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Harold D. Beeson and Richard D. McClenagan, Lockheed–ESC
Frank J. Benz, NASA
NASA White Sands Test Facility
Las Cruces, NM

W. J. Pitz and C. K. Westbrook
Lawrence Livermore National Laboratory
Livermore, CA

John H. S. Lee
McGill University
Montreal, Canada

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William J. Pitz and Charles K. Westbrook
Lawrence Livermore National Laboratory
Livermore, California

John H.S. Lee
McGill University
Montreal, Canada

ABSTRACT

Liquid hydrocarbon fuels are used extensively in propulsion systems, and explosion hazards associated with fuel vapors (or droplets) mixed with air must be assessed. In this paper, the detonation of gas phase mixtures of n-hexane and the commercial fuel, JP-4, with oxidizers varying from pure oxygen to air, have been studied both experimentally and theoretically via kinetic modeling. Experiments were carried out in a detonation tube 150 mm in diameter and 1.75-m long. The detonation tube was heated to control the vapor pressure of the fuel. An exploding bridge wire with 2000 J was used for initiation, except for less sensitive mixtures when a solid explosive charge was used. Detonation velocities and cell sizes, λ, were measured as a function of stoichiometry and diluent concentration. The theoretical model calculates the induction length, Δ, of a one-dimensional ZND detonation using the detailed kinetics for the reaction of the hydrocarbon fuel used. Using the same constant of proportionality of 29 (i.e. $\lambda = 29\Delta$) found previously for other hydrocarbons, the theoretical prediction for the cell size of n-hexane is found to agree well with the experimental data. Due to the non-standard composition of the JP-4, no detailed modeling was carried out for this fuel. Because n-hexane is the principal component of JP-4, however, this fuel would be expected to behave similarly to n-hexane. This similarity is confirmed experimentally. The cell size data obtained for n-hexane and JP-4 was found to be slightly less than that of the other lighter hydrocarbons in the same alkane family with the exception of methane (i.e. ethane, propane, n-butane, etc.). Critical energy and critical tube diameter are compared for a relative measure of the detonability of the heavy hydrocarbon fuels studied, and it appears from kinetic modeling that the detonation sensitivity increases slightly with increasing carbon number; however, this trend cannot be distinguished experimentally with the error in cell size measurement.

INTRODUCTION

Detonations represent a major source of hazard in the use of hydrocarbon fuels in practical combustion systems. The study of detonations also provides insight into the fundamental interactions between the fluid mechanics and chemical kinetic properties of combustion. Detonations have been the subject of many experimental, theoretical, and computer modeling studies, and it is beyond the scope of the present paper to survey this extensive literature. The entire field was reviewed quite recently [1], and other reviews have appeared [2].

Most previous detonation studies have dealt with relatively small hydrocarbon-fuel molecules, both in experimental work [3,4] and modeling analyses [5-7]. From the kinetic modeling point of view, one important reason for the focus on smaller fuels has been the fact that only very recently have mechanisms for fuels as large as n-pentane [8] and n-octane [9,10] been developed.

From the experimental point of view, a different factor has been responsible for the past concentration on smaller fuels: larger fuels (those with about six or more carbon atoms) exist as liquids under normal conditions of temperature and pressure. While it is not impossible to produce detonable fuel-oxidizer mixtures for these larger hydrocarbon molecules, their lower volatility certainly complicates experimental studies of their combustion and detonation properties. However, many practical hydrocarbon fuels, particularly those often used for aviation fuels and other propellants, include large fractions of these liquid fuels. Therefore, it is very important to be able to study these fuels, in spite of the difficulty of dealing with them in well-posed experimental conditions.

With liquid fuels such as n-hexane, two distinct types of detonations are very important: those involving aerosols or sprays, and those consisting of purely gas-phase fuel-oxidizer mixtures. Of particular interest are detonations that propagate through a droplet or aerosol spray. Bull [11] reported studies of spray detonations in which n-hexane was the fuel, while experiments [12] indicated that under conditions very similar to those for n-hexane, n-decane would not support a spray detonation. A great deal of work remains to be done to unravel the mysteries of spray detonations, including the identification of the controlling physical and chemical processes in these detonations.

To provide insight into some of those processes, gas-phase detonations can be studied as a form of limiting condition. The purely chemical kinetic factors that influence detonability can be examined in detail by eliminating complicating factors such as the formation and vaporization of a spray, the interaction of a shock wave with arrays of droplets, the mixing of the vaporized fuel with the oxidizer, and chemical ignition in a fuel-oxidizer medium that is not homogeneous. These results can then be integrated into a future, more complex model that includes the additional factors important in a true spray detonation. Without a thorough description of the gas-phase problem, analysis of the spray case would be overly speculative. The present study reports the results of exactly this type of problem: the detonability of gas-phase mixtures of n-hexane, oxygen, and nitrogen, and mixtures of JP-4, oxygen, and nitrogen.

For practical applications, mixtures of fuels with air are of primary importance. The spatial scales for such detonations and the amounts of energy required to initiate such detonations are often quite large, however, making it inconvenient and even dangerous to carry out the fuel-air experiments. It is therefore common to study fuel-oxygen mixtures, for which the relevant scales are much smaller, and systematically dilute these mixtures with increasing amounts of nitrogen until the scales become larger. These results are then used to extrapolate, in terms of further dilution by nitrogen, to mixtures that have a nitrogen/oxygen ratio equal to 3.76, the ratio in normal air. This approach has been used productively in many experimental studies [3,13,14], and modeling studies have provided further refinements for this extrapolation procedure [5,7]. These approaches are employed in the present study.

EXPERIMENTAL DETAILS

The experiments were carried out in a 150-mm diameter and 1.75-m long insulated detonation tube (Figure 1). The tube could be heated above ambient temperatures by electrical tape to maintain the hydrocarbon fuel in the vapor phase. A 1-liter heated vaporizer vessel was used to evaporate the liquid fuel so that the fuel vapor could be introduced into the evacuated detonation tube. The fuel concentration was monitored by partial pressure.

The rest of the mixture components (oxygen and nitrogen) were added to the detonation tube, and mixing was accomplished by a propeller fan at the end of the tube.

