producing the measured pressure profile, and the ineffective
parts, $x_1$ and $y_1$, expended primarily on energy lost by heat transfer to the walls of the enclosure, i.e.

$$x_F = x_E + x_1 \quad \text{and} \quad y_P = y_E + y_1$$

Their profiles are displayed by Fig. 1.2 in terms of the normalized time, $\tau \equiv (t - t_i)/T$, where $T = t_f - t$ is the lifetime of the exothermic process. As demonstrated in Chapter 3, the initial state, $i$, is a fundamental sharp singularity of combustion, while the final state, $f$, is a smooth singularity at the maximum of the exothermic process.

![Fig. 1.2. Profiles of effective and ineffective mass fractions of fuel and products](image)

Global properties of a combustion system are established by pressure diagnostics – a procedure for solution of an inverse problem based on measured pressure, $p$, and given mass averaged specific volume, $v$. The procedure of pressure diagnostics consists of two perspectives:

1. Dynamic Aspect (Dynamic Stage in former publications) in physical space, expressed in terms of a set of relationships of volume profiles, $v(t)$, and pressure profiles $p(t)$, establishing among others the profile of the dynamic potential, $w(t) \equiv p(t)v(t)$ in the form of an analytic function.
2. Thermal Aspects (Exothermic Stage in former publications) in thermodynamic phase space, for which \( w(t) \) provides the fundamental reference coordinate of the state diagram where the trajectories of the processes carried out by the system are delineated and the profiles of the temperature, \( T(t) \), as well as of the effective mass fractions of products, \( y_P(t) \), and hence of fuel, \( x_F(t) \), expended to create pressure.

1.2 Dynamic Aspects

The dynamic aspects provide analytic expressions for the exothermic process (popularly referred to as ‘heat release’) of combustion. Its life time is identified by the coordinates of its bounds: the initial state, \( i \), and the final state, \( f \). State \( i \) is an essential singularity of combustion, a saddle point at which the specific volume of the products at this state, \( v_i = V_i / M_i = 0/0 \) (!) – the raison d'être of what is known in combustion literature as the “cold-boundary difficulty” for laminar flames (Williams 1985). Since nature abhors corners, it is bypassed by experimental data and, hence, state \( i \) is not identifiable by a data point.

State \( f \), is at a singular point of maximum in the evolution of the combustion system, where its support by the deposition of exothermic energy is at equilibrium with the endothermic loss of energy incurred by heat transfer to the walls.

1.2.1. Dynamic Potential

Of particular significance to pressure diagnostics is the dynamic potential

\[
\omega \equiv p v \equiv \frac{p}{\rho} \equiv h - e
\]

whose time profile is a prominent variable of dynamic aspects, while for thermal aspects it plays the role of a fundamental thermodynamic reference parameter replacing in this role the temperature that is delegated then to the position of a dependent variable. For convenience, the specific volume is often expressed in a non-dimensional, normalized form; \( \omega \) is then measured in units of pressure. Its magnitude can be readily determined from the equation of state for given values of \( p \) and \( \omega \), or \( v \), of the substance. The
concept of $w$ is popularly called flow work - a term demeaning its cardinal nature, as pointed out by Kestin 1966 (Sections 4.1 and 4.2). The significance of $w$ is brought up by the virial equation of state, according to which

$$w = A(\Theta) + B(\Theta)p + C(\Theta)p^2 + \ldots$$

where, with subscript $m$ denoting the dynamic potential, $w$, per mole and $\mathcal{R}$ the universal gas constant,

$$\Theta \equiv \frac{w_m}{\mathcal{R}}$$

It is on this basis that an equation of state for a system in equilibrium can be determined experimentally without measuring the temperature – a procedure engendering the concept of an absolute temperature scale (vid. e.g. Kestin 1966-68)

The general utility of $w$ is demonstrated by most equations of state, to wit:

Van der Waals:

$$w = \frac{R}{M} T \frac{v}{v-b} - \frac{a}{v}$$

Dietrich:

$$w = \frac{R}{M} T \frac{v}{v-b} e^{w/R\Theta}$$

Beattle-Bridgeman:

$$w = \frac{R}{M} T \left[ \frac{\beta}{v} + \frac{\gamma}{v^2} + \frac{\delta}{v^3} \right]$$

BKW$^1$:

$$w = \frac{R_a}{M} T \left[ 1 + xe^{\text{fr}} \right]$$

$$x = \frac{k}{v(T + \Theta)^k}$$

JWL$^2$:

$$w = A \left[ 1 - \frac{v}{c_{x1} v_c} \right] v e^{\gamma v/v_c} + B \left[ 1 - \frac{v}{c_{x2} v_c} \right] v e^{\gamma v/v_c} + \frac{R}{c_v} u$$

1.2.2. Data.

The procedure for establishment of the dynamic aspects is illustrated here by a specific example of a HCCI (Homogeneous Charge Compression Ignition) engine – a system that today is at the crest of popular research on

$^1$ Becker-Kistiakowski-Wilson

$^2$ Jones-Wilkins-Lee
novel piston engines. The data of the engine adopted for the present purpose are provided by Table 1.1. The operating conditions of its dynamometer test are listed in Table 1.2.

**Table 1.1. HCCI engine data**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (cm)</td>
<td>7.95</td>
</tr>
<tr>
<td>Stroke (cm)</td>
<td>9.56</td>
</tr>
<tr>
<td>Length of piston rod (cm)</td>
<td>14.4</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>16.5</td>
</tr>
<tr>
<td>Intake valve closing, $\Theta_a$</td>
<td>205</td>
</tr>
<tr>
<td>$p_a$ (bar)</td>
<td>1.39</td>
</tr>
<tr>
<td>$T_a$ (K)</td>
<td>325</td>
</tr>
<tr>
<td>Exhaust valve opening $\Theta_z$</td>
<td>512</td>
</tr>
</tbody>
</table>

**Table 1.2. Operating conditions**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed</td>
<td>rpm 1200</td>
</tr>
<tr>
<td>Torque</td>
<td>Nm 75</td>
</tr>
<tr>
<td>Fuel (gasoline)</td>
<td>Octane No. 87</td>
</tr>
<tr>
<td>Stoichiometric air/fuel ratio</td>
<td>$\nu_{st}$, mol/mol 12.305</td>
</tr>
<tr>
<td></td>
<td>$\sigma_{st}$, gm/gm 15.064</td>
</tr>
<tr>
<td>Air-equivalence ratio, $\lambda_{st}$</td>
<td>- 2.2</td>
</tr>
<tr>
<td>Cylinder pressure at $\Theta_a$, $p_a$</td>
<td>atm 1.39</td>
</tr>
<tr>
<td>Gas temperature at $\Theta_a$, $T_a$</td>
<td>K 325</td>
</tr>
</tbody>
</table>

The air equivalence ratio cited in Table 1.2 was obtained from by exhaust gas analysis and pertains therefore to the system, S, rather than the reactants, R.

Parameter profiles of the dynamic aspects, obtained from the dynamometer test, are presented in Figs. 1.3-1.6, where, according to convention, their measured data are displayed by open circles. Figure 1.3 presents the record of the measured pressure, $p(\Theta)$. Figure 1.4 displays the data of the work cycle (positive loop of the indicator diagram), $p(\nu)$, where $\nu \equiv v_{S}/v_{c}$, subscript S denoting the displacement volume of the cylinder-piston enclosure and subscript c its clearance volume, $v_{c}$. Figure 1.5 depicts the profile of dynamic potential, $w$. Figure 1.6 presents the work cycle in logarithmic scales.
Fig. 1.3. Data of the pressure record

Fig. 1.4. Data of the work cycle in linear scales
Fig. 1.5. Data of the dynamic potential

Fig. 1.6. Data of the indicator diagram in logarithmic scales
1.2 Dynamic Aspects

1.2.3. Functions

To provide a rational interpretation of the profiles presented by these figures, their data are expressed in terms of analytic functions.

