Mild Ignition Phenomena in Rapid Compression Machines

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1 Introduction

Rapid compression machines (RCMs) [1] are commonly used to study fuel decomposition and ignition behavior at elevated temperature and pressure conditions that are representative of combustion engine environments. RCMs are designed to isolate chemical kinetic phenomena from other complex processes that occur within the combustion chamber during engine operation. There is a long history of development of RCMs, and modern configurations are generally well-characterized over a range of conditions. RCMs typically explore ignition behavior using realistic fuel loadings, which is similar to what is employed in operating engines. Other devices, such as shock-tubes, are usually operated under highly diluted conditions in order to minimize thermal feedback and inhomogeneities that can result from exothermic and endothermic processes, as well as other operational challenges such as excessive pressure rise rates.

Idealized reactors like RCMs can be influenced by physical processes which result in coupled chemico-physical phenomena, and this leads to non-ideal experimental conditions. Measurements and interpretation of datasets under these scenarios can be complicated. In RCMs such processes can include heat loss and complex fluid dynamics, as well as turbulent fluctuations and the development of non-uniform or deflagrative ignition.

Deflagrative ignition, which is referred to as "mild ignition" in this work, occurs when flames develop within the reaction chamber. Mild ignition differs from strong ignition phenomena due the inhomogeneous nature of the ignition event, which is characterized by ignition kernel formation. Additionally, mild ignition can be succeeded by a strong ignition event in the bulk fluid; this ignition variety is referred to as "mixed ignition" in this work. Ignition delay times are generally shortened during mild ignition events, while the rates of pressure rise are much slower than under uniform ignition conditions.

The objective of the present work is to better understand and quantify physical processes that influence mild ignition phenomena within RCMs. Specifically, by employing essential scaling analysis of processes involving hydrodynamics, turbulence, and ignition, demarcations are developed that are indicative of the occurrence of mild ignition.

The remainder of this paper is organized as follows: a description of the various physical phenomena affecting ignition is provided in the next section, and scaling relationships distinguishing different ignition regimes are derived; these derivations are followed by a comparison with experimental data available in the literature and discussion; and finally, conclusions are presented.

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2 SWACER and the strong ignition limit

Shock Wave Amplification by Coherent Energy Release (SWACER) [2, 3] is a mechanism that explains the transition of isolated ignition kernels to detonation. SWACER theory predicts a spontaneous transition into a detonation wave if there is a coherent coupling of pressure waves and heat release at the ignition kernel [4]. The transition criterion is given as

$$\frac{a}{u_{\mathrm{RF}}} = 1 \,, \tag{1}$$

where a is the speed of sound in the mixture, and u_{RF} is the speed of the reaction front. Using Zeldovich's relation for the speed of the ignition front [5], the following criterion is obtained:

$$a \frac{\partial T}{\partial \xi} \frac{\partial \tau_{\mathrm{ign}}}{\partial T} = 1 \,, \tag{2}$$

where ξ is the spatial coordinate normal to the reaction front, and τ_{ign} is the ignition delay time of the mixture. Gu *et al.* [6] studied the transition of a flame kernel to a detonation wave in one-dimensional simulations and found acceptable agreement between Eq. (2) and the computed transition. The SWACER mechanism has been found to be relevant in inhomogeneous ignition phenomena [7]. Additional mechanisms for deflagration-to-detonation transition (DDT), including kernel-wall-interaction and kernel-kernel-interaction, are discussed by Blumenthal *et al.* [8].

Assuming an Arrhenius form, the ignition delay is given by

$$\tau_{\mathrm{ign}} = B \exp\left(\frac{E_{\mathrm{A}}}{\mathcal{R}T}\right) \,, \tag{3}$$

where B is an exponential prefactor that is generally a function of density, $E_{\mathrm{A}}$is the activation energy, and $\mathcal{R}$ is the universal gas constant. Taking the partial derivative of Eq. (3) with respect to temperature and defining the Arrhenius factor as $\mathcal{A} = E_{\mathrm{A}}/\mathcal{R}T$, the partial derivative of the ignition delay is given as

$$\frac{\partial \tau_{\mathrm{ign}}}{\partial T} = -\frac{\mathcal{A}}{T} \tau_{\mathrm{ign}} \,. \tag{4}$$

Following Peters *et al.* [9], the Taylor microscale, λ_{T}, is employed as the characteristic dimension of a flame kernel. From this, the temperature gradient is approximated as

$$\frac{\partial T}{\partial \xi} \approx -\frac{T'}{\lambda_{\mathrm{T}}} = -\mathcal{T}_T \frac{T}{\lambda_{\mathrm{T}}} \,, \tag{5}$$

where $\mathcal{T}_T$ is the temperature fluctuation level. Substituting Eqs. (4) and (5) into Eq. (2) the following is obtained:

$$a \mathcal{T}_T \tau_{\mathrm{ign}} \frac{\mathcal{A}}{\lambda_{\mathrm{T}}} = 1 \,. \tag{6}$$