The initiation of the detonation was achieved with a 2000 J exploding bridge wire for the sensitive mixtures. For the less sensitive, highly dilute mixtures, however, a solid explosive charge of PETN (or various lengths of primacord) initiated by a #8 blasting cap was used. A short length of schelkhin spiral was also placed at the ignition end to ensure the formation of the detonation. For diagnostics, four PCB piezoelectric transducers were used to measure the detonation velocity. Detonation cell sizes were measured by inserting a metallic smoked foil at the end of the detonation tube.

The vapor pressure (as a function of temperature) of the JP-4 used in the experiment and of n-hexane is shown in Figure 2. For the mixtures studied with the highest fuel concentration, the vapor pressure corresponds to about 8.1 kPa. This vapor pressure corresponds to a temperature of 293 K. Similar results were obtained for the JP-4 liquid fuel used. The maximum initial temperature of the heated detonation tube required to maintain the fuel in the vapor phase was, therefore, about 293 K. This modest initial temperature above ambient played a negligible role in the equilibrium detonation properties and induction kinetics of the mixture.

THEORETICAL MODELING

The Zeldovich-von Neumann-Doring (ZND) model was employed, in which a detonation (locally) consists of a shock wave traveling at the Chapman-Jouguet (CJ) velocity, followed by a reaction zone. The shock wave compresses and heats the fuel-oxidizer mixture, which then begins to react. In most mixtures, the fuel oxidation consists of a relatively long induction period, during which the temperature and pressure remain nearly constant, followed by a rapid release of chemical energy and temperature increase. For each fuel-oxidizer mixture considered, the CJ conditions were computed using the TIGER code [15]. From the detonation velocity, D_{CJ}, the conditions in the von Neumann spike (including the temperature T_1, pressure P_1, and the particle velocity u_1 of the post-shock unreacted gases) were computed and used as initial conditions for the chemical kinetics model. In actuality, the shock velocity and other physical properties of the detonation varied within a single detonation cell; therefore, the CJ conditions (and the computed induction times) represented average values.

The reactive mixture volume was assumed to remain constant over the mixture's reaction time, and the induction time was defined in terms of the mixture's temperature history. The mixtures considered in the present study experienced a temperature increase of more than 1000 K, and the induction time was defined as the time of maximum rate of temperature increase. This coincided closely with the time at which the temperature had completed about half of its total increase. This is not, strictly speaking, a true induction period (which is often defined as the time required for a small [1 - 5 percent] temperature or pressure increase), but it represents a time scale for the release of a significant amount of energy. In a detonation, it is this macroscopic energy release that reinforces the shock wave and permits a detonation to propagate; therefore, the definition of the characteristic time used here was motivated by the properties of a detonation. In addition to the induction time, τ, it is useful to define the induction length $\Delta = \tau (D_{CJ} - u_1)$, which represents a characteristic length scale in the post-shock unreacted gas mixture.

The computed induction times and lengths defined characteristic time and length scales rather than the precise history of a gas element through the detonation front. The evolution of the reacted gas subsequent to the induction period considered here was dominated by the fluid mechanics of the post-induction expansion of the reaction products. This expansion reduced the pressure and density of the products and altered the kinetic equilibrium, leading eventually to the CJ state. Because virtually all of the reactants had been consumed by this time, the kinetics of this final expansion phase were controlled by relatively slow radical recombination processes. The present model does not attempt to follow that entire relaxation phase, concentrating on the details of the induction kinetics in the von Neumann spike. Shepherd has constructed a model that follows the entire process (combining the fluid mechanics with the reaction kinetics in the case of hydrogen-air mixtures), and found results that were very similar to those obtained using the present simplified approach [16].

This model of the detonation neglects some potentially significant effects associated with the fluid mechanics parts of the gas history. Variations of density, temperature, and particle velocity in the post-shock unreacted mixture were not considered. Multiple shock wave reflections, rarefactions, interactions with confining walls, cellular structure, and related effects were also not treated directly by the present simplified model.

For the kinetic model, the same type of approach employed presently has been used in the past to study detonation parameters for fuels such as hydrogen, methane, ethane, ethylene, methanol, acetylene, and propane [5-7,17,18]. Recent applications have included a wide variety of larger fuels, including ethers, nitrates, and other complex fuels [19]. In the present case of n-hexane, the reaction mechanism was assembled by adding reactions for n-hexane and its immediate products to an existing reaction mechanism for the oxidation of n-pentane [8]. Reactions for the unimolecular decomposition of n-hexane were based on those for n-pentane. Abstraction reaction rates of H atoms from n-hexane were based on the principle that rates of abstraction of primary and secondary H atoms from a hydrocarbon fuel are relatively insensitive to the size and structure of the parent fuel, so these rates could be estimated from analogous reactions in n-pentane and other comparable fuels. Subsequent reactions of hexyl radicals were assumed to be dominated by the process of β-scission, producing smaller olefins and alkyl radicals. In this formulation, the reaction mechanism for the oxidation of n-hexane was viewed as a perturbation of mechanisms for n-pentane and smaller hydrocarbon fuels.

The second fuel used in the present study was JP-4, a complex mixture of hydrocarbon fuels. Modeling was not attempted with this particular fuel, but it is known that its combustion characteristics are quite closely related to those of n-hexane, and n-hexane is a major component in JP-4. Most of the conclusions of the present kinetic analysis of n-hexane would be expected to apply closely to the case of JP-4.

The important kinetic features of the ignition of n-hexane at the high temperatures characteristic of detonation conditions were dominated by the reactions of the H_2-CO-O_2 submechanism. In particular, the chain branching reaction,

$$H + O_2 \rightarrow O + OH \qquad (1)$$

which produces two radicals O and OH for each H atom radical, is particularly important. Those reactions that produce H atoms accelerate the overall rate of ignition, because the H atoms then produce two new radical species via Reaction (1). Smaller radical species, which lead to H atom production, also accelerate the overall rate of ignition. An example of this is the ethyl radical C_2H_5, which decomposes at elevated temperatures to produce H atoms and ethylene through the reaction

$$C_2H_5 \rightarrow C_2H_4 + H \qquad (2)$$

In contrast, those reactions that produce methyl CH_3 radicals actually retard the overall rate of ignition, because many of those methyl radicals recombine to produce ethane,

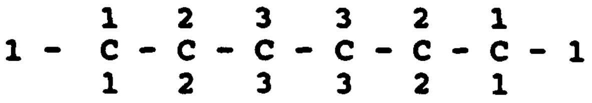
$$CH_3 + CH_3 \rightarrow C_2H_6 \qquad (3)$$

which, because it is relatively stable, does not produce new radical species.

