

## Review

## Advances and challenges in laminar flame experiments and implications for combustion chemistry

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## ABSTRACT

The state of the art and the further challenges of combustion chemistry research in laminar flames are reviewed. Laminar flames constitute an essential part of kinetic model development as the rates of elementary reactions are studied and/or validated in the presence of temperature and species concentration gradients. The various methods considered in this review are the flat, low-pressure, burner-stabilized premixed flame for chemical speciation studies, and the stagnation, spherically expanding, and burner-stabilized flames for determining the global flame properties. The data derived using these methods are considered at present as the most reliable ones for three decades of pressures ranging from about 50 mbar to over 50 bar. Furthermore, the attendant initial and/or boundary conditions and physics are in principle well characterized, allowing for the isolation of various physical parameters that could affect the flame structure and thus the reported data. The merits of each approach and the advances that have been made are outlined and the uncertainties of the reported data are discussed. At the same time, the potential sources of uncertainties associated with the experimental methods and the hypotheses for data extraction using each method are discussed. These uncertainties include unquantified physical effects, inherent instrument limitations, data processing, and data interpretation. Recommendations to reduce experimental uncertainties and increase data fidelity, essential for accurate kinetic model development, are given.

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## 1. Introduction

In his Nobel Lecture on December 11, 1956, Nikolai Semenov stated that “mechanisms of chemical reactions and in particular chain reactions” is essential towards the understanding of “combustion and explosion processes.” Since then, the key role of chemical kinetics in a wide range of combustion phenomena has been recognized further through advances in flame theory and the characterization of rate constants of elementary reactions relevant to the oxidation and/or pyrolysis of simple fuels such as  $H_2$  and the small molecular weight hydrocarbons. An important outcome of this process is the realization that detailed kinetic models can be compiled to describe the elementary pathways of the oxidation of fuels to the final products. Experience with reaction kinetics has revealed though that accurate prediction of the rate constants can be quite challenging [1–6] and complicated by the presence of unknowns that frequently exceed the number of equations, given the limited knowledge on the quantum states, potential energy surface, anharmonicity and the third body collisional energy transfer, especially for a large fuel molecule consisting of many atoms. On the other hand, carrying out experiments that could isolate elementary reactions with confidence in a broad parametric range is equally challenging due to equipment limitation in capturing accurately events of intermediate species at the (sub)-picosecond level and in the unavoidable coupling with other reactions. Thus, both theory and experiments have to rely on assumptions that “combine” several unknowns so that the problem becomes tractable.

While chemical knowledge on combustion reactions was essential in the time of Semenov and beyond as a theoretical background to describe the general flame structure and to derive important practical criteria such as the flammability and explosion limits, the role of chemical reaction pathways towards the fundamental understanding and intelligent design of practical combustion devices today has become even more prominent: with in-depth chemical knowledge, substantially cleaner combustion strategies can be explored and made available for a flexible mix of conventional and alternative fuels, so that current and future emission regulations are met.

The aforementioned challenges motivated the need to validate reaction models indirectly by constraining the attendant uncertainties against data obtained through a wide range of combustion phenomena. For the last 50 years this approach has been followed closely and at present such validations are attempted for fuel molecules whose oxidation/pyrolysis is described by thousands of species and even more reactions [7–11], as shown in Fig. 1; we note in passing that references cited on subjects of general nature are meant to be representative instead of exhaustive.

The reacting systems that have been used for validation purposes have evolved through the years and at present they include a variety of homogeneous reactors and laminar flames. Given the close interplay between chemical kinetics and molecular diffusion in the presence of convective transport and thermal radiation, complex reaction systems are not suitable for kinetic model validation given the increased uncertainties associated with the boundary conditions as well as with multi-dimensional flow and transient effects. Thus, it is highly desirable that data are derived in low-dimensional experiments.

In homogeneous reaction systems, all spatial dependencies are suppressed and the evolution of an oxidation or a pyrolysis process depends only on time and can be modeled rather conveniently even for very large number of species. The homogeneous reaction systems that are used extensively at present are shock tubes, flow reactors, jet-stirred reactors (JSR), and rapid compression machines (RCM). Each system operates at different thermodynamic conditions, although in recent years their ranges have been extended to provide overlaps as is the case of the shock tube that operates at lower temperatures thus overlapping with the RCM [11]. The data obtained in homogeneous reaction systems constitute the basis for studying kinetic pathways and the attendant rate constants for a specific elementary reaction, which is an essential first step towards the compilation of complex reaction models. However, it must be recognized that experimental deviations from ideality frequently assumed in modeling can be potential sources of uncertainty. More specifically, the assumptions of spatial uniformity, adiabaticity, fast mixing, absence of catalytic reactions, radical quenching, hot spots, fluid mechanics effects, constant pressure, temperature, residence time, zero or pre-specified initial radical concentration, and the definition of “zero time” or time-shifting could be questioned under many instances; meeting these assumptions is a non-trivial undertaking. Thus, the data derived in homogeneous reaction systems need to be evaluated critically and reported properly, along with uncertainties given their relevance in quantifying rate constants.

Most of the heat release in practical engines such as gasoline, diesel, and gas turbines is produced by flames. Models developed based on kinetics experiments in homogeneous reactors need to undergo a more stringent validation process in low-dimensional, stable laminar flames in which a wide range of temperature, species concentration, and temperature/species gradients are

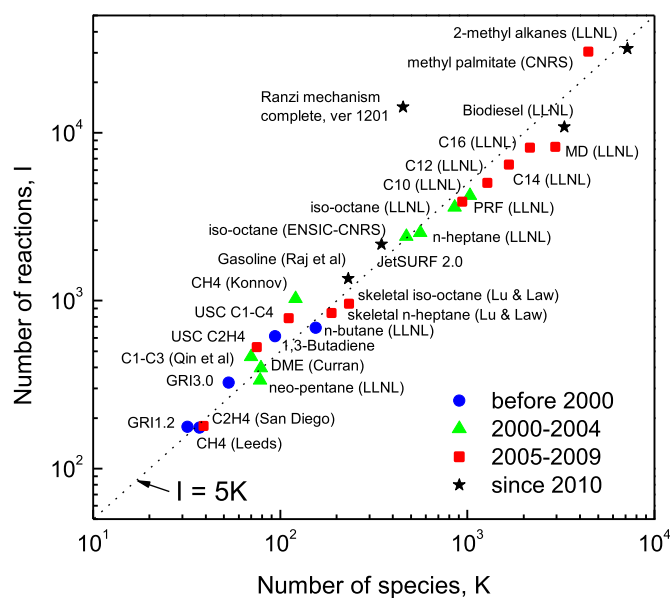


Fig. 1. Correlation between number of reactions and number of species for various published kinetic models for selected hydrocarbons and bio-derived fuels. Updated from Ref. [8]; courtesy of T.F. Lu.

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