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Program

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Design and operation of gas turbines and engines are very sensitive to the underlying fuel chemistry. Practical fuels are complex mixtures of several hundreds of individual species, which can be divided in four hydrocarbon families (n-/i- paraffins, naphthenes (cycloparaffins) and aromatics). The kinetics of all of the fuel components and intermediate species are not fully determined and investigated.

The present study reports results of further develop of the DLR reaction kinetic mechanism for the benzene (C_6H_6) oxidation, which is the base chemistry for an oxidation of the larger aromatic molecules. The DLR C_6H_6 reaction sub-mechanism was extended with 15 new species, $C_6H_5O_2$, C_6H_4OOH, OOC_6H_4OOH, C_6H_5OOH, C_6H_4O,$\cdot OC_6H_4OO$, C_2H_2O, C_6H_4O, OC_6H_4O,$\cdot OC_6H_4OH$, C_6H_4, C_6H_3, C_5H_4OH, C_5H_5OH, C_5H_5O, C_5H_4O to describe the low-temperature ($T < 1500$ K) ignition. For some of these molecules the thermodynamical and transport properties were evaluated with the empirical rules. Also the reaction pathways of PAH formation and growth in benzene flames were investigated and improved. For the new adopted reactions the uncertainty intervals of reaction rate coefficients have been evaluated. The developed reaction mechanism has been validated on the experimental data for ignition delay times, laminar flames speeds and concentration profiles obtained in laminar flames of benzene.

REACTION MECHANISM OF THE BENZENE OXIDATION

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INTRODUCTION

Design and operation of gas turbines and engines are very sensitive to the underlying fuel chemistry. Practical fuels are complex mixtures of several hundreds of individual species, which can be divided in four hydrocarbon families (n-/i- paraffins, naphthenes (cycloparaffins) and aromatics). The kinetics of all of the fuel components and intermediate species are not fully determined and investigated.

Benzene is the first aromatic compound, a relevant intermediate of several combustion processes and also a key precursor to soot formation.

There is considerable current interest in the kinetics and mechanism of benzene oxidation because of the increasing use of aromatics as fuel components. A number of modeling studies of benzene (C_6H_6, A1) oxidation have been reported. The detailed chemical kinetic mechanism for the combustion, oxidation and pyrolysis of benzene have been developed by Norrish and Taylor, Asaba, Fujii, McLain, Santoro and Glassman, Bittner and Howard, Venkat and Brezinsky, Kern et al., Hsu co-workers, Rotzoll, Brezinsky, Bittker, Lovell, Lindstedt and Skevis, Richter, Wang and Djurisic, Alzueta and et al., Costa and coworkers, Blanquart et al., Ranzi and et al., Saggese, and Yang validated on the measured data obtained in shock tube, jet stirred reactor (JSR), plug flow reactors (PFR) and premixed laminar flames.

METHODOLOGY

On the basis of existing detailed kinetic schemes [1,2] a general and consistent mechanism of the oxidation of hydrocarbons and the formation of higher hydrocarbons was compiled for computational studies covering the characteristic properties of a wide range of combustion processes.

The DLR C_6H_6 reaction sub-mechanism was extended with 15 new species, $C_6H_5O_2$, C_6H_4OOH, OOC_6H_4OOH, C_6H_5OOH, C_6H_4O,$\cdot OC_6H_4OO$, C_2H_2O, C_6H_4O, OC_6H_4O,$\cdot OC_6H_4OH$, C_6H_4, C_6H_3, C_5H_4OH, C_5H_5OH, C_5H_5O, C_5H_4O to describe the low-temperature ($T < 1500$ K) ignition. For some of these molecules the thermodynamical and transport properties were evaluated with the empirical rules. Also the reaction pathways of PAH formation and growth in benzene flames were investigated and improved.

Numerical modelling was performed using the SENKIN (for simulation of ignition delay time) and PREMIX (for simulation of laminar flame speed, species concentration profiles and sensitivity analysis) code from the CHEMKIN II package [3] and Chemical Workbench [4].

