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LABORATORY OF NONEQUILIBRIUM PROCESSES

# Influence of minor impurities of acetone on soot formation in acetylene shock wave pyrolysis

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## Motivation

Processes of polyaromatic hydrocarbons (PAH) and soot formation are attracting steady scientific interest.

**Acetylene** is a major product of decomposition of several hydrocarbons and plays an important role as a building block towards PAH and soot formation, thus investigated in many experimental studies using various setups.

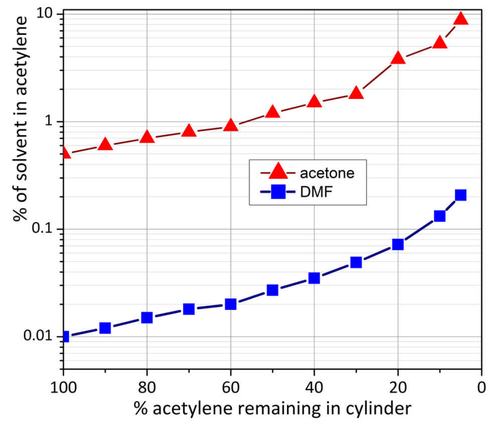
Accurate prediction of features of soot yield dependencies in acetylene is still a tough problem for many suggested kinetic mechanisms.

## Acetone presence

Due to positive heat effect of polymerization acetylene is an explosive substance and could not be stored compressed at high pressure in cylinders of a common design. Special cylinders are used which are filled with a porous material and contain notable amount of a solvent (rarely other than acetone).

Acetone vapors are inevitably present in acetylene exhausting from the cylinder. Often that 0.5% impurity considered as neglectable, and many works have no mentions of acetylene purification at all or do not underline its importance.

*Solvent carry-through in acetylene stream*



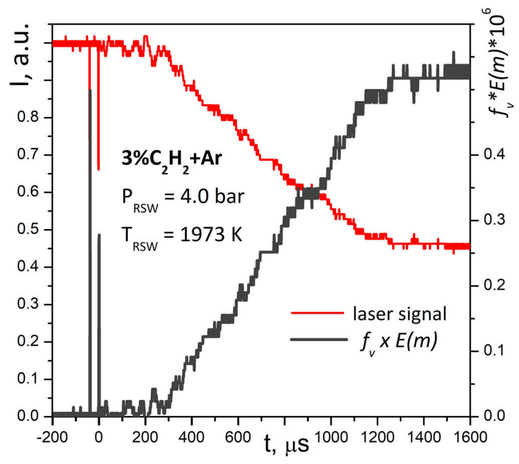

## Experimental results

Results of shock tube measurements performed at 1700-2400 K in mixtures 3%$C_2H_2$ + Ar at 3.5-4.5 bar are presented. Results previously obtained in 1%$C_6H_6$ + Ar (at 1.7-2.7 bar) are used as a reference.

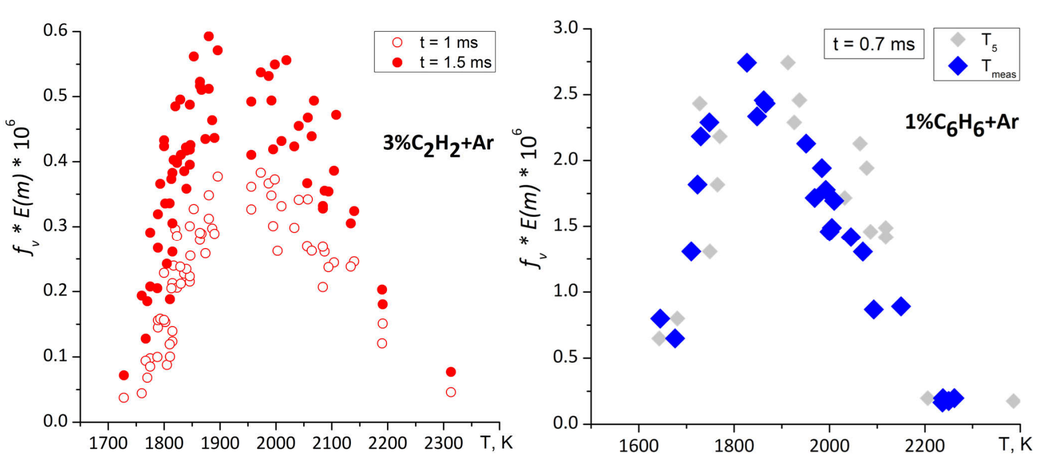
Acetylene of technical grade A in a standard cylinder was used (*UN 1001 / GOST 5457-75, Linde, Russia*).

