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Chemical-Kinetic Modeling of Ignition Delay: Considerations in Interpreting Shock Tube Data

MARCOS CHAOS, FREDERICK L. DRYER

Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544-5263

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ABSTRACT: High-pressure shock tube ignition delays have been and continue to be one of the key sources of data that are important to characterizing the combustion properties of real fuels. At pressures and temperatures of importance to practical applications, concerns have recently been raised as to the large differences observed between experimental data and chemical-kinetic predictions using the common assumption that the shock tube behaves as a constant volume (V) system with constant internal energy (U). Here, a concise review is presented of phenomena that can considerably affect shock tube data at the extended test times (several milliseconds or longer) needed for the measurement of fuel/air ignition at practical conditions (i.e., high pressures and relatively low temperatures). These effects include fluid dynamic nonidealities as well as deflagrative processes typical of mild ignition events. Proposed modeling approaches that attempt to take into account these effects, by employing isentropic assumptions and pressure- and temperature-varying systems, are evaluated and shown to significantly improve modeling results. Finally, it is argued that at the conditions of interest ignition delay data do not represent pure chemical-kinetic observations but are affected by phenomena that are in some measure facility specific. This hampers direct cross

Correspondence to: Frederick L. Dryer; e-mail: fldryer@princeton.edu.

Present Address of Marcos Chaos: Fire Explosions and Dynamics Group, Fire Hazards and Protection Unit, FM Global Engineering and Research, Norwood MA 02062.

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comparison of the experimental ignition data collected in different venues. In such cases, pressure/temperature histories should be provided in order to properly interpret shock tube ignition data. © 2010 Wiley Periodicals, Inc. *Int J Chem Kinet* 42: 143–150, 2010

INTRODUCTION

Interest in the combustion characteristics of practical fuels and their surrogates at conditions relevant to those encountered in automotive as well as gas turbine engines has led to a number of recent shock tube studies involving high-density, undiluted fuel/air mixtures (e.g., [1–11]). These high-pressure studies extend to relatively low temperatures (below ~ 1100 K), well below typical dilute shock tube investigations aimed at achieving fundamental kinetic information on elementary reactions or validating chemical-kinetic models. The observations of chemical ignition delays that have emerged at these extended conditions are frequently used as validation data for developing insights to and detailed kinetic models for hydrocarbon oxidation chemistry that encompass negative temperature coefficient and hot ignition behavior, presenting valuable information for designers of combustions systems as well as modelers.

However, there has been an emerging concern about the interpretation of these shock tube data, most prominently raised by recent discussions concerning the ignition behavior of syngas mixtures [8]. There, similarities in ignition delay measurements from various shock tube, flow reactor, and rapid compression observations were noted to differ considerably from kinetic model predictions generated using homogeneous, zero-dimensional, isochoric modeling assumptions (i.e., constant internal energy, U , and volume, V) typically employed by kineticists. As a result, the fundamental understanding of syngas elementary chemical kinetics was brought into question. In considering these observations [12–14], we emphasized that the high sensitivity of induction chemistry to any type of experimental perturbations or nonidealities is what principally led to similarities in observations among the various experimental venues. Furthermore, we argued that disparities in observations and kinetic predictions were a result of the ideal modeling assumptions applied and their inability to represent experimental conditions appropriately. In the particular case of shock tube observations, we noted the multidimensional nature of the ignition event in the weak ignition regime where characteristic kinetic times are strongly influenced by induction chemistry involving HO_2 and H_2O_2 reactions, and we hypothesized a number of potential perturbing phenomena that would not be captured by modeling approaches that assume uniform,

constant U , V (or constant enthalpy, H , and pressure, P) conditions in the reflected shock gases. Finally, noting that hydrocarbon ignition delay data at similar temperatures, pressures, and energy densities were also commonly treated in the same ideal manner, we indicated that similar misinterpretations were likely to exist.

Recently, several papers have drawn attention to the fact that significant pressure variations can occur during ignition of syngas as well as hydrocarbon-oxidizer mixtures featuring long ignition times (several milliseconds or longer). These revelations have significant impact on the arguments made with regard to syngas combustion as well as hydrocarbon model validation based upon shock tube data presently in the literature. This communication is intended to bring wider attention to these issues and to review and summarize their implications in interpreting and modeling ignition delay data collected in shock tubes, as well as species–time histories that may be observed subsequent to ignition.

