Dynamic Characteristics of Kinetically Controlled Combustion and Their Impact on Thermoacoustic Instability

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Combustion in high performance engines utilizes strong swirl, recirculation and interacting jets to enhance the mixing rate of the fuel, air and products, and hence maximize the burning rate. The ideal limit for these systems is often modeled as a well-stirred reactor [1]. The operation of a well-stirred reactor is governed by a characteristic residence time, t_{res}, which is the nominal time the reactants spend inside the reactor. Stable operation is achieved when the residence time is larger than the characteristic chemical time, otherwise blow-out should be expected.

Combustion dynamics, resulting from coupled heat release-pressure oscillations, has been suspected to occur when oscillations in the mass-flow rate, equivalence ratio, inlet temperature and pressure, etc., occur at the same time-scale. The condition under which a combustion system becomes unstable has been expressed in terms of the Rayleigh criterion [2], which states that a combustion system becomes unstable when the heat release increases at a moment of a rise in pressure.

In a former study [3], we investigated the linear response of a WSR model to residence time oscillations using a single-step kinetics mechanism. We showed that as the mean equivalence ratio or the mean residence time approach the blow-out limit, the operating point may transition from stability to instability due to a sudden phase change between pressure and heat release oscillations. In this paper, we use the same approach with a multi-step kinetics mechanism instead of a single-step mechanism to examine its impact on the instability characteristics.

The governing equations of a well-stirred reactor are obtained using the conservation laws and a set of reaction-rate equations. The conservation equations of the mass, energy and species in the WSR are given by:

$$\text{Mass : } \frac{dM}{dt} = \dot{m}_i - \dot{m} \ , \qquad (1)$$

$$\text{Energy : } \frac{dE}{dt} = \dot{m}_i \bar{h}_i - \dot{m}\bar{h} + \dot{Q}_r \ , \qquad (2)$$

$$\text{Species : } \frac{dM_k}{dt} = \dot{m}_i Y_{k,i} - \dot{m} Y_k - \dot{W}_k \ , \qquad (3)$$

where M, E, and M_k are a total mass, energy and mass of species k inside the combustor, respectively, $\dot{Q}_r = \sum_k \dot{W}_k h_k(T_i)$ is the heat release rate due to the chemical reaction, $\dot{W}_k$ is a consumption rate of species k, $\dot{m}$ is the mass flow rate, h is the enthalpy per unit mass, Y is the mass fraction, and subscript i refer to the inlet condition.

For a single-step mechanism, the source terms can be represented as function of Y and T [4] as follow:

$$\dot{W}_f = A_f V (rY_f)^{n_f} (rY_{o_2})^{n_{o2}} \exp\left(\frac{-T_a}{T_o}\right) \text{ and } \dot{Q}_r = \Delta h_r \dot{W}_f \qquad (4)$$

where A_f is the frequency factor, Δh_r is the enthalpy of reaction (measured per unit mass of fuel), and $T_a = E_a / R$ where E_a is activation energy and R is the gas constant. Linearlizing Eq. (4) and using Eqs. (1)-(3), we obtain the following linear heat release rate model [3]:

$$\dot{Q}_r' = J(s)\dot{m}' = \frac{b}{s+a}\dot{m}' \qquad (5)$$

where

$$a = \frac{\bar{\dot{m}}}{\bar{r}V}(1+\Gamma) \ , \qquad (6)$$

where $\Gamma = n\frac{(\bar{T}-T_i)}{\bar{T}} - \frac{(\bar{T}-T_i)}{\bar{T}^2}T_a + n\frac{(Y_i-\bar{Y})}{\bar{Y}}$,

and

$$b = A_f' \Delta h_r \bar{r}^{\,n-1} \bar{Y}^{\,n} \exp\left(\frac{-T_a}{\bar{T}}\right)\Gamma \ . \qquad (7)$$

The cut-off frequency a and the static gain b are functions of the mean residence time, the equivalence ratio, and the inlet temperature. At a fixed equivalence ratio, if the residence time is much larger than the chemical reaction time, almost all the fuel is burnt, i.e., $\bar{Y} \approx 0$. In this case, a and b are much larger than the acoustic frequency, and the heat release responses instantaneously to the acoustic perturbations. As the residence time decreases, the unburned fuel $\bar{Y}$ increases, and the values of a and b decrease. Moreover, the change of the residence time affects the equilibrium temperature $\bar{T}$. As the residence time decreases, the equilibrium temperature $\bar{T}$ decreases, while a and b change from positive to negative values because of the $-\frac{(\bar{T}_o - T_i)}{\bar{T}_o^2} T_a$ term. When a becomes negative, the heat release model itself becomes unstable. The system is critically stable when $a = 0$. It is shown that this corresponds to blow-out [3].

