Dynamic Characteristics of Kinetically Controlled Combustion and Their Impact on Thermoacooustic 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 the 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:

Mass Conservation: $$\frac{dM}{dt} = \dot{m}_i - \dot{m} \quad , \tag{1}$$

Energy Conservation: $$\frac{dE}{dt} = \dot{m}_i \bar{h}_i - \dot{m}\bar{h} + \dot{Q}_r \, , \tag{2}$$

Species Conservation: $$\frac{dM_k}{dt} = \dot{m}_i Y_{k,i} - \dot{m} Y_k - \dot{W}_k \, , \tag{3}$$

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:

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

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. By linearlizing Eq. (4) and with Eqs. (1)-(3), we obtain the following linear heat release rate model [3]:

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

where

$$a = \frac{\dot{\bar{m}}}{\bar{r}V}\left[1 + n\frac{(\bar{T}-T_i)}{\bar{T}} - \frac{(\bar{T}-T_i)}{\bar{T}^2}T_a + n\frac{(Y_i-\bar{Y})}{\bar{Y}} \right] \quad (6)$$

,and

$$b = A_f' \Delta h_r \bar{r}^{n-1}\bar{Y}^n \exp(\frac{-T_a}{\bar{T}})\left[n\frac{(\bar{T}-T_i)}{\bar{T}} - \frac{(\bar{T}-T_i)}{\bar{T}^2}T_a + n\frac{(Y_i-\bar{Y})}{\bar{Y}}\right] \quad (7)$$

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 (due to the $\bar{Y}$ term in the denominator in Eqs (6) and (7)), and the heat release responses instantaneously to the acoustic perturbations. As the residence time decreases, the unburned fuel $\bar{Y}$ increases, so 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 since a perturbation grows exponentially as e^{-at}. 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) and gain. Based on this, one expects b to become negative before a as the 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 $\bar{T}$. Therefore, the linearized model shows that by decreasing the residence time or the equivalence ratio, one expects phase change or blow-out to occur.

Now, we use a multi-step mechanism instead of Eq. (4). 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:

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

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

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

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:

$$\dot{x}' = A\, x' + B\, \dot{m}_i' \tag{11}$$

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

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

,and $D = \frac{\partial h}{\partial \dot{\bar{m}}_i}$. (13)

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

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

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). These poles represent the time constants of five first-order equations. Also, the zeros represent the interactions between equations (e.g. coupling by temperature and mass fractions of species). The frequencies of four of these zeros and four of the poles are located over 10kHz and one zero and one pole are 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 the zero which are located near the origin (Figure 1, (b)) as follows:

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

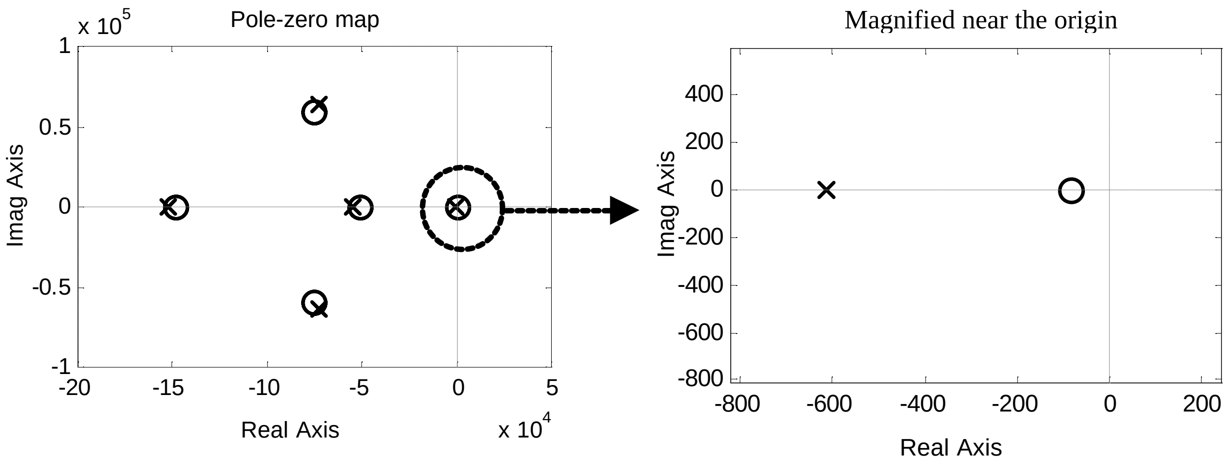
where a_2 represents the location of the pole, b_2 is the gain and s represents the location of the zero. As before, the parameters, a_2, b_2 and s in Eq. (15) are functions of mean residence time and mean equivalence ratio.