The changes of state taking place immediately before and after the exothermic process are expressed by polytropes, \( \pi_k = p v^\nu_k \), where subscript \( k = c, e \) for, respectively, compression and expansion, whence \( n_k = \frac{d \log p}{d \log v} \).

The polytropic exponents are evaluated, accordingly, from data of \( \log p \) vs. \( \log v \) presented on Fig. 1.6 by least square fit regression of these data for sectors of the processes of compression and expansion where their profiles are linear. For compression, the selected sector is between point \( b \) and the estimated location of the initial state, \( i \). For expansion, it is between the estimated location of the final state, \( f \), and point \( c \).

The key to an analytic expression for the exothermic process is provided by the polytropic pressure model,

\[
\pi = p v^\nu_S \quad (1.6)
\]

In contrast to polytropes, the exponent of the exothermic process is variable, its value being expressed by a linear function of the crank angle, \( \Theta \), so that

\[
n(\Theta) = n_c + (n_e - n_c) \tau(\Theta), \quad (1.7)
\]

where

\[
\tau \equiv \frac{\Theta - \Theta_i}{\Theta_f - \Theta_i} \quad (1.8)
\]

is the progress variable for time, \( t \), or crank angle, \( \Theta \). In an enclosure of variable volume, the polytropic pressure model is equivalent to pressure in an enclosure of constant volume.

The progress parameter for the polytropic pressure model

\[
x(\tau) = x(\tau) \equiv \frac{\pi(\tau) - \pi_i}{\pi_f - \pi_i} \quad (1.9)
\]

is expressed by the life function introduced in Chapter 2, namely
1. Thermodynamic Aspects

\[ x = \frac{e^\zeta - 1}{e^\alpha - 1} \]  \hspace{1cm} (2.49)

where

\[ \zeta = \frac{\alpha}{\chi + 1} \left[ 1 - (1 - \tau)^{\chi+1} \right] \]  \hspace{1cm} (2.48)

And \( \zeta_f = \frac{\alpha}{\chi + 1} \). The two parameters, \( \alpha \) and \( \chi \), are evaluated by regression of data between point \( i \) and \( f \). As demonstrated in Chapter 2, the life function is in shape akin to the profile of the polytropic pressure model depicted by Fig. 1.6, and it satisfies both the conditions imposed by the singular bounds of the exothermic process.

Its profile is presented by Fig. 1.7 together with profiles of the polytropes for compression and expansion.

![Fig. 1.7. Profile of the polytropic pressure model](image)

Concomitantly with evaluation of the life function parameters: \( \alpha \) and \( \chi \), the polytropic indices, \( n_c \) and \( n_e \), together with the crank angles of point \( i \) and point \( f \), \( \Theta_i \) and \( \Theta_f \), are determined by iterative procedures. The values of all these parameters are listed, together with the crank angles of all the bounds of analytic functions, in Table 1.3.
Table 1.3. Parameters of dynamic aspects

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crank angle of point a</td>
<td>205°</td>
</tr>
<tr>
<td>Crank angle of point b</td>
<td>320°</td>
</tr>
<tr>
<td>Crank angle of point i</td>
<td>366°</td>
</tr>
<tr>
<td>Crank angle of point f</td>
<td>375°</td>
</tr>
<tr>
<td>Crank angle of point c</td>
<td>500°</td>
</tr>
<tr>
<td>Crank angle of point z</td>
<td>512°</td>
</tr>
<tr>
<td>Life function coefficient, $\alpha$</td>
<td>13.55</td>
</tr>
<tr>
<td>Life function exponent, $\chi$</td>
<td>2.19</td>
</tr>
</tbody>
</table>

