Flame structure studies of ethyl pentanoate

Haddy MBUYI KATSHIATSHIA, Véronique DIAS*, Hervé JEANMART
Institute of Mechanics, Materials and Civil engineering
Université catholique de Louvain, Belgium
Veronique.dias@uclouvain.be

Few results are available to characterize esters combustion at high pressure and none available at low pressure. The characterization of ethyl pentanoate (also ethyl valerate, EPE) combustion at low pressure is studied in this work.

One of the main challenges was the setup of the test bench, combining an evaporation system for high boiling point compounds, a combustion chamber, a compression system and a gas chromatography. The present complete test bench allows us to study ethyl pentanoate flat flames.

Three flat flames of ethyl pentanoate at different equivalence ratios, 0.81, 0.95 and 1.31, have been stabilized at 55 mbar. The reactants, intermediate species and products such as EPE (ethyl pentanoate), O_2, C_4H_9COOH (valeric acid), CH_3CHO (acetaldehyde), CH_2O (formaldehyde), CH_3COCH_3 (acetone), HOCHO (formic acid), CH_4 (methane), C_2H_2 (acetylene), C_2H_4 (ethylene), H_2, CO, CO_2 and H_2O, have been separated and analyzed using gas chromatography as the analysis technique.

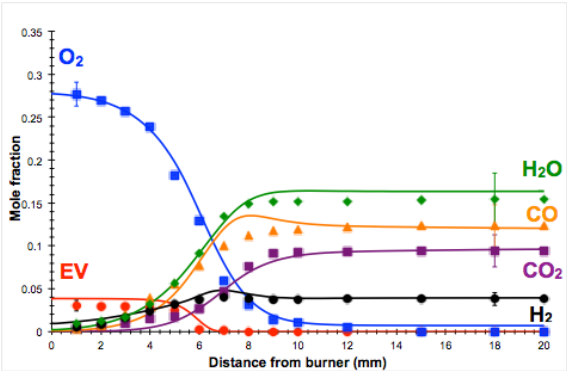
Inlet compositions for the three stabilized flames

Flame	$X_{C7H14O2}$	X_{O2}	X_{Ar}	**Φ**	**C/O**
Lean	0.037	0.435	0.527	0.81	0.274
stoichiometric	0.038	0.379	0.583	0.95	0.319
Rich	0.039	0.282	0.679	1.31	0.425

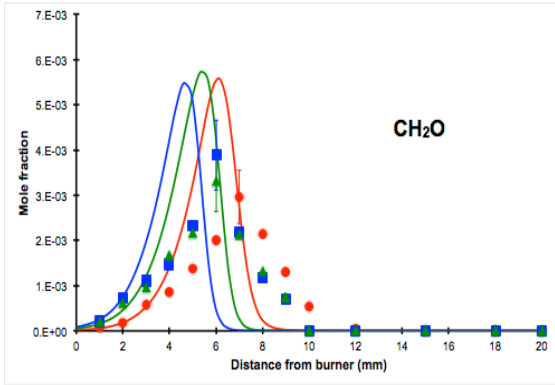
Based on the experimental results, a detailed kinetic model of ethyl pentanoate combustion, containing 211 species and 1368 elementary reactions, has been elaborated. The mechanism is based on the “UCL” model (http://veroniquedias.github.com) extended for the ethyl pentanoate sub-model from Dayma et al. (Energy and Fuels, 2012). The agreement between the experimental results and the model is good.