The major reactions consuming n-hexane under the present conditions are its unimolecular decomposition, followed by reactions with OH, H, O, CH_3, and HO_2. The important decomposition reactions are:

$$nC_6H_{14} \text{ --> } pC_4H_9 + C_2H_5$$
$$nC_6H_{14} \text{ --> } nC_3H_7 + nC_3H_7$$

The former leads to the production of H atoms from both the p-butyl and ethyl radicals, while the second reaction leads to two methyl radicals. The H atom abstraction reactions produce three logically different hexyl radicals, those in which the H atom has been taken from the 1, 2, and 3 sites in the hexane molecule,



$$\begin{array}{ccccccccccccccc} & & 1 & & 2 & & 3 & & 3 & & 2 & & 1 & & \\ 1 & - & C & - & C & - & C & - & C & - & C & - & C & - & 1 \\ & & 1 & & 2 & & 3 & & 3 & & 2 & & 1 & & \end{array}$$

where the numbers 1, 2, and 3 indicate logically distinct H atoms in the n-hexane molecule. These sites must be kept distinct, because the subsequent decomposition of the product alkyl radicals leads to different products. The dominant decomposition paths are as follows:

1) $1\text{-}C_6H_{13} \text{ --> } C_2H_4 + 1\text{-}C_4H_9$

$$1\text{-}C_4H_9 \text{ --> } C_2H_4 + C_2H_5$$
$$C_2H_5 \text{ --> } C_2H_4 + H$$

2) $2\text{-}C_6H_{13} \text{-->} C_3H_6 + 1\text{-}C_3H_7$

$1\text{-}C_3H_7 \text{-->} C_2H_4 + CH_3$

3) $3\text{-}C_6H_{13} \text{-->} 1\text{-}C_4H_8 + C_2H_5$

$C_2H_5 \text{-->} C_2H_4 + H$

$3\text{-}C_6H_{13} \text{-->} 1\text{-}C_5H_{10} + CH_3$

Thus the abstraction of H atoms from the 1 sites in n-hexane leads eventually to the production of H atoms and acceleration of the overall rate of ignition, while the 2 site leads to a slower rate of ignition, and the 3 site leads to both H atoms and CH_3 radicals. In addition to the thermal decomposition of the alkyl radicals, the $1\text{-}C_6H_{13}$ and $2\text{-}C_6H_{13}$ radicals are inter-related through internal H atom abstraction reactions. The subsequent reactions of the ethylene, propene, and 1-butene are already well understood from previous modeling studies; therefore, the most important features of the n-hexane mechanism can be presented in terms of the ways that they eventually impact the mechanisms for smaller fuels and lead to H atom or CH_3 radical production. There are minor paths in the n-hexane reaction mechanism that are also included (paths that lead to production of hexenes and other intermediate hydrocarbon species), but these play a minor part in the induction process.

RESULTS AND DISCUSSION

Measurements for the detonation velocity deduced from the time of arrival at the various pressure transducers are shown in

Figure 3. Velocities were obtained for hexane and JP-4 at two fuel compositions of $\phi = 1$ (stoichiometric) and $\phi = 1.5$, and for various nitrogen dilutions, β. Also shown are the theoretical curves for the CJ detonation velocity computed using the Gordon-McBride code [20]. The experimental results are in accordance with the theoretical CJ values with typical velocity deficits of less than 10 percent for most cases. For the high nitrogen diluted mixtures when very large amounts of initiation energy were used, the detonation velocities appear to be slightly overdriven because the detonation tube was only 1.75-m long. Results for both hexane and JP-4 showed insignificant differences between the two fuels, within the experimental error of the present study.

The cell sizes for hexane and JP-4 detonations are shown in Figures 4 and 5, respectively. The detonation sensitivity (as inferred from the cell size) for both JP-4 and hexane are about the same, indicating that the presence of other hydrocarbons in JP-4 are not important in influencing its induction kinetics. Due to the limitation of the present detonation tube (short length and small diameter), the less sensitive mixtures with higher values of β could not be studied. For JP-4, the cell size was measured in support of this study in a larger tube at Sandia National Laboratory. The Sandia heated detonation tube was 43 cm in diameter and 13.1 m in length. The Sandia cell size data for JP-4/air mixtures ($\beta = 3.76$) are also plotted in Figure 5, and are consistent with the data obtained for more sensitive mixtures obtained in the smaller apparatus. Additionally, recent results reported by Sandia National Laboratories for hexane/air ignitions are plotted in Figure 4 [21].

For kinetic modeling, computations were carried out using the approach outlined earlier, which has been used in previous studies for other similar hydrocarbon fuels. Only n-hexane was included in the modeling analysis. Kinetic induction times were computed for stoichiometric n-hexane/oxidizer mixtures and for fuel-rich mixtures with $\phi = 1.5$. The entire range from pure oxygen to air as the oxidizer was included for both equivalence ratios.

As outlined previously, the computed induction length $\Delta - \tau (D_{CJ} - u_1)$ has been related to the cell size by a simple constant of proportionality. In earlier work, the majority of the fuel-oxidizer mixtures were best correlated if this constant of proportionality was approximately 29 [5,6]. If exactly the same relationship between computed induction time and cell size is used, the model predictions for cell sizes agree quite well with the experimentally measured values over the range of conditions studied. These results are indicated in Figure 6, in which the computed cell sizes (using the proportionality of $\tau = 29\Delta$) are indicated as filled symbols.

Over the range of conditions studied experimentally, the agreement between kinetically predicted and measured cell size is very good. This is particularly true in the middle range where $1.0 < \beta < 2.5$. This suggests strongly that n-hexane, in the gas phase, is very similar to most other hydrocarbon fuels in the way that the chemical kinetics of ignition influences detonability. This result was expected, because it is well established that the ignition of n-alkane fuels under high temperature conditions is a very weak function of fuel size [22]. Those factors that affect the relationship between induction length and cell size are very much the same for all of these fuels. One of the most important of these factors must be the wave propagation velocity, and because all of these mixtures are dominated by oxygen and nitrogen, this conclusion is consistent with the fact that the hydrocarbon fuel does not contribute very much to the thermodynamic properties of the combustible mixture. The amounts of water and carbon dioxide in the product gases in these mixtures were roughly constant as well.

