



# NO formation in rich premixed flames of C<sub>1</sub>–C<sub>4</sub> alkanes and alcohols

Graeme M.G. Watson, Philippe Versailles, Jeffrey M. Bergthorson\*

*Department of Mechanical Engineering, McGill University, Montréal, Québec, Canada*

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## Abstract

A comprehensive study of prompt nitric oxide (NO) formation is presented for rich ( $\phi = 1.3$ ) premixed flames of alkanes and alcohols. Measurements of the flame burning rate, the temperature, and the CH radical and NO species are performed in atmospheric-pressure laminar premixed stagnation flames. New data, obtained for all isomers of the C<sub>4</sub> fuels, butane and butanol, are merged with existing data for C<sub>1</sub>–C<sub>3</sub> fuels obtained by the same methodology. The combined dataset consists of all isomeric combinations of the fuel molecules, and provides a complete description of pollutant trends related to fuel type and branching structure for C<sub>1</sub>–C<sub>4</sub> alkanes and alcohols. These data show alcohols produce less NO than alkanes of equivalent carbon chain length. This behavior is linked to the tendency of alcohols to produce lower concentrations of the CH radical, due to inhibition of the formation of methyl radicals. The results show a linear scaling of prompt-NO formation with the CH radical concentrations, when these are scaled by the characteristic residence time in the flame. This residence time depends on the burning velocity of the fuels, which decreases with increasing fuel branching. These data are useful for thermochemical model development using detailed simulations of the experiments and a comparative diagnostics approach. Further adjustments to all of the thermochemical models are needed to capture the observed trends. This dataset is made available and provides validation and optimization targets for future model revisions.

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## 1. Introduction

The formation of nitrogen oxides, NO<sub>x</sub>, has environmental and health implications. These compounds have received much attention result-

ing in the identification of numerous chemical pathways for the formation and destruction of nitrogen species. Rate parameters for the elementary reactions of these pathways have also been determined [1,2], allowing for the development of detailed thermochemical models to predict NO<sub>x</sub> in conventional fuels [3–6].

Progress has been made to reduce world-wide NO<sub>x</sub> emissions in response to increasingly stringent environmental regulations. Mitigation strategies focus on the reduction of combustion temperatures

\* Corresponding author.

E-mail addresses: [graeme.watson@mail.mcgill.ca](mailto:graeme.watson@mail.mcgill.ca) (G.M.G. Watson), [jeff.bergthorson@mcgill.ca](mailto:jeff.bergthorson@mcgill.ca) (J.M. Bergthorson).

to inhibit the thermal (Zel'dovich) formation route, the primary contributor in traditional combustion systems, and have reduced total  $\text{NO}_x$  emissions by at least an order of magnitude.

There are plans to make  $\text{NO}_x$  regulations more stringent. These new regulations will put added pressure on present technologies [7]. For many clean combustion systems, thermal  $\text{NO}_x$  is mitigated so that its contribution to the total  $\text{NO}_x$  emissions is of the same order as other major formation routes, including prompt, NNH, and  $\text{N}_2\text{O}$  [8]. These mechanisms are less understood and accurate thermochemical models are needed as design tools.

There is also interest in meeting strict emissions regulations while providing combustion technologies that are fuel-flexible. This will be especially important as the fuel base expands to non-standard petroleum and natural gas blends, and to unconventional, non-petrochemical sources. Current thermochemical models are unable to meet such requirements, given that most models are developed for low-molecular weight fuels, such as methane [1,4].

A diverse and comprehensive experimental database of  $\text{NO}_x$  targets must be assembled for further thermochemical model development and validation. Such targets include fundamental reaction data for key NO elementary reactions [2],  $\text{NO}_x$  sensitization data from ignition delay measurements [9], and speciation data from flow reactors and low-pressure burner stabilized flames [10, 11]. These  $\text{NO}_x$  investigations should be supplemented by data from a wider fuel range to capture fuel-dependent emissions. For short-chain fuels, without bounded nitrogen, a significant source of these dependencies is from the prompt route [12]. This route is coupled to intermediate chemistry and the CH radical through the initiation reaction:  $\text{CH} + \text{N}_2 \leftrightarrow \text{NCN} + \text{H}$  [13]. The strength of this route is linked to the concentration and structure of the fuel, and is thus strongest in rich combustion conditions.