SCRUTINY OF SHOCK TUBE PRESSURE–TIME HISTORIES

Shock-induced self-ignition of undiluted fuel/air mixtures at the conditions of interest noted above are characterized by relatively long ignition delay times on the order of a few milliseconds. The ignition event is accompanied by marked changes in pressure and heat release. Hence, ignition under these conditions is strongly coupled to the thermodynamic state and fluid dynamics of the gas behind the reflected shock wave. Unidimensional analyses predict that the gas behind a reflected shock should be stationary and have uniform thermodynamic properties over the entire test volume. In the case of syngas/air mixtures, ideal analyses further predict that no significant preignition heat release can occur without substantial depletion of reactants, which could then be considered “ignition” as little chemical enthalpy is present in intermediates in comparison to reactants and products. On the other hand, preignition chemistry might occur in the case of hydrocarbons, as a result of negative temperature coefficient behavior (i.e., two-stage ignition), leading to observable radical and intermediate production. We also recently commented on similar chemical induction

processes that might occur during the compression phase in rapid compression machine studies that can perturb measured ignition delay times after compression ceases [15].

Practically, however, even for dilute mixture studies, unavoidable nonidealities exist in the shocked gases, due to the ubiquitous presence of boundary layers. Incident shock attenuation, boundary layer growth, and shock-wave/boundary-layer interactions lead to nonuniform pressures and temperatures behind the reflected shock, which gradually increase with time [16–18]. Furthermore, residual gas velocities may exist behind the reflected shock wave that also contribute to pressure gradients along the shock tube axis [19,20]. These nonidealities can be minimized by using large-diameter shock tubes, dilute fuel/oxidizer mixtures in monoatomic gases, and short test times (less than about 500 μ s) [16,17,20]. The latter two options typically are not applicable to ignition studies of undiluted fuel/air mixtures.

For highly reactive mixtures, the above-mentioned phenomena are further compounded by the fact that at high pressures and lower temperatures, shock tube ignition is inhomogeneous with observed localized “hot spots” in a deflagrative manner leading to a homogeneous transition to detonation [1,21–25]. Gas expansion due to the finite exothermicity of the initial, localized, heterogeneous reaction sites coupled with the high speed of sound in the shocked region can induce further increases in pressure throughout the gases behind the reflected shock, prior to the main ignition event. These features are typical of the well-known mild ignition process recently reviewed in [12–14]. For nonreactive mixtures, Petersen and Hanson [16] reported temperature increases (due to observed pressure gradients behind the reflected shock) of up to 40 K over 500 μ s for representative pressure and temperature ranges of 24–530 atm and 1275–1900 K, respectively, for a 5-cm tube. This temperature rise value was found to be highly dependent on shock tube diameter, and Petersen and Hanson [16] reported nonreactive temperature increases of \sim 20 K for a 12.7-cm shock tube and conditions similar to those mentioned above. However, for conditions relevant to practical fuels (i.e., 25–50 atm and 700–1000 K) and due to their relatively long ignition times, and the potential for localized reaction centers to be formed in the reflected gases during the experiments, more severe pressure and temperature increases are to be expected.

From the discussion above, it is clear that changes in the thermodynamic state of the gas behind the reflected shock wave are likely to be significant (especially for longer observation times and higher energy density fuel/oxidizer mixtures) and, thus, can have a pro-

nounced effect on kinetic observations as well as the ignition process [12–14]. Figure 1 shows pressure–time histories during ignition of several different fuel/air systems [1,3,5,26]. Pressure increases of nearly a factor of 2 prior to ignition can be observed (see Figs. 1a and 1c). In such instances, kinetic modeling of ignition delay should no longer be performed under the common assumption that the shock tube behaves as a constant volume system with constant internal energy. The pressure history in these cases is needed; however, this information is infrequently provided along with reported shock tube ignition delay measurements. Some experimental shock tube studies offer sample pressure profile plots where the ordinate scaling chosen (large enough to capture pre- and postignition pressure values) is such that pressure increases prior to ignition are not evident.