Of particular interest are the limiting conditions for the cell sizes as $\beta \rightarrow 0$ and as $\beta \rightarrow 3.76$ (normal air). For n-hexane/oxygen mixtures, the predicted cell size is slightly smaller than that observed experimentally, but the two values are quite close together. If the experimental results are extrapolated to $\beta = 0$, the estimate of the cell size is larger than that observed by more than a factor of 2. The kinetic model, therefore, provides an improved basis for extrapolation of the experimental results. This really means that linear extrapolation to the experimental data in Figures 4 and 5 is not valid, in part because the variations in induction length with nitrogen dilution are very non-linear. Similar curvature as $\beta \rightarrow 0$ is seen for other hydrocarbon fuels [5-7]. At the other limit, the predicted cell size for stoichiometric n-hexane/air is $\lambda = 111$ mm. When an extrapolation to n-hexane/air conditions is made solely on the basis of the experimental results, the best estimate is $\lambda = 85$ mm for $\phi = 1.0$ and $\lambda = 79$ mm for $\phi = 1.5$, while the direct measurement of cell size is reported to be 55 mm [21]. Clearly, the kinetic model provides a significantly larger estimate of the cell size under n-hexane/air conditions.

Several overall observations can be drawn from the present computational results. First, the constant of proportionality between the computed induction length and the cell size data (≈ 29) is the same as that determined previously for many other hydrocarbon fuels [5]. This indicates that the same type of scaling can be applied for a very wide range of hydrocarbon fuels, including many for which experiments may not have been carried out but kinetic mechanisms may exist. It also indicates that the reaction mechanism and numerical model are generally reliable.

For stoichiometric fuel-air mixtures with hydrocarbon fuels larger than methane or ethane, the predominant species in the reactive mixture are oxygen and nitrogen. This means that physical quantities such as the sound speed and heat capacity of the reactant mixtures will vary only slightly from one hydrocarbon fuel to another. The adiabatic flame temperature and heat of reaction are also very similar for these fuels. Combined with the near-constancy of the computed induction times for these fuels [20], this suggests very strongly that the cell sizes will also be very similar for the same gaseous fuels. Therefore, if major differences are observed experimentally between detonation cell sizes for hydrocarbon/air mixtures (particularly for n-alkane/air mixtures with 4 to 10 carbon atoms), they are probably attributable to variations in parameters (such as vapor pressure) that affect the ability of the fuel to support stoichiometric gas-phase mixtures. There is very little distinction between the kinetic factors of any n-alkane fuels; therefore, the only remaining conclusion is that differences are due to variability in the abilities of these fuels to provide detonable fuel-oxidizer mixtures.

The cell size data for stoichiometric fuel-air mixtures for the alkane family (i.e. ethane, propane, hexane, and JP-4) are shown in Figure 7a. With the well known exception for methane, all of the fuels given show similar cell sizes. Although there is a slight trend in decreasing cell size with increasing carbon number, this trend is well within the experimental error in cell size measurements. From the cell size data, all the dynamic detonation parameters can be estimated (e.g. critical tube diameter, $d_c = 13\lambda$, etc.). The critical initiation energy for these fuels are compared in Figure 7b. With the exception of methane, stoichiometric mixtures of alkanes in air typically require 100 kJ of energy (about 25 g of high explosive) for initiation.

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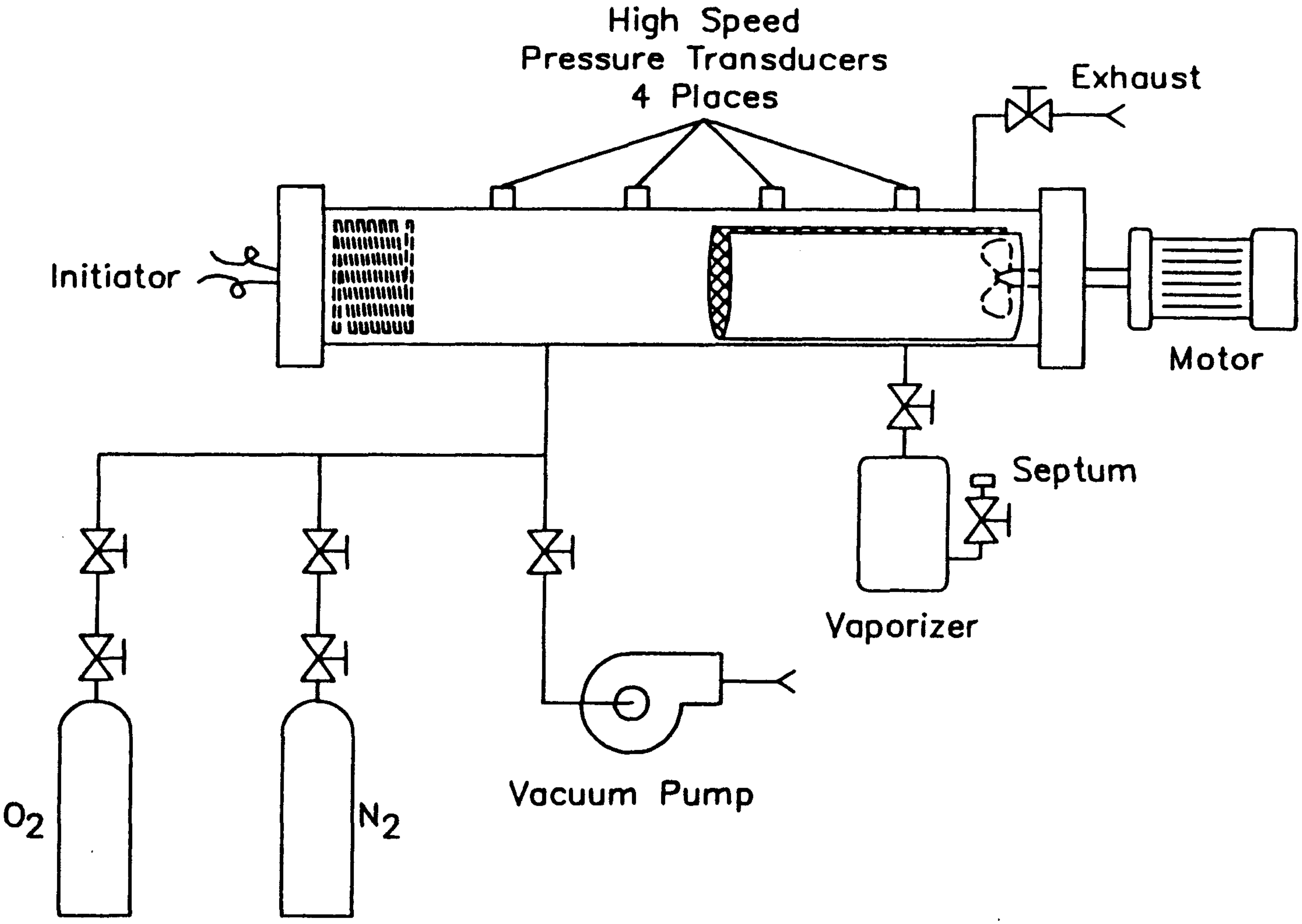