Common method of laser extinction time profile registration was used for investigation of processes of soot particles growth and estimation of their relative volume fraction.

*Typical time profiles of laser extinction and relative soot volume fraction*




*Experimental dependencies of relative soot volume fraction for acetylene and benzene mixtures*




## Modeling results

Modeling of hydrocarbons pyrolysis, PAH formation and soot growth was performed in OpenSMOKE++ software package using kinetic mechanism of CRECK.

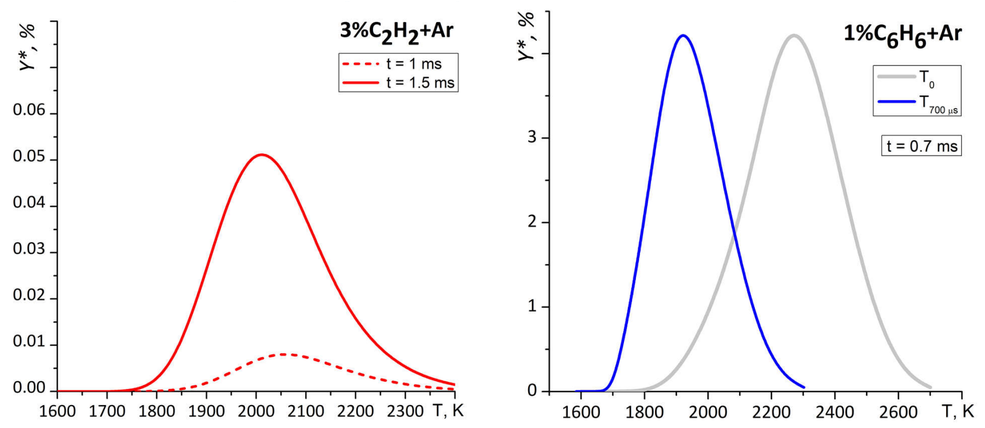
OpenSMOKE++ — Modeling Group CRECK

Ratio of number of carbon atoms in "sooty" species and total number of carbon atoms in mixture were denoted as "supposed soot yield" and used for analysis.

Quite good agreement of modeling and experimental result was achieved for benzene mixtures.

Contrary, calculated temperature dependence for acetylene looks shifted 100-200 K to high temperature region, and the value of supposed soot yield is severely underpredicted.

*Modeled temperature dependencies of supposed soot yield Y* for acetylene and benzene mixtures*




## Analysis

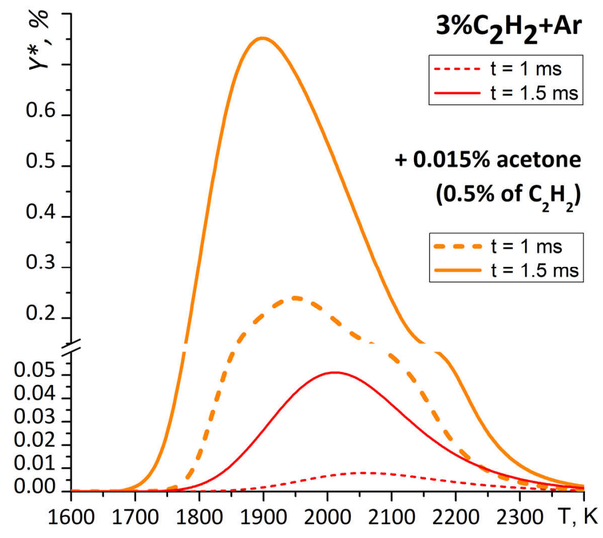
The influence of acetone impurity was estimated while analyzing dramatic discrepancy of modeled and observed soot yield in acetylene.

Supposed soot yields in given conditions increased 20-50 times providing much better agreement of modeling and experimental results.