Although the aforementioned nonidealities present in shock tubes at the conditions of interest have been known for some time across the community and noted by a number of shock tube experimentalists [1,3,16–24], some recent shock tube studies of fuel/air mixtures have omitted that these phenomena might have considerable impact on modeling the reported data [4–11]. Even with this information in hand, the general modeling approach for analyzing shock tube data has typically been to apply constant U , V zero-dimensional modeling predictions to interpret the reported data. An interesting example is provided by the study of Davidson et al. [5] who acknowledged the presence of the preignition pressure rise seen in Fig. 1c and noted that existing kinetic models failed to predict this preignition activity. In their study, Davidson et al. [5] considered this behavior to be due to a chemical-kinetic process not predicted by the chemical-kinetic models used and postulated that matching the preignition pressure–time history (and associated heat release) would be a constraint and a good validation test for future model development and validation. Below, it is suggested that this result is from a misinterpretation of the experimental observations as occurring under constant U , V conditions.

Further evidence of similar disparities can be found in the study of Cadman et al. [27]. They reported a distinct decrease in the activation energy of propane–air ignition data for ignition times longer than approximately 1 ms. Such behavior could not be reproduced using available chemical-kinetic models. Cadman et al. [27] identified the importance to their observations of hydroperoxyl, propyl, and methyl radical chemistry, which they then considerably modified; the updated chemical-kinetic scheme, however, still could not reconcile the observed model–experiment differences. Furutani et al. [23,24] reported similar changes in the