Fig. 1.8. Profile of dynamic potential

\textit{Data and analytic functions}
Fig. 1.9. Work cycle

Data and analytic functions

Fig. 1.10. Pressure profile

Data and analytic functions

Figures 1.8-10 demonstrate the remarkable accuracy with which the pressure data are, on this basis, modeled by analytic functions except, notably, in the immediate vicinities of the two singularities at \( i \) and \( f \) that, as a rule, are obviated by the data. Besides points \( i \) and \( f \), marked in Fig. 1.9
are points a, b, c and z, whose crank angles are listed in Table 1.3. Points a and z denote the bounds of the closed system, the first at the closure of the inlet valve, and the second at the opening of the exhaust valve. Points b and c mark, respectively, the crank angle designated as the start of the process of compression and that chosen as the end of the expansion process.

1.3 Thermal Aspects

In accord with the zero-dimensional nature of dynamic aspects, the variables of thermal aspects are expressed in terms of time-dependent mass averaged thermodynamic parameters of state: the pressure, $p_K(t)$, the temperature, $T_K(t)$, the specific volume, $v_K(t)$, the internal energy, $e_K(t)$, and the dynamic potential, $w_K(t)$, where $K = F, A, B, C, R$ and $P$, providing a link between the dynamic and thermal aspects. Moreover, since all the parameters of the dynamic aspects are expressed in terms of analytic functions, the time coordinate can be expressed in terms of any of them, in particular pressure whose time profile provides the basis for their evaluation.

1.3.1 Thermodynamic State

The state of a constituent is identified by three parameters of its own equilibrium. The conventional equation of state, expressing a relationship between pressure, $p$, specific volume, $v$, and temperature, $T$, does not provide a comprehensive specification of state, because, to evaluate internal energy, $e$, specific heats are, moreover, required. If, however, internal energy is included among the parameters of state, then, according to the fundamental principle of the First Law provided by Gibbs (1875-1878) and formulated by Poincaré (1892) and Carathéodory (1909), the state of a constituent is thereby completely specified.

Accordingly, the thermodynamic state of a constituent is expressed by a point in a three-dimensional thermodynamic phase space whose coordinates are specific internal energy, $e$, specific dynamic potential, $w$, and pressure, $p$. If internal energy is expressed in molar (volumetric) basis, the fundamental role of a reference coordinate is played by the temperature, $T$, rather than $w$. However, since in system undergoing a chemical reaction mass is conserved rather than volume, the latter is for this purpose more appropriate.
### 1. Thermodynamic Aspects

#### Table 1.4: Thermodynamic parameters of components in the HCCI engine

<table>
<thead>
<tr>
<th>States</th>
<th>p (atm)</th>
<th>T (K)</th>
<th>v (m³/kg)</th>
<th>e (kJ/g)</th>
<th>h (kJ/g)</th>
<th>w (kJ/g)</th>
<th>M (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td></td>
<td></td>
<td></td>
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<td>29.50</td>
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<tr>
<td>P</td>
<td></td>
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<tr>
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<td>1832</td>
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<td>-0.03</td>
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<td>0.53</td>
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<tr>
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<td>0.086</td>
<td>0.57</td>
<td>1.25</td>
<td>0.68</td>
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</tr>
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</table>

![Diagram of states for an adiabatic and isochoric combustion system](image)

**Fig. 1.11.** Diagram of states for an adiabatic and isochoric combustion system

The reactants, R, are considered as an air/fuel mixture at their own air-equivalence ratio, \( \lambda_R \). The products, P, are specified by the molecular composition of the system at thermodynamic equilibrium. The states of both of them are established by appropriate algorithms. Their thermodynamic parameters are presented by Table 1.4 upon evaluation by means of STANJAN (Reynolds 1996), and CEA (Gordon and McBride 1994, McBride and Gordon 1996)\(^3\), on the basis of thermodynamic data provided by the JANAF Tables (Stull and Prophet 1971), as well as the

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\(^3\) <http://www.grc.nasa.gov/WWW/CEAWeb>
Chemistry WebBook of NIST\(^4\), for a mixture of iso-octane and normal heptane in proportions provided by the octane number and the air-equivalence ratio cited in Table 1.2.