Figure 1. Schematic of Experimental Apparatus

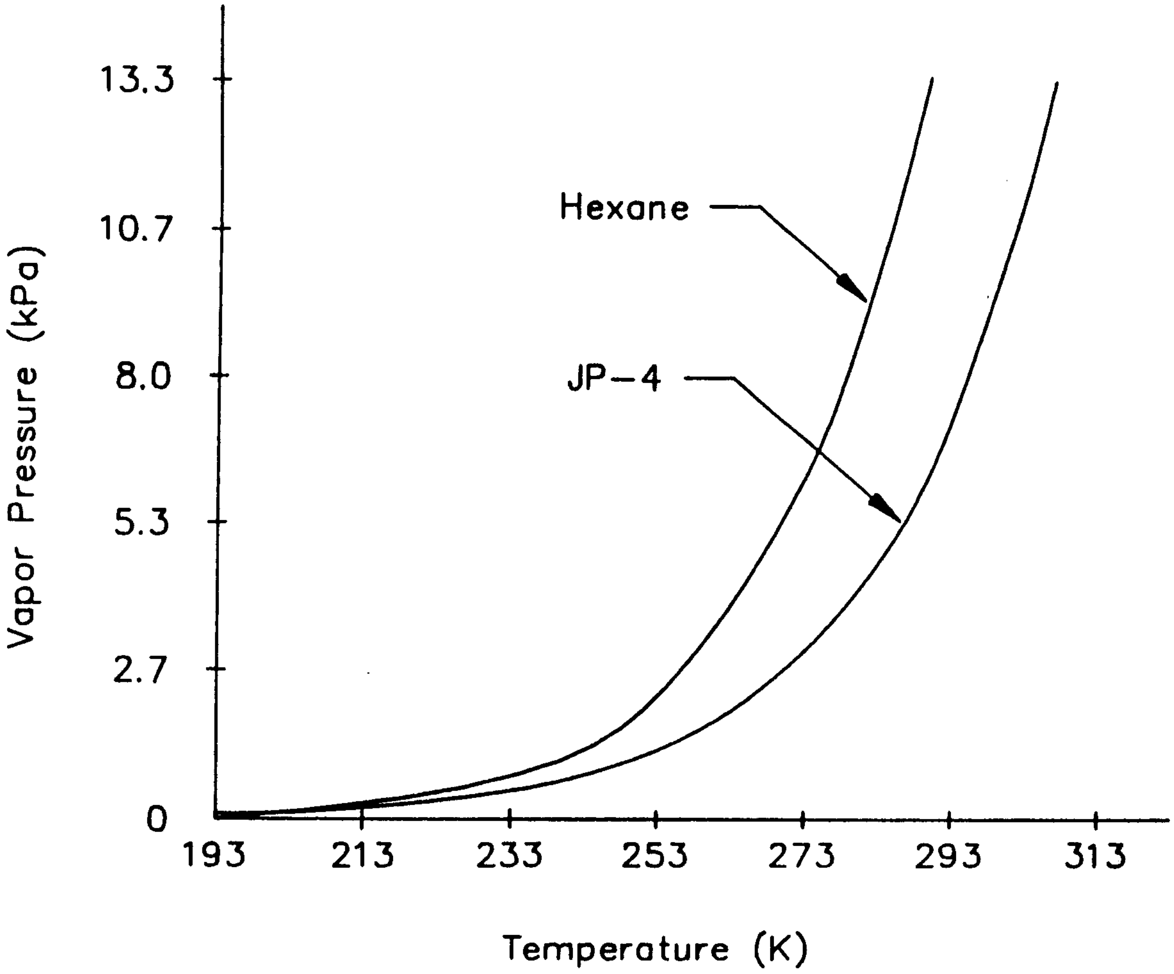

Figure 2. Vapor Pressure Curve for JP-4 and Hexane

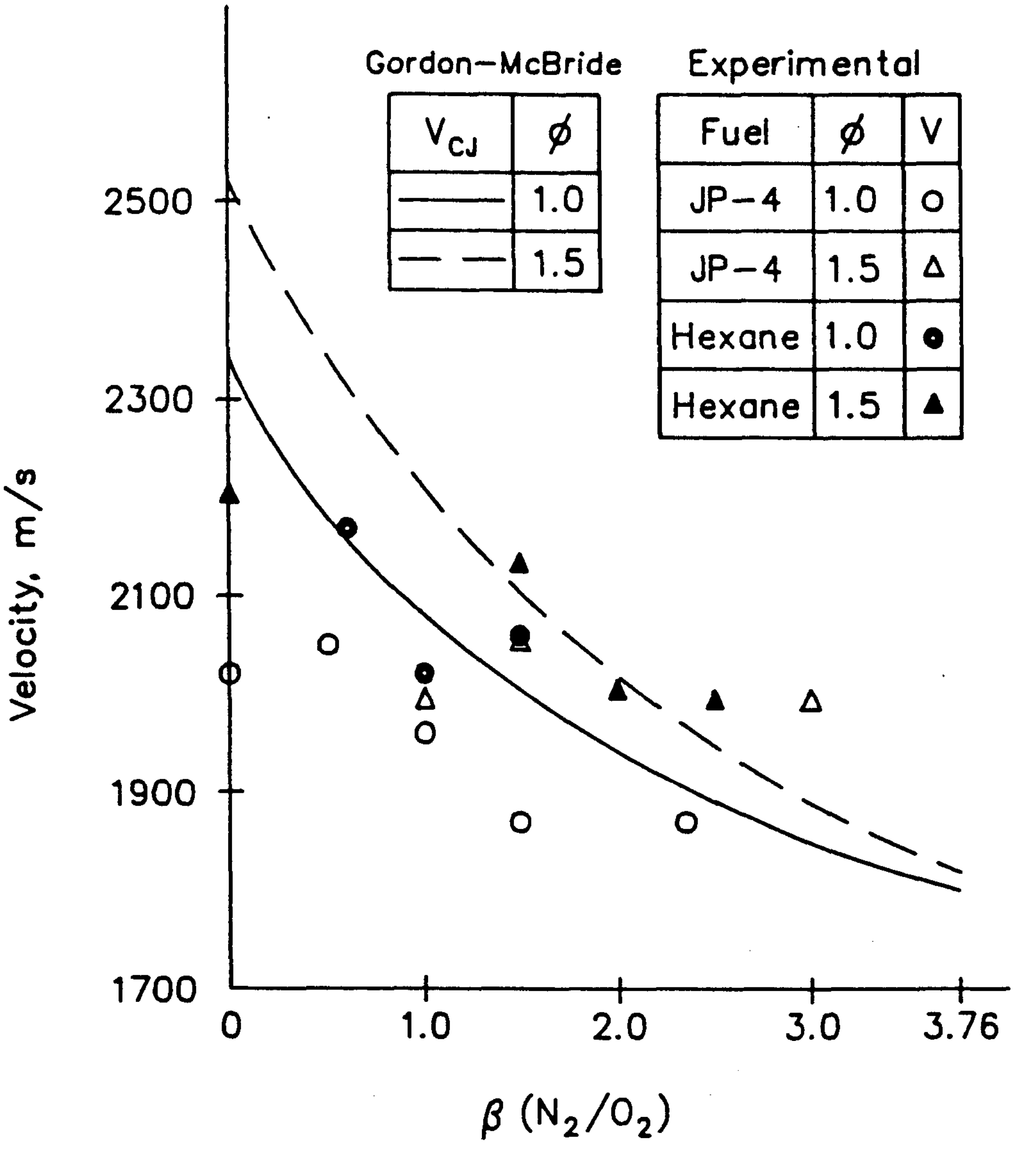

Figure 3. Theoretical Detonation Velocity as