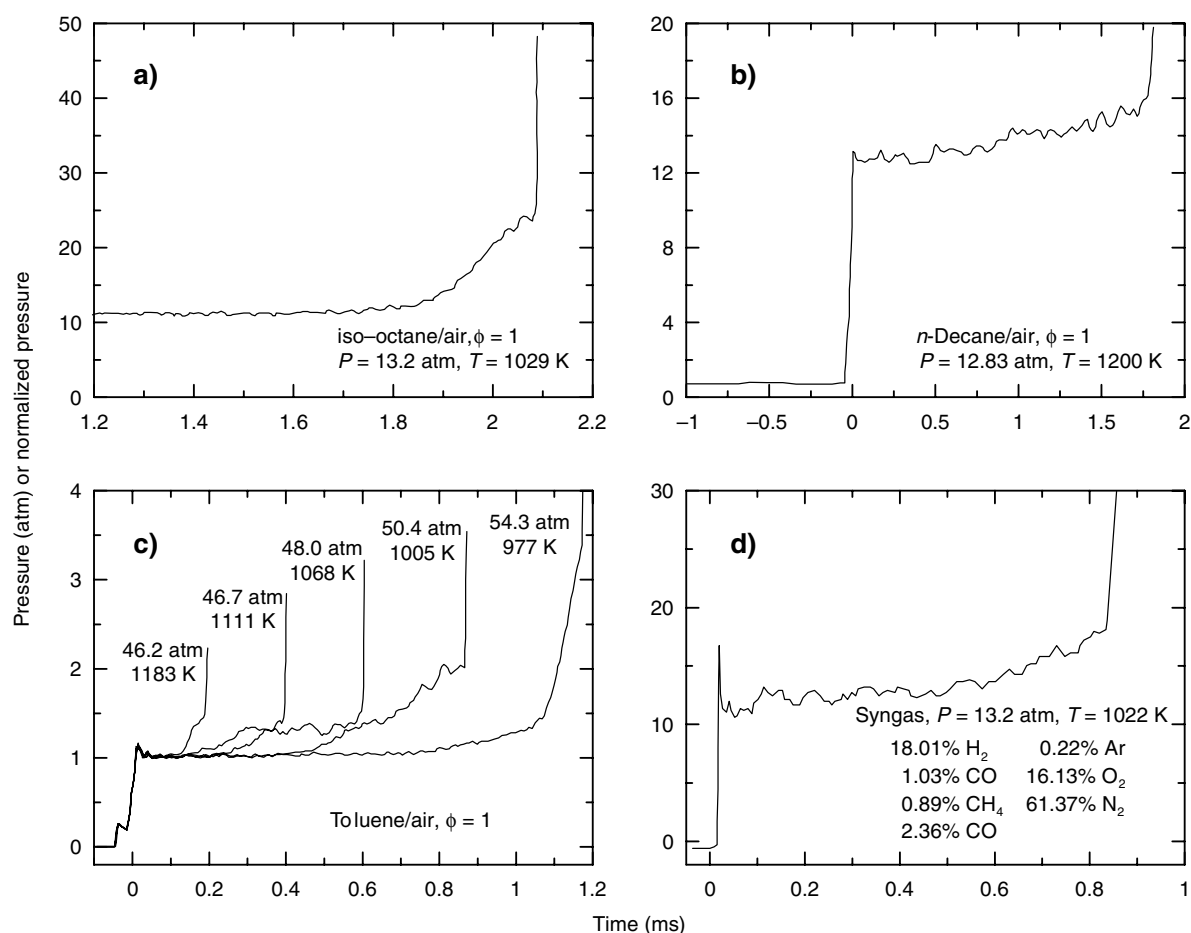


Figure 1 Typical experimental pressure traces during fuel/air ignition in shock tubes: (a) data from Fieweger et al. [1]; (b) data from Misawa et al. [3]; (c) normalized data from Davidson et al. [5]; (d) data from Reehal et al. [26].

activation energy of methane as well as isooctane ignition delays as those shown by Cadman et al. [27]. Based on the results of Furutani et al., however, it is clearly evident that the change in the activation energy of the data at lower temperatures and longer ignition times is solely due to the nonidealities discussed above rather than being dependent on chemical processes.

The issues outlined above have received considerable attention recently, evidenced by reports [28–34] where ignition delay data are further examined and pressure variations prior to ignition are identified and taken into account when interpreting and modeling the data. Their implications into how ignition delay chemical-kinetic modeling should be approached are discussed in the next section.

CHEMICAL-KINETIC MODELING APPROACHES

In several previous investigations, it has been suggested that preignition pressure variations in reflected

shock tube observations can be assumed to manifest in the system as polytropic processes [2,3,16,17,20]. Pressure histories and associated temperatures deduced from isentropic relations have been used by Fieweger et al. [2] to adjust isooctane/air ignition data affected by preignition pressure rise. Others [3,28,32] have opted to compute an effective or average pressure and temperature based on the observed pressure history and plot the data with respect to these adjusted values. The presence of dynamic pressure features prior to ignition can have considerable effects on radical initiation processes, as discussed by Mittal et al. [15]. Therefore, it is important to include measured pressure histories in modeling approaches rather than using averaged or effective values.

Li et al. [29] propose a specific modeling tool for shock tube applications, CHEMSHOCK, which allows for the treatment of time-varying pressures coupled with chemical kinetics. CHEMSHOCK solves the coupled energy and chemical species system of differential equations using a two-step process: at every time

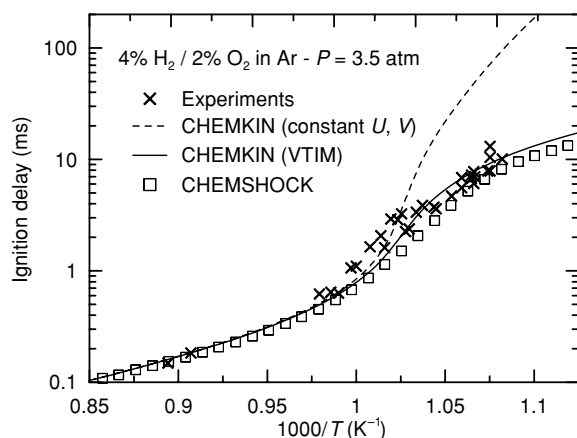


Figure 2 Comparison between calculations performed using CHEMSHOCK [29] and SENKIN [35] employing the VTIM option (see the text). Predictions with constant U , V assumptions are also shown. Model results are compared with the data of Pang et al. [30]. Both CHEMSHOCK and VTIM approaches use a linear pressure rise of 2%/ms prior to ignition.

step the system is first solved assuming constant U , V conditions, and then pressure and temperature are adjusted isentropically to match the measured pressure profile while keeping the chemical composition fixed. Pang et al. [30] showed promising results using CHEMSHOCK in modeling ignition delay data of H_2/O_2 mixtures (see Fig. 2).