Equation (5) shows that when b changes sign, it introduces 180° phase change between $\dot{m}'$ and $\dot{Q}_r'$. If the heat release dynamics is coupled with acoustics, this phase change may trigger a thermoacoustic instability as an out-of-phase relationship between (p', q') becomes in-phase. That is, at $b = 0$, the system can transition from stability to instability, and $b = 0$ corresponds to burning at the maximum heat release rate [3]. Equations (6) and (7) are similar expect for the extra "1" in Eq. (6). Thus, one expects b to become negative before a as he residence time decreases. Therefore, immediately before blow out ($a = 0$), the heat release experiences a phase change. That is, the onset of thermoacoustic instability may occur before blow-out. The change of the equivalence ratio at a fixed residence time also changes the equilibrium temperature $\bar{T}$, thereby affecting a and b . One can expect that a and b become negative as the equivalence ratio decreases due to the drop of the equilibrium temperature $\bar{T}$.

Now, we use a multi-step mechanism. For C_3H_8 , the following 4-reaction step has been suggested [5].

$$C_3H_8 \rightarrow 3/2C_2H_4 + H_2$$
$$C_2H_4 \rightarrow 2CO + 2H_2$$
$$CO + 1/2O_2 \rightarrow CO_2$$
$$H_2 + 1/2O_2 \rightarrow H_2O$$

In this case, the WSR model is governed by four rate equations and the energy equation, increasing its order to 5. To get a linearized model, we define the following states variables:

$$x = [Y_{C_3H_8}\ Y_{C_2H_4}\ Y_{H_2}\ Y_{O_2}\ Y_{co}\ Y_{CO_2}\ Y_{H_2O}\ T]^T \qquad (8)$$

$$\dot{x} = [\,f_1(x,\dot{m}_i)\ f_2(x,\dot{m}_i) \cdots f_8(x,\dot{m}_i)] \qquad (9)$$

$$\dot{Q}_r = h(x,\dot{m}_i) \qquad (10)$$

where $f_k = \frac{\dot{m}_i}{\bar{r}V} \cdot (Y_{k,i} - Y_k) - \frac{\dot{W}_k}{\bar{r}V}$, $h(x,\dot{m}_i) = \sum_k \dot{W}_k h_k(T_i)$, $\bar{r}$ is the mean density and V is the volume of the combustor.

The linearized model is:

$$\dot{x}' = A\,x' + B\,\dot{m}_i' \qquad (11)$$

$$\dot{Q}_r' = C\,x' + D\,\dot{m}_i' \qquad (12)$$

$$\text{where } A = \begin{bmatrix} \frac{\partial f_1}{\partial Y_{C_3H_8}} & \frac{\partial f_1}{\partial Y_{C_2H_4}} & \cdots & \frac{\partial f_1}{\partial T} \\ \vdots & \cdots & & \vdots \\ \frac{\partial f_8}{\partial Y_{C_3H_8}} & \frac{\partial f_8}{\partial Y_{C_2H_4}} & \cdots & \frac{\partial f_8}{\partial T} \end{bmatrix}, B = \begin{bmatrix} \frac{\partial f_1}{\partial \dot{m}_i} \\ \vdots \\ \frac{\partial f_8}{\partial \dot{m}_i} \end{bmatrix}, C = \begin{bmatrix} \frac{\partial h}{\partial Y_{C_3H_8}} & \cdots & \frac{\partial h}{\partial T} \end{bmatrix},$$

$$\text{and} \quad D = \frac{\partial h}{\partial \dot{m}_i} \ . \qquad (13)$$

The derivatives are obtained numerically around an equilibrium point. The transfer function previously defined in Eq. (5) becomes

$$J(s) = \left\lfloor C(sI - A)^{-1} B + D \right\rfloor . \tag{14}$$

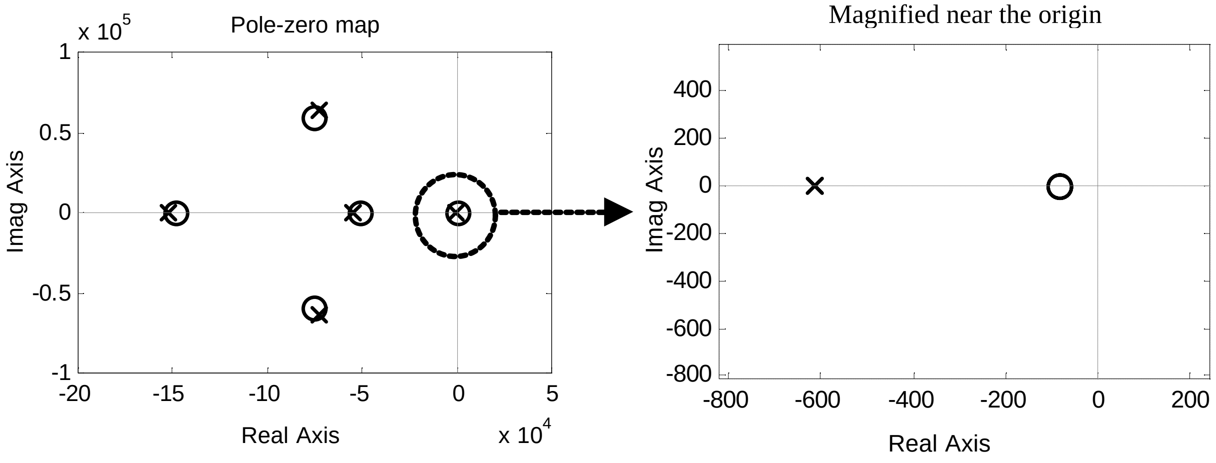
Now, we examine the heat release dynamics model acquired by linearizing the four step mechanism. The model has five poles and five zeros as shown in Figure 1 (a). The poles represent characteristic time scales of the coupled chemical processes, while the zeros represent the interactions among them. The frequencies of four of these modes are located over 10kHz and one pole is near the origin. Considering that the frequency range of the acoustic modes in a typical combustor is 100-1000Hz, the effect of the high frequency dynamics on the system is negligible. Therefore, we approximate the model in the range of interest using the pole and zero which are located near the origin (Figure 1, (b)) as follows:

$$\dot{Q}_r' = J(s)\dot{m}_i' = \frac{b_2(s+s)}{s+a_2}\dot{m}_i' . \tag{15}$$

As before, the parameters, a_2, b_2 and s are functions of mean residence time and mean equivalence ratio. Compared to Eq. (4) acquired using a single–step mechanism, Eq. (15) has an additional zero at $s = -s$. It is observed from a typical calculation that s changes from positive to negative values when either equivalence ratio or residence time are reduced. Moreover, the critical point, where $s = 0$, corresponds to the maximum heat release rate point. The static gain b_2 does not change its sign in this case remaining positive over the entire range. This shows that the phase change mechanism around the condition of maximum heat release is no longer due to a sign change of the static gain. As a result, we observe that in multi-step mechanism

1) The phase between $\dot{Q}_r$ and $\dot{m}_i$ varies continuously as the mean conditions change,
2) The phase between $\dot{Q}_r$ and $\dot{m}_i$ depends on the perturbation frequency in $\dot{m}_i$.

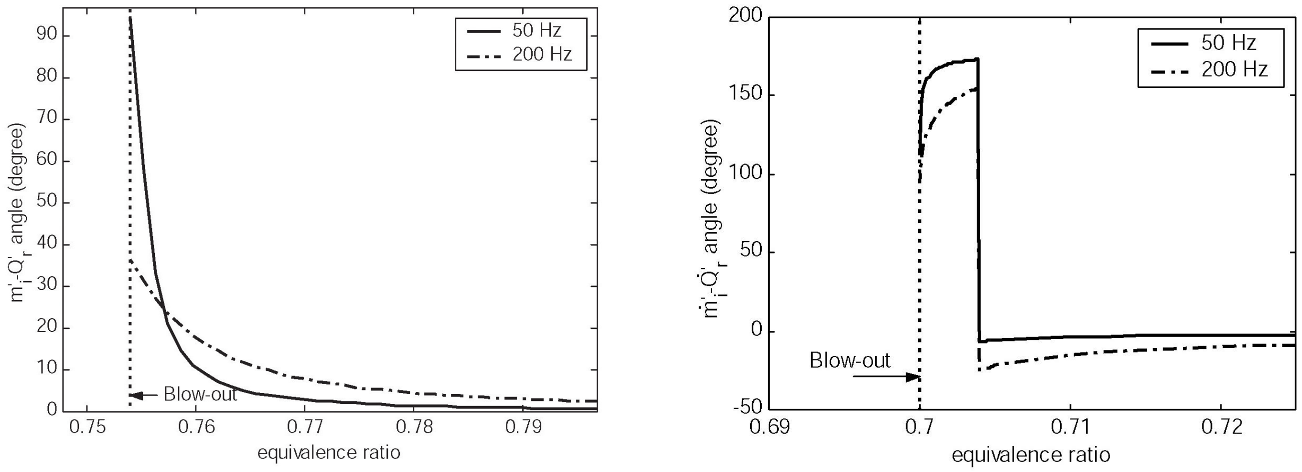
Figure 2 (a) clearly shows the above characteristics. First, the $\dot{Q}_r$ - $\dot{m}_i$ phase changes rapidly around $f = 0.76$. Contrary to the single-step kinetics model result, this change is "continuous" for the 50 Hz acoustic mode (Using Eq. 5, a jump in the phase is observed at the maximum reaction point, as shown in Figure 2 (b)). The 50 Hz mode experiences this phase change over a narrower range of equivalence ratio than for the higher mode (200 Hz). As mentioned before, the time constant of the zero, s , decreases "continuously" as the equivalence ratio decreases introducing that phase change. Moreover, in Eq. (5), the phase change is observed when the sign of the gain changes at maximum heat release, thereby generating a jump in a phase. Also, one can expect that the higher frequency oscillation mode will experience a phase change first because the zero moves towards lower values thereby affecting the higher mode first.



(a)

(b)

Figure 1 Pole and zero map of WSR model for C_3H_8 at $f = 0.7$, $\bar{\dot{m}}_i = 732kg/m^3s$ and $T_i = 600K$.



(a)

(b)

Figure 2 Phase change between $\dot{Q}_r$ and $\dot{m}_i$ of WSR model for C_3H_8 at $T_i = 600K$, $\bar{\dot{m}}_i = 1000kg/m^3s$ using (a) a four-step mechanism and (b) a single-step mechanism.

References

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