a Function of Equivalence Ratio for JP-4 and Hexane

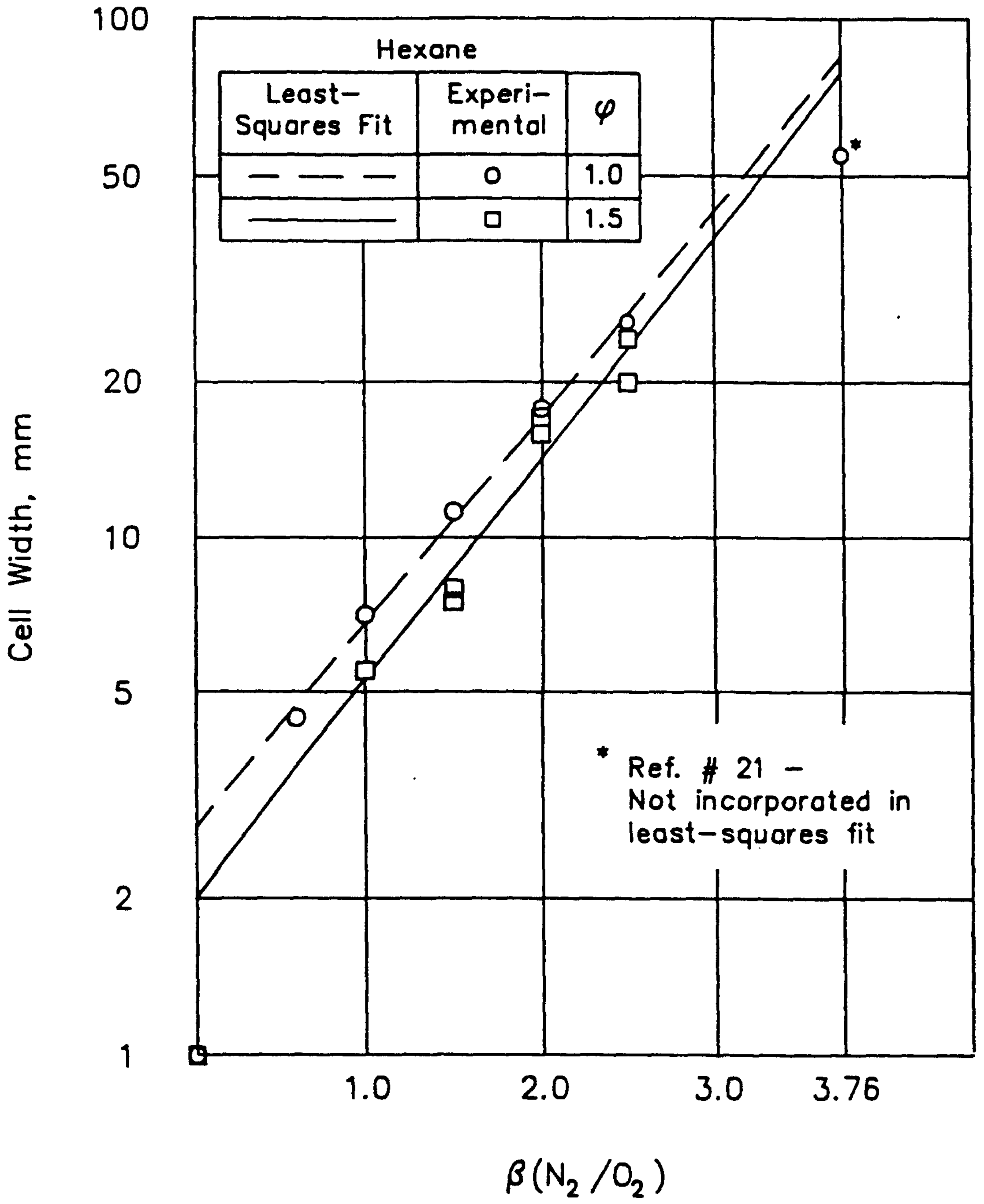

Figure 4. Experimentally Determined Detonation Cell-Widths at Varying Diluent-to-Oxidizer Ratios and Equivalence Ratios for Hexane