RESULTS AND DISCUSSION

The reaction sub-mechanism for C_6H_6 oxidation was validated in literature experimental data obtained in laminar premixed flames (flame speed and concentration profiles for small and PAH molecules) and ignition delay time (Table 1). The good agreement was obtained for the modeling experimental data for ignition delay times, laminar flames speeds and concentration profiles obtained in laminar flames of benzene. There is special focus was on the benzene oxidation at low-temperature ($T < 1500$ K) in this work. So the modelling results match experimental data of the laminar flame speeds, ignition delay times, and species concentration profiles both at high ($T > 1500$ K) and low temperatures ($T < 1500$ K).

Reference

1. N.A. Slavinskaya et al. Kinetic study of the effect of ethanol addition on PAH and soot formation in ethylene flames // Comb. and flame (impress) (2015)
2. N.A. Slavinskaya, U. Riedel, S.B. Dworkin, M.J. Thomson, Combust. Flame 159 (3) (2012) 979-995.
3. R.J. Kee, F.M. Rupley, J.A. Miller. Report No. SAND89-8009B, Sandia Laboratories Report, (1993)
4. http://www.kintechlab.com/products/chemical-workbench/

Table 1. Proposed kinetic mechanisms of benzene and validation data base.

Shock tube		**Flame**	**Pyrolysis**	**Laminar flame speed**	**JSR**	**PFR**
Ignition delay time	*Concentration profiles*					
p_5 = 1.7-7.89 atm T_5 = 1212-1748 K φ = 1.0	p_5 = 1.1-1.7 atm T_5 = 1700-2800 K φ = 1.0	p = 2.67 kPa (0.0267atm) T_0 = 700-1900 φ = 1.8-1.9	p = 0.2-3 atm T_0 = 1515-2500 K $\varphi = \infty$	p = 1atm T_0 = 298, 500, 588, 700 K φ = 0.8-1.3	p = 350 torr T_0 = 900-1300 K φ =0.19, 1.02	p = 1 atm T_0 = 900-1450 K φ = 0.8-1.3
p_5 = 13-40 bar T_5 = 800-1400 K φ = 1.0	p_5 = 0.4-0.5atm T_5 = 1704-2192 K $\varphi = \infty$	p = 0.04 atm T_0 = 298 K φ = 1.78		p = 3 atm (304 kPa) T_0 = 450 K φ = 0.8-1.4	p = 1 atm T_0 = 950-1350 K φ = 0.3-1.5	p = 1 atm T_0 = 1118-1280 K φ = 0.39-1.5
p_5 = 6.5-9.5 atm T_5 = 1230-1970 K φ = 1.0-3.0	p = 0.05 atm T = 298 K Φ = 2.0	p = 1 atm T_0 = 1100-1810 K φ = 1.98		p = 1 atm T_0 = 353 K φ = 0.7-1.5	p = 1 atm T_0 = 923 K φ = 1.9-3.6	p = 1 atm T_0 = 1096-1217 K φ = 0.76-1.36
p_5 = 5.4-7.4 atm T_5 = 1210-1615 K φ = 0.2-2.8	p = 0.045 atm T = 298 K φ = 2.0	p = 1.8 atm T_0 = 500-1800 K φ = 1.8		p = 1 atm T_0 = 298 K φ = 0.7-1.7		p = 1 atm T_0 = 1108 K φ = 0.65
p_5 = 25-45 atm T_5 = 920-1100 K φ = 0.5, 1	p_5 = 1 atm T_5 = 875-1500 K φ = 1.0			p = 1 atm T_0 = 298 K φ = 0.8-1.3		p = 1 atm T_0 =1110-1280 φ = 1.0
p_5 = 4 atm T_5 = 1110-2220 K φ = 1.0	p_5 = 7.3-9.5 atm T_5 = 1230-1970 K φ = 0.5-3.0					p = 400 mbar T_0 = 950-1150 K φ = 1.0
	p_5 = 30-50 atm T_5 = 1200-1800 K $\varphi = \infty$					p = 1 atm T_0 = 1118-1280 K φ = 0.39-1.5