More generally available codes can also be used to consider pressure variations in shock tube ignition delay predictions. SENKIN [35], part of the CHEMKIN-II [36] suite of programs, is completely capable of handling this situation. A time-dependent polytropic compression (or expansion) results in both volume and density changing with time. In contrast to other options such as CONP (constant enthalpy and pressure) and CONV (constant internal energy and volume, commonly used for shock tube modeling), the VTIM (i.e., volume as a function of time) option in SENKIN can be employed to emulate a time-dependent polytropic state change. The user must only provide time functions for variations in the specific volume of the system. Knowing the functional variation of pressure from the measured data and assuming isentropic compression/expansion, the functions to be provided are

$$v(t) = \frac{1}{\rho_0} \left[\frac{P(t)}{P_0} \right]^{-1/\gamma}$$

$$\frac{dv}{dt} = -\frac{1}{\gamma} \frac{v(t)}{P(t)} \frac{dP}{dt}$$

where v is the specific volume, P the measured pressure, γ the specific heat ratio, and P_0 and ρ_0 are the initial pressure and density, respectively, behind the reflected shock wave. This approach has been successfully used in the modeling of rapid compression machine ignition and is further detailed in [37]. Petersen and Hanson [16] also used a similar methodology to account for observed pressure variations behind reflected shock waves.

Figure 2 shows computations performed using both SENKIN and CHEMSHOCK against data collected by Pang et al. [30] for validation of the CHEMSHOCK model. In the experiments, for $\text{H}_2/\text{O}_2/\text{Ar}$ (4/2/94 mol) mixtures, a linear pressure rise of about 2%/ms was observed for pressure and temperature conditions of 3.3–3.7 atm and 924–1118 K, respectively. For consistency the present SENKIN chemical-kinetic calculations shown in Fig. 2 were performed using GRI-Mech 3.0 [38] and implementing the same updates for the heat of formation of OH [39] and the reaction $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$ [40] as those used by Pang et al. [30]. For ignition times less than approximately 1 ms, the SENKIN constant U , V model agrees fairly well with the data. At longer test times, the gradual pressure (and temperature) increase can have considerable effects on the ignition process, as noted above. In this case, Fig. 2 shows that the constant U , V approach fails to provide a good estimate of ignition delay for temperatures lower than 975 K. SENKIN modeling with VTIM assuming a linear pressure profile provides much improved predictions and yields very similar values to those computed with CHEMSHOCK.

Unlike the trends observed in the study of Petersen and Hanson [16] and Pang et al. [30], for higher concentrations of reactants (i.e., fuel/air mixtures) and due to the mild ignition processes discussed above, observed pressure rises are seldom linear, as shown in Fig. 1. In the case of toluene, the pressure traces shown in Fig. 1c can be used to further demonstrate the application of the SENKIN/VTIM approach described above. Davidson et al. [5] showed that an available toluene model [41] considerably overpredicted ignition delays of stoichiometric toluene/air mixtures (see Fig. 3) while providing reasonable results for lean mixtures. Fieweger et al. [1] indicated that significant pressure increases, as shown in Fig. 1a, occurred for isooctane/air mixtures only at stoichiometric conditions; toluene may, thus, exhibit similar behavior. Figure 3 shows the model–data discrepancies discussed by Davidson et al. [5]. Note, however, that data collected at 17 atm exhibit relatively short ignition delays at lower temperatures, comparable to those at 50 atm. This is not a result of chemistry leading to negative temperature coefficient behavior as toluene exhibits no such behavior [42,43].

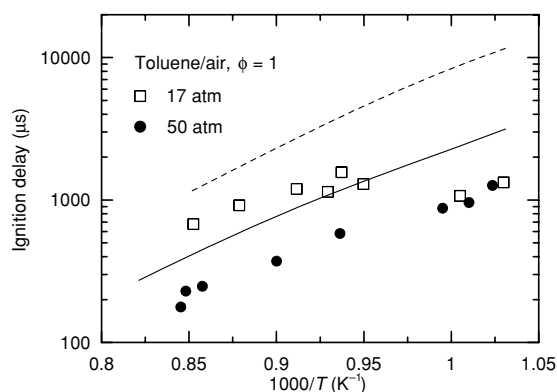


Figure 3 Experimental [5] (symbols) and model [41] predictions (lines, employing constant U , V assumptions) for stoichiometric toluene/air mixtures; the dashed line corresponds to open symbols. The experimental data have been normalized to the pressures shown assuming proportionality to P^{-1} . Pressure traces for data represented by solid symbols can be found in Fig. 1c.