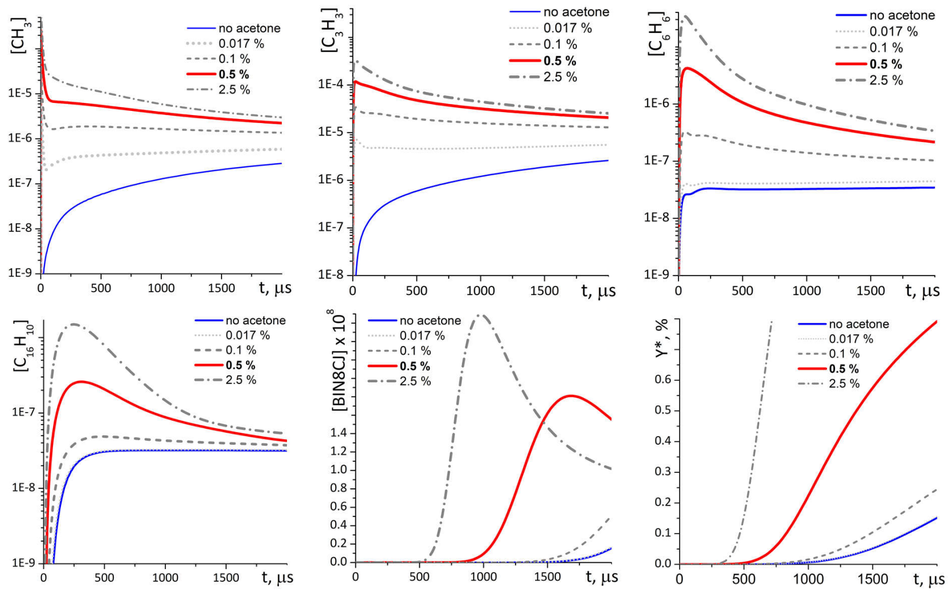
Influence of acetone impurity is exceptionally strong in considered case of relatively low pressures and concentrations when the soot formation processes are slow and soot yield is low.

Chain reactions play key role in acetylene pyrolysis thus its kinetics is quite sensitive to small changes of active radical concentration.

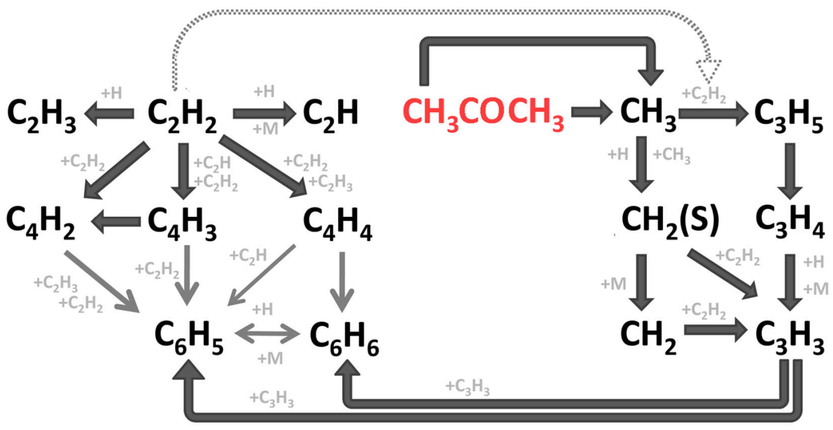
*Influence of acetone impurity on modeled temperature dependencies of supposed soot yield Y* in acetylene*




*Concentration of active radicals, PAH and soot yield are dramatically increased in presence of acetone*




*Suggested kinetic pathway of acetone impurity influence on $C_6H_6$ formation and following growth of PAH and soot*




## Conclusion

- It was shown that small acetone impurity which is typical for technical acetylene could not be neglected and, moreover, determine observed features of soot yield temperature dependencies at investigated conditions
- Presence of acetone impurity as minor as 0.5% of acetylene, which is typical for stream of technical grade acetylene from the cylinder, may lead to increase of soot volume fraction at given time up to few orders of magnitude
- That result should be considered in fundamental studies of PAH and soot formation as well as in estimation of safety risks in industrial processes using acetylene

## Acknowledgments

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DFG RFBR