Using homogeneous turbulence theory [10], the Taylor microscale is given by

$$\lambda_{\mathrm{T}} = \sqrt{10 \nu \tau_{\mathrm{t}}} \,. \tag{7}$$

Defining the relevant Mach number as

$$\mathrm{M} = \frac{U_{\mathrm{p}}}{a} \,, \tag{8}$$

with U_{p} being the characteristic piston speed, the SWACER criterion is found to be

$$\mathrm{Da_t} = \left(\frac{\mathcal{T}_T}{\mathcal{T}_u}\right) \frac{\mathcal{A}}{\mathrm{M}\sqrt{10}} \mathrm{Re_t}^{1/2} \,. \tag{9}$$

where $\mathrm{Da_t}$ is the turbulent Damköhler number, and $\mathrm{Re_t}$ is the turbulent Reynolds number. The turbulent Damköhler number is defined as

$$\mathrm{Da_t} = \frac{\tau_\mathrm{t}}{\tau_\mathrm{ign}} \,, \tag{10}$$

where τ_t is the turbulent time scale defined as the ratio of the integral length scale to the turbulent velocity fluctuation ($\tau_\mathrm{t} = l/u'$). The ignition delay is considered to be unaffected by turbulence and heat transfer in this definition. Additionally, this paper defines all relevant variables in algebraic expressions with respect to the conditions at the end of the compression stroke unless otherwise noted. The turbulent Reynolds number is defined as

$$\mathrm{Re_t} = \frac{u'l}{\nu} \,, \tag{11}$$

where ν is the kinematic viscosity.

Equation (9) shows the influence of compressibility and chemistry by the appearance of the Mach number and the Arrhenius factor, respectively; however, independence of the SWACER criterion to the design of the RCM is shown since it is likely that $\mathcal{T}_T \propto \mathcal{T}_u$. This criterion designates a mixtures propensity to ignite either as a detonation or as supersonic autoignition wave. The latter is interpreted in the context of an RCM as a strong ignition event.

3 Sankaran criterion

Sankaran *et al.* [11] postulated that a comparison between the velocity of the reaction front of an ignition kernel to the laminar flame speed yields a demarcation that indicates the propensity of a mixture towards mild ignition. This criterion is given as

$$\frac{S_\mathrm{L}}{u_\mathrm{RF}} = 1 \,, \tag{12}$$

where S_L is the laminar flame speed, and u_RF is the speed of the ignition front. The Sankaran criterion is qualitatively similar to the SWACER criterion. However, the Sankaran criterion is meant to demarcate the regime in which the mixture forms flame kernels, and the SWACER criterion is meant to indicate a flame kernel's propensity to transition to a detonation. Hence, the region bounded by these criteria is a transitional regime where a flame kernel readily transitions into a detonation wave or experiences mixed ignition. A mixed ignition event is characterized as a transient ignition state where flame fronts are produced before the mixture undergoes uniform ignition.

The evaluation of the speed of the reaction front is the same as that for the SWACER criterion. Using a two-zone model for a laminar premixed flame [12], the laminar flame speed is approximated as

$$S_\mathrm{L}^2 \approx 2\alpha \frac{\dot{\omega}_\mathrm{F}(T_\mathrm{f})}{\rho_\mathrm{F}} \,, \tag{13}$$

where α is the thermal diffusivity, $\dot{\omega}_\mathrm{F}$ is the consumption rate of the fuel, and ρ_F is the initial density of the fuel in the mixture. The consumption rate of the fuel is evaluated at the flame temperature of the fuel since the high temperature kinetics in the reaction zone dominate. For an autoignition event, a linear relationship between the ratio of fuel density to fuel consumption rate and ignition delay is assumed:

$$\frac{\rho_\mathrm{F}}{\dot{\omega}_\mathrm{F}(T_\mathrm{f})} = C_\mathrm{ign}\tau_\mathrm{ign} \,, \tag{14}$$

where C_ign is a proportionality constant.

Using the high activation energy asymptotics for a thermal explosion, given in Law [13], and comparing it to Eq. (14), the coefficient C_{ign} is deduced to be

$$C_{\mathrm{ign}} = \gamma\beta\mathcal{A}\, Y_{\mathrm{F}} \exp\left(-\mathcal{A}\frac{\beta}{\beta+1}\right), \tag{15}$$

where γ is the heat capacity ratio, and β is the heat release parameter, and Y_{F} is the mass fraction of the fuel. The heat release parameter, $\beta = \Delta H_{\mathrm{C}}/c_p T = (T_{\mathrm{f}} - T)/T$, compares the heat of combustion, ΔH_{C}, to the initial enthalpy of the mixture, $c_p T$.