Even though pressure profiles were not reported for the 17-atm data [5], the traces shown in Fig. 1c for the 50-atm data set indicate strong preignition activity that cannot be approximated using a linear pressure increase assumption. Here, for modeling purposes, we have approximated the traces shown in Fig. 1c as having constant pressure for a finite amount of time and then increasing linearly until the moment of ignition (see Fig. 4a). Applying this assumption to the five conditions shown in Fig. 1c and using SENKIN/VTIM, the computed ignition delays show considerably improved agreement with the experimental data as shown in Fig. 4b.

Shen et al. [44] recently presented additional data on toluene ignition that contrary to the data of Davidson et al. [5] showed no evidence of preignition activity, consistent with rapid compression machine measurements performed by Mittal and Sung [45]. They speculated, again consistent with Mittal and Sung's conclusions, that wall contamination might have been responsible for producing preignition phenomena in the work of Davidson et al. However, very recently, Vasu et al. [33] have reexamined toluene ignition delays and concluded that contamination was not the source of the preignition events observed by Davidson et al. They conclude that preignition events can be correlated with experimental conditions that result in mild, strong, and mild to strong ignition regimes. This conclusion is completely consistent with the observation of localized ignition centers under conditions in the mild and transition regimes in other shock tube research. We have noted earlier that under such conditions ignition chemistry is strongly influenced by chemical induction

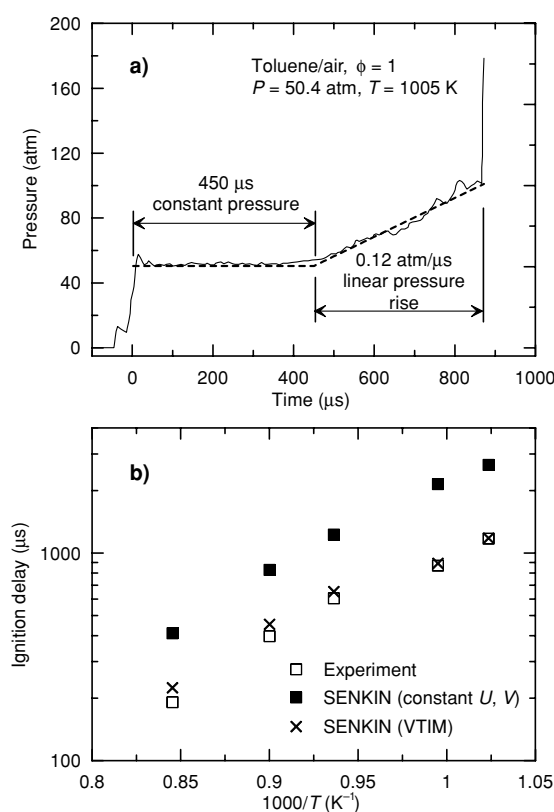


Figure 4 Effect of pressure rise on the modeling of toluene/air ignition delays: (a) pressure profile approximation used as input for SENKIN/VTIM; similar profiles were used for the traces shown in Fig. 1c; (b) experimental data [5] and computational results (using the model of Pitz et al. [41]) using constant U , V and including the effect of preignition pressure rise.

processes, which inherently have high sensitivity to chemical and fluid dynamic perturbations [13,14].

As noted previously, similar considerations warrant revisions in the analyses of the syngas data of Petersen et al. [8]. Furthermore, emission from the hydroxyl radical collected at the shock tube's endwall [26,32] indicates that these data show severe mild ignition characteristics that, as explained above, in conjunction with boundary layer effects, help compress the test mixture prior to a more general ignition event behind the reflected shock. Pressure profiles for the data reported by Petersen et al. [8] are not available; therefore, Fig. 5 shows results using assumed linear pressure gradients of 2%, 5%, and 10%/ms prior to ignition. These values are conservative as the presence of mild ignition events will certainly change pressure signals considerably (see [32]). It can be seen that these simplified assumptions yield good agreement with the data over the entire temperature range. Although Petersen et al. [8] did not discuss the characteristics of the pressure signals associated with their shock tube data, in recent work [26,32]