The main decomposition pathways of ethyl pentanoate have been identified for the three flames.
In the lean flame the decomposition leads to $CH_3(CH_2)_3COOCHCH_3$ (EPEEj), CH_3CHO, CH_3CO and CH_3.
For the stoichiometric flame, the ethyl pentanoate main consumption pathway produces C_4H_9COOH, BuCOOH-4 ($CH_2(CH_2)_3COOH$), C_4H_7COOH, CH_2COOH, CH_2CO and CH_3.
Finally, in the rich flame, from ethyl pentanoate to pentenoic acid (C_4H_7COOH), the decomposition pathway is the same as in the stoichiometric

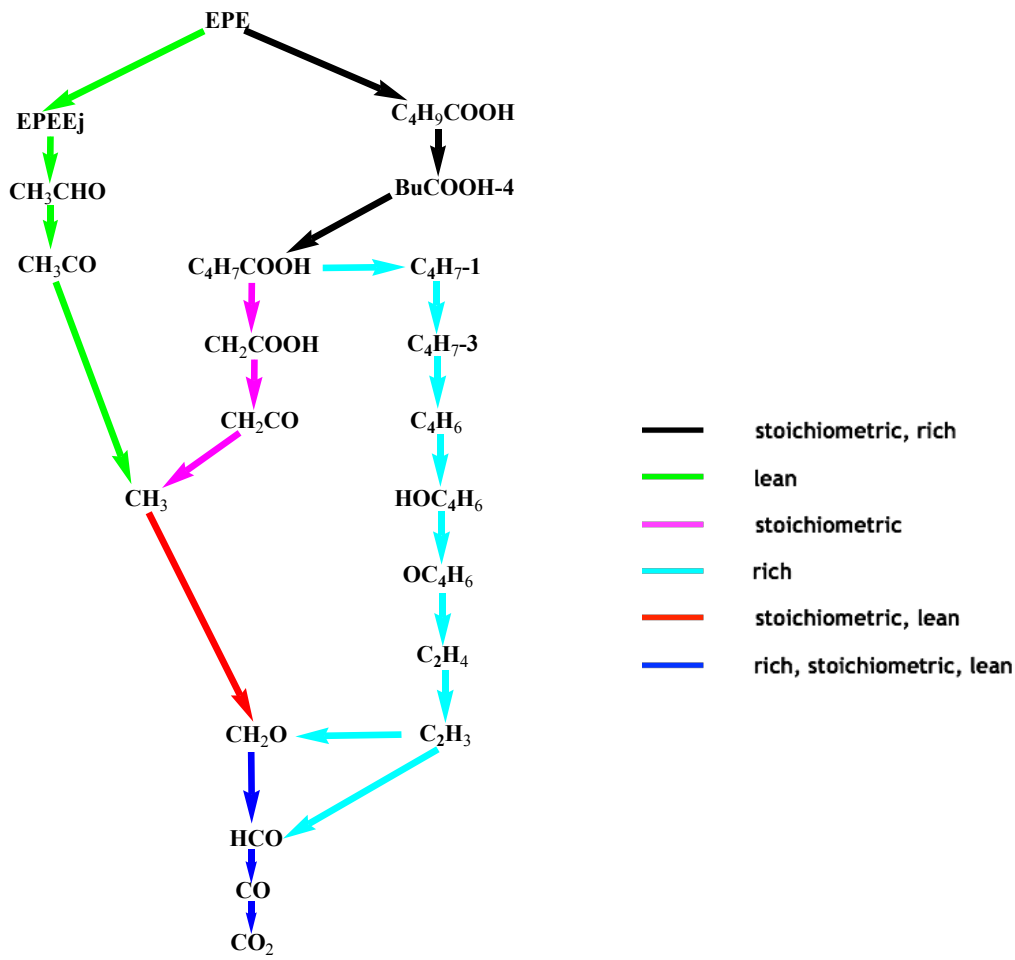
flame. It then leads to C_2H_4 via C_4H_6 and C_3H_6. From the formaldehyde to the carbon dioxide, the consumption pathway is the same in the three flames.



Experimental (symbols) and simulated (lines) mole fraction profiles for the main species in the rich EPE/O_2/Ar flame



Experimental (symbols) and simulated (lines) mole fraction profiles for CH_2O in the EPE/O_2/Ar flames : lean (blue), stoichiometric (green) and rich (red).



Reaction pathways of consumption of ethyl pentanoate for the three equivalence ratios