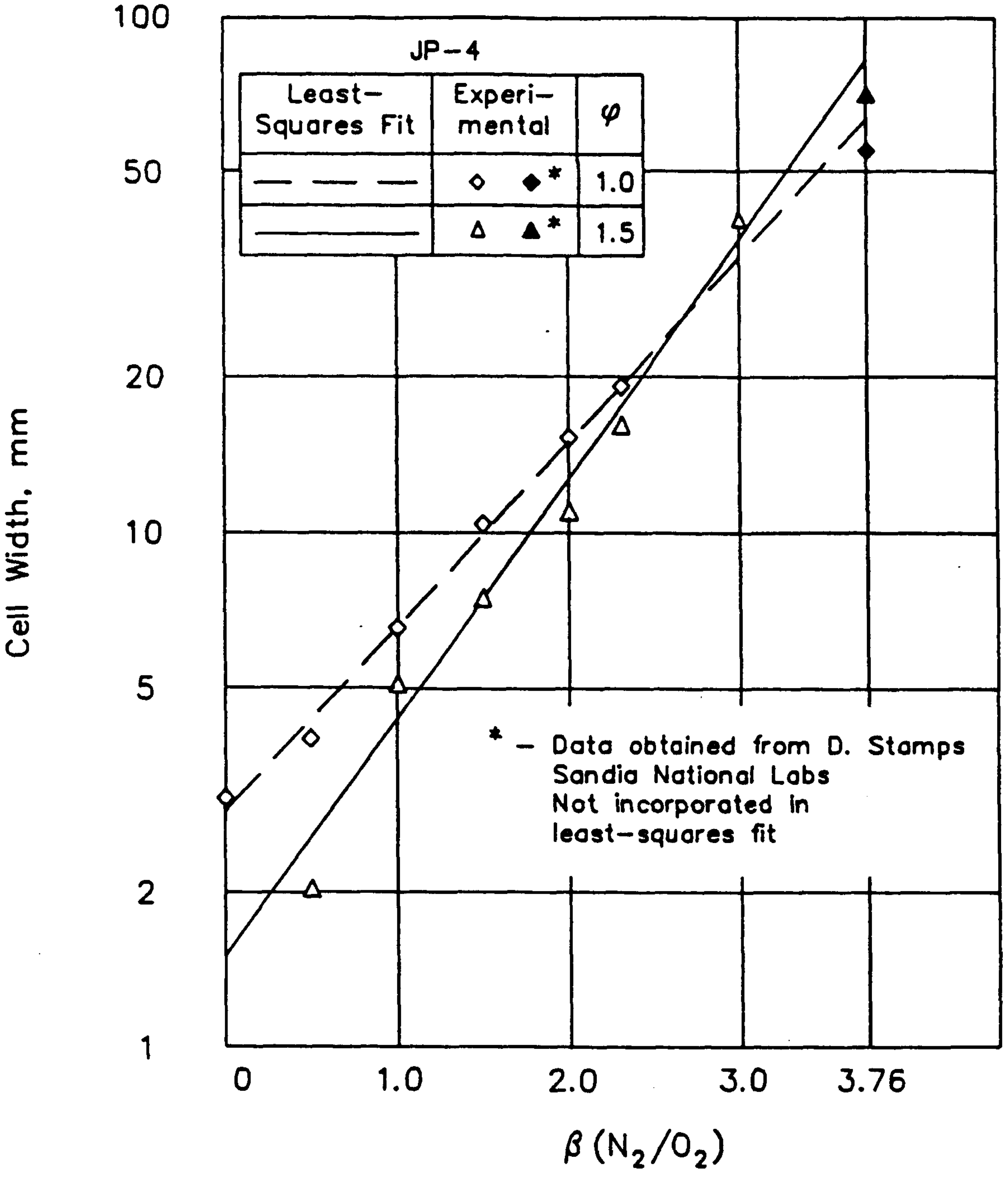

Figure 5. Experimentally Determined Detonation Cell-Widths at Varying Diluent-to-Oxidizer Ratios and Equivalence Ratios for JP-4