Compared to Eq. (4) acquired using a single–step mechanism, Eq. (15) has an additional zero at $s = -s$. It is observed from typical calculation that s changes from positive values 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 difference between $\dot{Q}_r$ and $\dot{m}_i$ varies continuously as the mean conditions change,

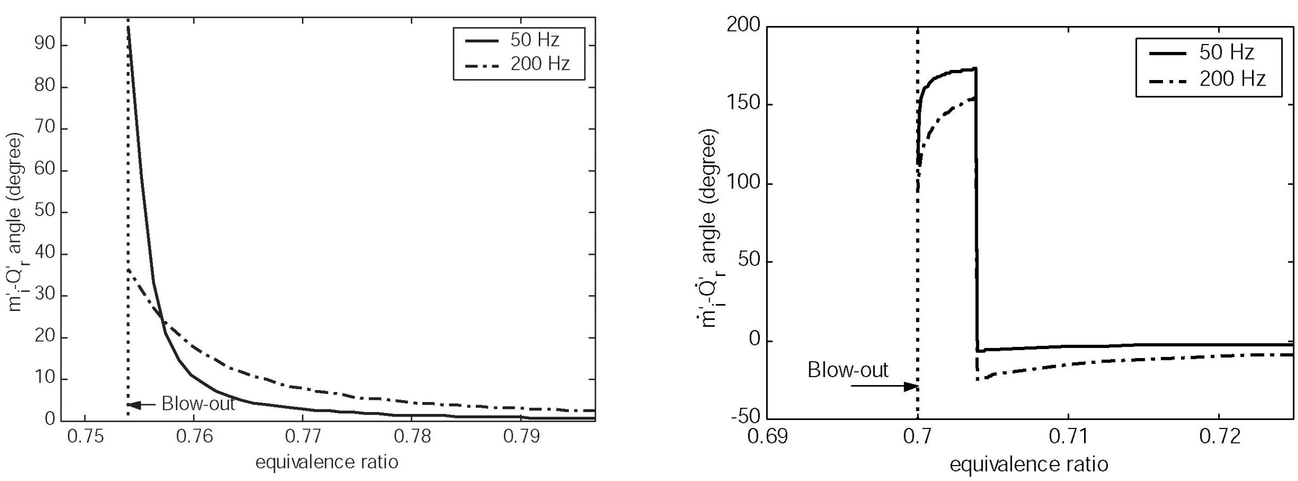
2) The phase difference between $\dot{Q}_r$ and $\dot{m}_i$ varies also by the perturbation frequency in $\dot{m}_i$.

Figure 2 (a) clearly shows the above characteristics. First, the phase change between $\dot{Q}_r$ and $\dot{m}_i$ happens around $f = 0.76$, and it is "continuous" for 50 Hz oscillations. Using Eq. 5, one gets a jump in the phase at the maximum reaction point as shown in Figure 2 (b). Also, the 50 Hz mode gets phase change in a narrower range of equivalence ratio than the higher mode (200 Hz). As mentioned before, the time constant of zero, s , decreases "continuously" as the equivalence ratio decreases introducing a phase change. However, in Eq. (5), the phase change is obtained when the sign of the gain changes at the maximum heat release "point", thereby generating a jump in a phase. Also, one can expect that the higher oscillation mode will get a phase change first because the zero moves from a higher value to a lower value thereby affecting the higher mode in advance.



(a) (b)

Figure 1 Pole and zero map of WSR model for C_3H_8 at $f = 0.7$, $\bar{\dot{m}} = 732 kg/m^3 s$ 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 $T_i = 600K$, $\bar{\dot{m}}_i = 1000 kg/m^3 s$ using (a) a four-step mechanism and (b) a single-step mechanism.

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