This work presents a new, comprehensive data set for the characteristics of  $\text{C}_1$ – $\text{C}_4$  alkane and alcohol fuels in rich, premixed combustion conditions at atmospheric pressure. This work expands our previous study of alkanes and alcohols in the  $\text{C}_1$ – $\text{C}_3$  range [14], by adding further measurements for butane and butanol. These data include all isomeric configurations of the fuels, and thus provide a complete description of fuel-dependent NO emissions linked to fuel structure.

This paper starts with descriptions of the methodology and numerical approach. These are similar to our previous works [14–16], and are therefore discussed briefly. Representative profile measurements for velocity, temperature and species are also shown, and a new data set is presented for CH and NO formation in rich premixed flames of  $\text{C}_1$ – $\text{C}_4$  alkane and alcohol fuels. This data set

is then examined to establish the fuel-dependent trends. Finally, the predictions generated from various detailed thermochemical models are compared to these data to assess their performance.

## 2. Methodology

This study obtains detailed measurements of strained premixed flames in a jet-wall stagnation flow. This configuration has boundary conditions that are reliably measured and controlled, facilitating simulations and detailed comparisons with experiments. This methodology has been shown to be a useful test-bed for  $\text{NO}_x$  [15] and CH [16] studies, and for thermochemical model development and validation [16,17,18].

### 2.1. Experimental apparatus and method

The experiments are conducted at ambient pressure (1 atm) and elevated inlet temperature ( $T_{\text{inlet}} \sim 350$  K), in a stagnation flame apparatus, shown in Fig. 1. The apparatus uses a co-flow nozzle, with a premixed fuel-air central jet of diameter  $D = 20$  mm installed at a separation distance of  $\sim 1.25$  jet diameters upstream of a water-cooled stagnation plate.

Rich premixed flames ( $\varphi = 1.3$ ) are hydrodynamically stabilized inside a stagnation flow profile between an impinging-flow nozzle and a cooled stagnation-wall. Thirteen fuels are chosen to represent the complete isomeric range of  $\text{C}_1$ – $\text{C}_4$  alkane and alcohol fuels. The flow rates are set such that these flames have the same flame position relative to the stagnation-wall. These lifted flames are readily accessible by optical laser diagnostics because they are detached from the burner boundaries. 1D profiles for velocity, temperature, and speciation profiles for NO and CH are measured along the centerline of the flow.

The experimental boundary conditions for the direct simulation of the flames are given in Table S.1, in the Supplementary material. Simultaneous measurements of the fuel / air equivalence ratio,  $\varphi$ , the velocity profile,  $u$ , and the inlet and wall temperatures,  $T_{\text{inlet}}$  and  $T_{\text{wall}}$ , allow accurate determination of all upstream and downstream boundary conditions. The upstream velocity and temperature boundary conditions,  $u_{\text{inlet}}$ ,  $V_{\text{inlet}} = du_{\text{inlet}}/dz$ , and  $T_{\text{inlet}}$ , are taken within the parabolic-diminishing, cold stagnation-flow region of the velocity profile to be consistent with model assumptions, while the downstream temperature is specified at the stagnation-wall surface.  $u_{\text{inlet}}$  and  $V_{\text{inlet}}$  are specified by laser velocity measurements and have approximate uncertainties of  $\sim \pm 1$  cm/s and  $\sim \pm 5$  s $^{-1}$ , respectively. The inlet gas temperature,  $T_{\text{inlet}}$ , is measured along the centerline after each experimental realization. The stagnation plate wall temperature is monitored throughout the experiment using embedded K-type thermocouples, and is held constant

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