Equation (14) implicitly assumes that a thermal explosion is the mechanism for ignition. For dilute strong ignition events in RCMs, chain branching is more likely the impetus for ignition. However, since temperature is the primary inhomogeneity due to heat loss to the walls and radical concentrations are assumed to vary negligibly throughout the mixture, flame kernels likely result from thermal explosion. Hence, the scaling given in Eq. (14) is considered appropriate for this demarcation.

Using Eq. (12) and substituting the Zeldovich relation for the speed of the ignition front and the turbulent Damköhler number in the same manner as discussed in Sec. 2, the Sankaran criterion is found to be

$$\mathrm{Da}_{\mathrm{t}} = \frac{\mathcal{T}_T^2\mathcal{A}}{5\,\mathrm{Pr}\,\gamma\beta Y_{\mathrm{F}}} \exp\left(\mathcal{A}\frac{\beta}{\beta+1}\right) . \tag{16}$$

Hence, the Sankaran criterion is independent of the Reynolds number. However, additional dependence on the chemical kinetics beyond that encapsulated by the turbulent Damköhler number appears in explicit form via the Arrhenius factor.

4 Comparision to experimental data and discussion

A comparison of the ignition demarcations with experimental data is presented in Fig. 1. All ignition delay data except for the University of Michigan syngas data were taken directly from experiments. For this data, adiabatic, isochoric reactors using the Li *et al.* [14] C_1-mechanism at the specified thermodynamic conditions were used since significant deviation in the experimental ignition delay time from the reactor model is found for the mixed/DDT and the mild ignition cases.

Since turbulence statistics are rarely measured in RCMs, the turbulent Reynolds number and turbulent Damköhler number were estimated using commonly reported details of RCM experiments. The turbulent time scale can be determined assuming the following relation:

$$\tau_{\mathrm{t}} = \left(\frac{C_l}{\mathcal{T}_u}\right)\frac{d}{U_{\mathrm{p}}} , \tag{17}$$

where the turbulence intensity is given by the ratio of the turbulent velocity fluctuation and the piston speed ($\mathcal{T}_u = u'/U_{\mathrm{p}}$), and the ratio of the integral length scale to the diameter of the RCM is given by $C_l = l/d$. The parameters $\mathcal{T}_u$ and C_l were assumed to be 1% and 10%, respectively. With the turbulent timescale estimated, both the turbulent Damköhler and turbulent Reynolds numbers were determined with available ignition delay and mixture property data.

Considering the highly stochastic nature of inhomogeneous ignition events, the demarcations show favorable agreement with the experimental data. The transition between the regimes is quite evident in the syngas data. However, the iso-octane data shows robustness in the mixed ignition regime; this is expected since two-stage ignition phenomena tend to homogenize the mixture, which decreases the propensity towards mixed or mild ignition. Additionally, fuels such as iso-octane exhibit a decreasing

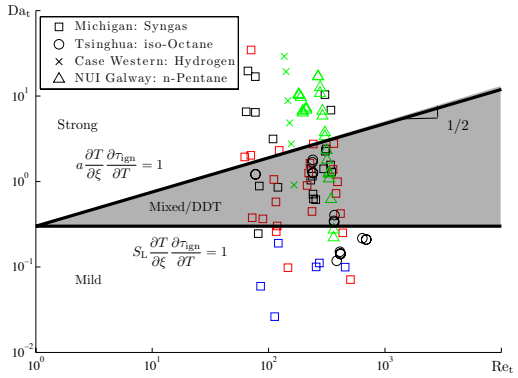

Figure 1: Comparison of the ignition demarcations to experiment. **BLACK** symbols indicate strong ignition, **RED** symbols indicate mixed/DDT ignition, **BLUE** symbols indicate mild ignition, and **GREEN** symbols indicate that the quality of ignition was not reported. □ taken from Mansfield *et al.* [15], ○ taken from Mansfield *et al.* [16], × taken from Mittal [17], and △ taken from Marks *et al.* [18].

Arrhenius factor as it approaches the NTC region; hence, the static demarcations with respect to the Arrhenius factor become increasingly conservative. The character of the ignition event is not reported for the NUI Galway and Case Western Reserve machines, but both are within the regimes where strong or mixed ignition is likely.

5 Conclusions

Rapid compression machines allow for low-temperature chemical kinetic studies in thermodynamic regimes under ideal conditions. However, mild ignition phenomenon can obfuscate the interpretation of these chemical kinetic studies. By considering the SWACER mechanism and the Sankaran criterion, demarcations were developed to indicate the prevalent ignition variety for a given turbulent Damköhler number and turbulent Reynolds number. These demarcations were compared against experiments, involving different RCM geometries, operating conditions, and fuel mixtures, and favorable agreement with the demarcations was found. Hence, mild ignition in RCMs can be predicted for many different configurations using only the turbulent Damköhler and turbulent Reynolds numbers.

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