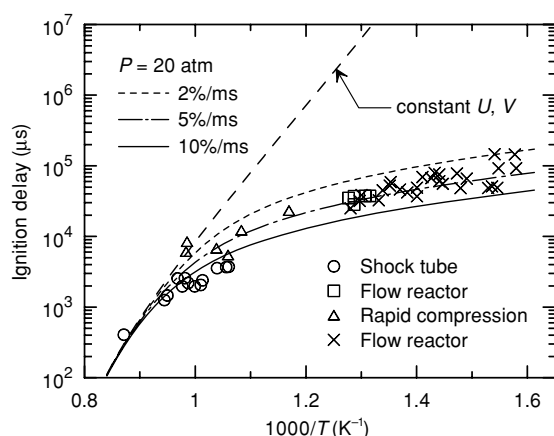


Figure 5 Effect of preignition linear pressure rise applied to the modeling of syngas/air ignition under the conditions of Petersen et al. [8]. Experimental conditions and associated references for the data shown can be found in [8,12,13].

they have shown that syngas shock tube ignition exhibits considerable pressure variations, and they themselves concluded that their data cannot be analyzed properly by constant U , V predictions. Even more recently, in considerations of propane rapid compression machine and shock tube ignition work, Aul et al. [34] have applied similar thinking to what is expressed herein as well as in [13,14] to reconcile disparities in experimental observations and modeling predictions.

CONCLUSIONS

High-pressure shock tube ignition delays have been and continue to be one of the key sources of data that provide insights into the combustion characteristics of real fuels. These are very important resources for our work and that of many others developing and validating chemical-kinetic models. The large differences seen between the experimental data and chemical-kinetic predictions using the more commonly applied assumption that shock tube observations are well reproduced by a constant volume (V) system with constant internal energy (U), needs to be carefully considered where significant preignition chemistry and pressure rise are noted in experimental observations. The non-idealities present in shock tube observations become more important at longer ignition delay conditions, characteristic of mild and mild-strong transition kinetic regimes and can considerably affect the data at extended tests times of several milliseconds needed for the measurement of fuel/air ignition at high pressures and lower temperatures. These effects, coupled with deflagrative processes typical of mild ignition events, serve to compress the test mixture prior to ignition leading to reduced ignition delays. Preignition pressure

(and associated temperature) changes have been shown to be reasonably approximated by isentropic assumptions and using well-established kinetic modeling approaches that take into account time-varying systems.

Although these nonidealities and mild ignition events reviewed herein have been known for a long time, their potential importance has frequently not been reflected in terms of the modeling assumptions used in attempting to predict experimental observations. This has led to misinterpretation of the data by both experimentalists and kinetic modelers alike, including ourselves, and to searching for kinetic model modifications and alterations that were inappropriate and unnecessary. For shock tube studies of fuel/air ignition that encompass mild and mild-strong ignition regimes, frequently encountered at high pressures and relatively low temperatures, the experimental data need to be reported along with pressure–time histories. At these conditions, it is clear that the ignition delay data do not represent pure chemical delay measurements under the ideal conditions, but are affected by phenomena that cannot be interpreted as pure homogeneous constant U , V kinetic measurements. Agreement of modeling predictions with experiments is dependent on the kinetic model, its response to dynamic variations in pressure and temperature caused by facility-dependent issues and polytropic compression if local thermal centers evolve during preignition. This precludes direct cross comparison of the experimental data collected in different venues without inferring adiabatic compression phenomena effects on end-gas conditions and the pressure–temperature response of the kinetic model to these phenomena.

Moreover, ignition delay measurements dominated by induction chemistry effects are in general extremely sensitive to numerous perturbation sources. Many have considered the experimental observations to be “imperfect,” and have attempted to determine and eliminate the source(s) of each and every perturbation to obtain “pure,” unperturbed results. It is highly probable that applied combustion configurations will result in one or more perturbations which substantially reduce chemical induction times and hence observed ignition delays. The “perturbed” measurements may thus be more relevant to some engineering design issues than the unperturbed results.

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