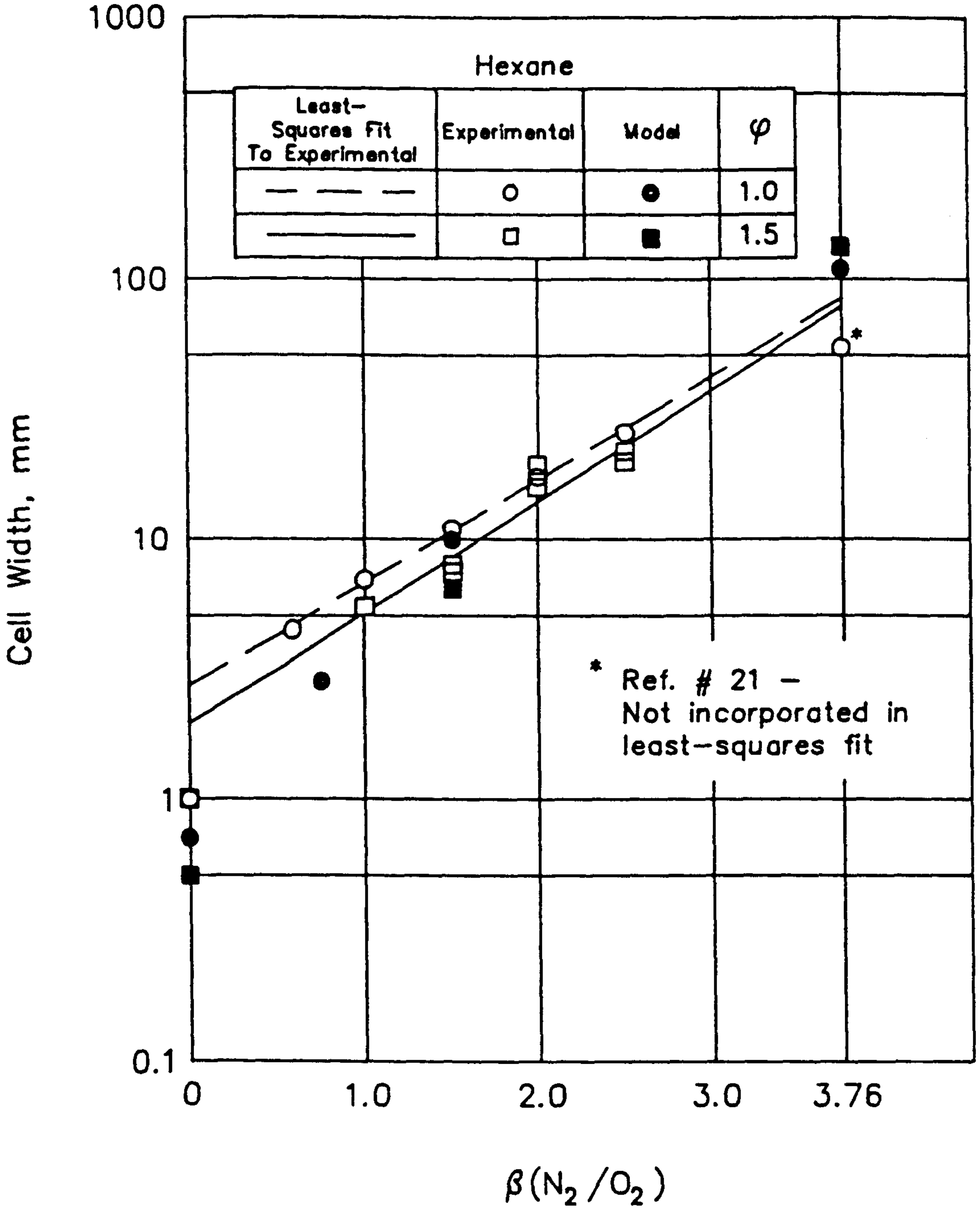

Figure 6. Comparison of Experimentally Determined Cell-Width Results and Model-Predicted Cell-Widths for Hexane

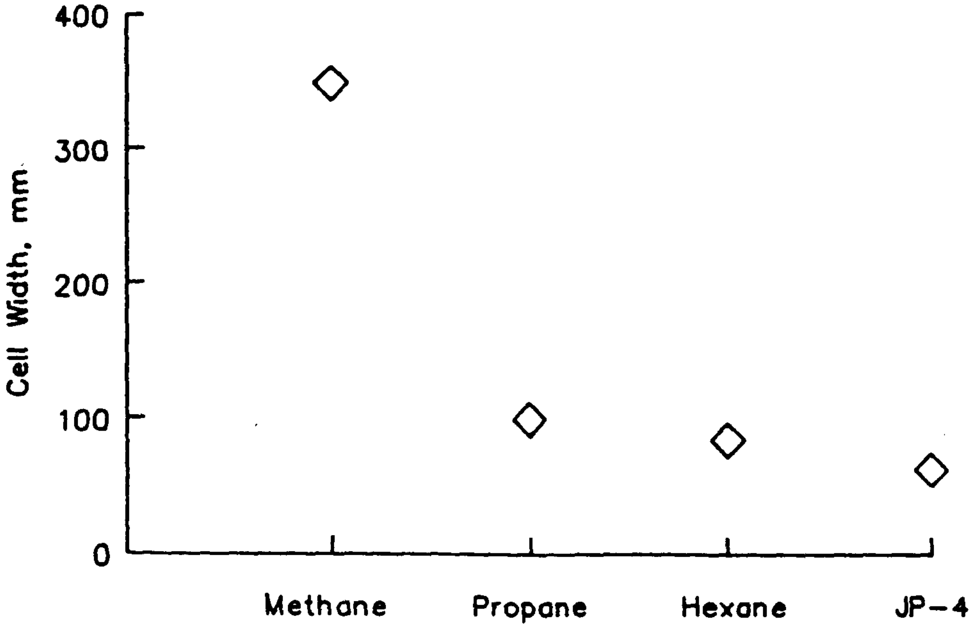

Figure 7a. Cell Widths for Several Hydrocarbon Fuels

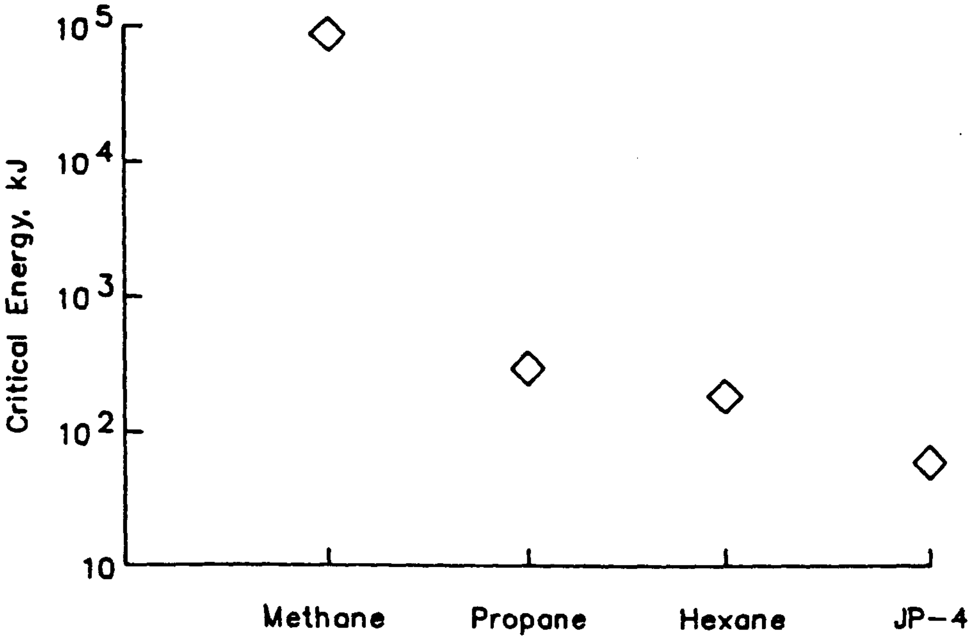

Figure 7b. Critical Energy for Several Hydrocarbon Fuels