Berlin Institute of Technology • Fasanenstr. 89 • 10623 Berlin

King Abdullah University of
Science and Technology (KAUST)
Yu Wang
CCRC
Thuwal, Makkah, Saudi Arabia

September, 21st - 24th 2014
FLAME STRUCTURE 2014
8th International Seminar on Flame Structure

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Prof. Dr. Frank Behrendt
Fakultät III: Prozesswissenschaften,
Institut für Energietechnik

Chair Energy Process Engineering and
Conversion Technologies for
Renewable Energies (EVUR)
Fasanenstr. 89
10623 Berlin

Contact
info@flame-structure-2014.com
frank.behrendt@tu-berlin.de

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Confirmation of paper submission

Name:	Yu Wang
Email:	yu.wang@kaust.edu.sa
Co-author:	Abhijeet Raj
2nd co-author:	Sukho Chung
3rd co-author:	-
Title of Paper:	Soot modeling of counterflow diffusion flames with ethylene-based binary mixture fuels
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Soot modeling of counterflow diffusion flames with ethylene-based binary mixture fuels

Yu Wang[1], Abhijeet Raj[2], Suk Ho Chung[1,*]

[1]Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia
[2]Department of Chemical Engineering, The Petroleum Institute, Abu Dhabi, UAE

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A soot model was developed based on the recently proposed PAH growth mechanism for C_1-C_4 gaseous fuels (KAUST PAH Mechanism 2, KM2), having molecular growth up to coronene (A7) to simulate soot formation in counterflow diffusion flames of ethylene and its binary mixtures with methane, ethane and propane based on the method of moments. The soot model included 36 soot nucleation reactions from 8 different PAH molecules including pyrene and larger PAHs. Soot surface growth reactions were based on a modified hydrogen-abstraction-acetylene-addition (HACA) mechanism, where CH_3, C_3H_3 and C_2H radicals were included in the hydrogen abstraction reactions in addition to H atoms. PAH condensation on soot particles was also considered. The experimentally measured profiles of soot volume fraction, number density, and particle size were well captured for the baseline case of ethylene along with the mixture cases.

The simulation results are shown in Fig.1. It can be seen that with 5% addition of propane (ethane) the soot volume fraction of the ethylene flame increased by 32% (6%), despite the fact that propane and ethane are less sooting fuels compared to ethylene. With 5% addition of methane simulation shows a reduction of 5% in soot volume fraction

while experiment exhibits a 6% increase. It was also noted that average soot particle sizes were only minimally influenced while soot number densities were increased by the fuel mixing. Further analysis of the numerical data indicated that the chemical cross-linking effect between ethylene and the dopants results in an increase in PAH formation, which leads to higher soot nucleation rates and therefore higher soot number densities. The predicted nucleation rates are plotted in Fig.2. On the other hand, the rates of soot surface growth per unit surface area through the HACA mechanism were similar among the different fuel mixing cases, although slightly lower compared to the ethylene base case. The increased soot nucleation rates by fuel mixing and similar soot surface growth rates (per unit surface area) help explain the increased soot volume fraction / number density and similar average sizes among the tested cases.

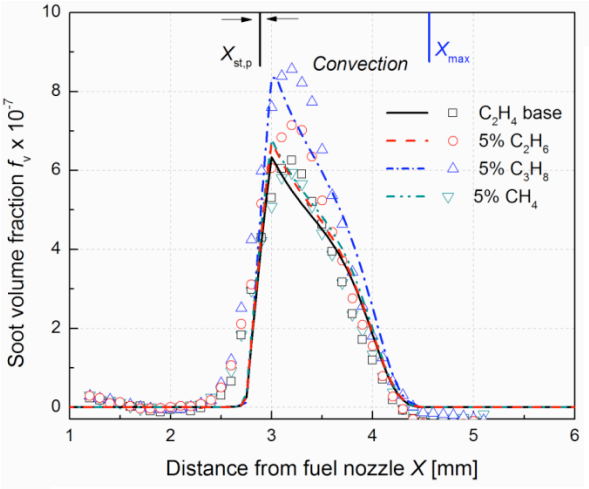

Fig.1 Experimental and predicted soot volume fraction in counterflow diffusion flames of ethylene-based binary fuel mixtures, the symbols represent experimental data and lines are from simulation results

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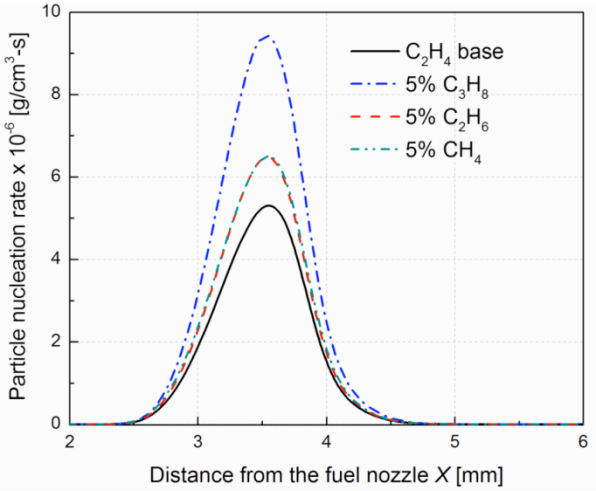

Fig. 2 Computed soot mass growth rate due to nucleation

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