

## Kinetic Analysis of the 2,5-Dimethylfuran Combustion Chemistry

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### INTRODUCTION

Biofuels, which can be obtained from renewable and abundant resources, have received much attention. Several molecules can be produced from biomass, however furan derivatives have received special attention.<sup>1-3</sup> Among these, 2,5-dimethylfuran (DMF) is a promising substitute for gasoline in a future scenario. A systematic study assessing the combustion profile of DMF and comparison with other typical fuels is, therefore, necessary.

In this work, a combustion model for DMF is evaluated, through numeric simulations.

### METHODS

The combustion model is based on an available mechanism,<sup>4</sup> which consists of 1456 reactions (in a total of 2820 steps, considering the reversible reactions) and 274 species. The corresponding differential equations were numerically solved using the DVODE method available in the Kintecus® software.<sup>5</sup> Rate Analysis (RA) has been performed in order to identify the most important reactions to the initiation of the mechanism and to the ignition. Simulations have been performed varying the equivalence ratio ( $\phi = 0.5$ ,  $\phi = 1.0$  and  $\phi = 1.5$ ), initial temperature (1300 – 1800 K) and total pressure (1 – 4 bar).

### RESULTS AND DISCUSSION

An important parameter for the evaluation of a combustion profile is the ignition delay time. In this work, this parameter has been calculated as the maximum point in the curve representing the first derivative of the system temperature in relation to the time. Ignition times were found in the range from 70 – 1700  $\mu$ s, increasing as the temperature decreases, in an Arrhenius-like trend. Our results were also found in good agreement with experimental data.

It can also be noted that the ignition time decreases as the DMF concentration increases. Moreover, ignition time is also shown to decrease as the total pressure increases and as the equivalence ratio decreases.

From the rate analysis, the combustion is initiated, at  $1 \times 10^{-8}$  s, from unimolecular dissociation reactions leading to ring opening and H atoms formation. Hydrogen atoms further reacts with DMF via H-abstraction channels. The importance of these reactions increase with time and H-abstraction reactions are shown to be the dominant channels at around  $5 \times 10^{-6}$  s. Moreover, H-abstraction channels initiated by OH reactions with DMF are also found among the most important steps at instants close to the ignition time ( $5.6 \times 10^{-4}$  s).

### CONCLUSIONS

The good agreement of our simulated combustion profile and the experimental results support the adoption of this chemical model for further studies aiming the evaluation of DMF as a biofuel in specific engine conditions.

### ACKNOWLEDGMENTS

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