In a three-dimensional state space, the planar platform of this diagram presented by Fig. 1.11 is at the level of the initial pressure, \( p_i \). For higher pressures, the e-w platform is at higher levels. For the regime of pressures and temperatures existing in internal combustion engines, the reactants are made out of fixed fuel and air fractions, while, according to the available source of thermodynamic data, these components are perfect gases. The locus of states of the reactants, \( R \), is, therefore, pressure independent. However, the locus of states of the products, \( P \), is dependent on pressure, because, in order to comply with the condition of thermodynamic equilibrium, their composition is variable. On the e-w plane, for higher pressures, the line of \( P \) tends to get straighter, so that, as indicated in Fig. 1.11, it is further away from the internal energy axis.

In the course of an exothermic process, the states of reactants, \( R \), and products, \( P \), move along their loci of states, starting from the initial point, \( i \), and ending at the terminal point \( t \), where the generation of products, and hence, consumption of fuel, is terminated, that, in principle, is different than the final point, \( f \). Nonetheless, as demonstrated in Chapter 3, they are coincident. The change of state taking place in the course of exothermic reaction, when the reactants are transformed into products at a fixed pressure, is presented by a straight line between a point on \( R \) and a point on \( P \).

In Fig. 1.11, the process of combustion is presented by vectors \( i - t \), on the lines of \( R \) and \( P \), while the processes of exothermic reactions promoting the transition between them are depicted by vectors \( i_\text{on} R - i_\text{on} P \), and \( t_\text{on} R - t_\text{on} P \).

### 1.3.2. Processes

#### 1.3.2.1 Mixing

For a chemical reaction to take place, its components must be first mixed to form a molecular aggregate. If, initially, the thermodynamic coordinates of fuel and air are different, they have to be brought to the same state \( i \) on \( R \) - a task accomplished physically by transport processes of molecu-
lar mass diffusion and thermal conduction, assisted by viscosity. In Fig. 1.11, the concomitant changes of state taking place in the course of mixing are expressed by broken curves between points o on A and o on F to point i on R, with their directions indicated by arrows. The effect of mixing is manifested by rotation of the end point of the state vector around point i on R. Irrespectively of the influence of molecular diffusion, which, as a rule, must be involved in forming the reacting mixture, its outcome can be identified right from the outset by the intersection of the straight line between points o on A and o on F with R.

1.3.2.2 Exothermic

Chemical reaction of combustion takes place in an exothermic center. The concept of exothermic centers has been known for a long time in detonation literature under the name of “hot spots.” Their non-steady behavior under the influence of molecular diffusion has been studied extensively as the process of ignition (e.g. Boddington et al 1971; Gray and Scott 1990; Griffiths 1990). Their diffusion dominated steady state model is a laminar flame. Their non-steady version in a turbulent field is referred to as the ‘flamelet model’ (Peters 2000). The fluid dynamic features of exothermic centers were investigated experimentally and theoretically in connection with their relevance to detonation and explosion phenomena, leading to the identification of mild and strong ignition centers. In a gasdynamic field where exothermic reaction takes place, exothermic centers occur at discrete sites. Each of them behaves then as a point singularity - a constant pressure deflagration where a finite change of state takes place locally at constant pressure - rather than across a straight line as it does in the classical version of a deflagration front.

1.3.3 System Parameters

The behavior of a combustion system is specified by the balances of mass, volume and internal energy. The mass balance is expressed simply by the fact that \[ Y_S = \sum y_K = 1, \] or \[ X_F = \sum x_K = Y_R, \] as depicted in Fig. 1.1. The balance of volumes, \( v_S = \sum y_K v_K \) is expressed by the balance of dynamic potential, \( w_S = \sum y_K w_K \), since by definition \( w(t) = p(t) v(t) \), where \( p(t) \) is the same for all the components. The balance of energy is