Electronic supplementary materials *Mendeleev Commun.*, 2019, **29**, 690–692

Combustion of ethyl acetate: the experimental study of flame structure and validation of chemical kinetic mechanisms

Ksenia N. Osipova, Artem M. Dmitriev, Andrey G. Shmakov, Oleg P. Korobeinichev, Sergey S. Minaev and Denis A. Knyazkov

Table of Contents

Experimental procedure

The burner was equipped with a perforated matrix of 16 mm in diameter, 3 mm thick, and maintained at 95 °C. Argon mole fraction in the mixtures and the total gas flowrate (1.374 SLM for near-stoichiometric and 0.841 SLM for fuel-rich flames, respectively) through the burner were adjusted in a manner so that the flames were nearly of the same temperature (~1550 K), which allowed us to compare the reaction pathways in the both mixtures under similar thermal conditions in order to distinguish kinetic effects. Ethyl acetate vapors were fed into the burner using a system consisting of a vaporizer and a syringe pump as described in our previous work.[S1] The flames were sampled by a sonic quartz probe with 0.07 mm orifice diameter. The procedure of species mole fraction measurements and data reduction were performed according to those reported in our previous works;[S1,S2] therefore, only the essential details are given hereinbelow. Ionizing electron energy was tuned individually for each species in such a way, that on the one hand (not too high) to eliminate the contribution from fragmented ions from other species, and on the other hand (not too low) to provide a sufficient signal-to-noise ratio. For reactants, major products (CO, CO_2, H_2, and H_2O), and stable intermediates (methane, acetylene, ethylene, ethane, and acetic acid), direct calibrations were carried out. For other intermediates (methyl radical, formaldehyde, acetaldehyde, propene+ketene), the method of relative ionization cross-sections was used.[S1–S3] Propene and ketene were not separated in our experiments, since the difference between their ionization energies is significantly smaller than the width of Maxwellian energy distribution of ionizing electrons (~0.25 eV). Temperature profiles in the flames were measured by S-type thermocouples (made of wires of 0.03 mm in diameter). The procedure of the measurements and thermocouple data reduction was also reported earlier.[S1,S2]

Kinetic analysis of the mechanisms for the fuel-rich conditions

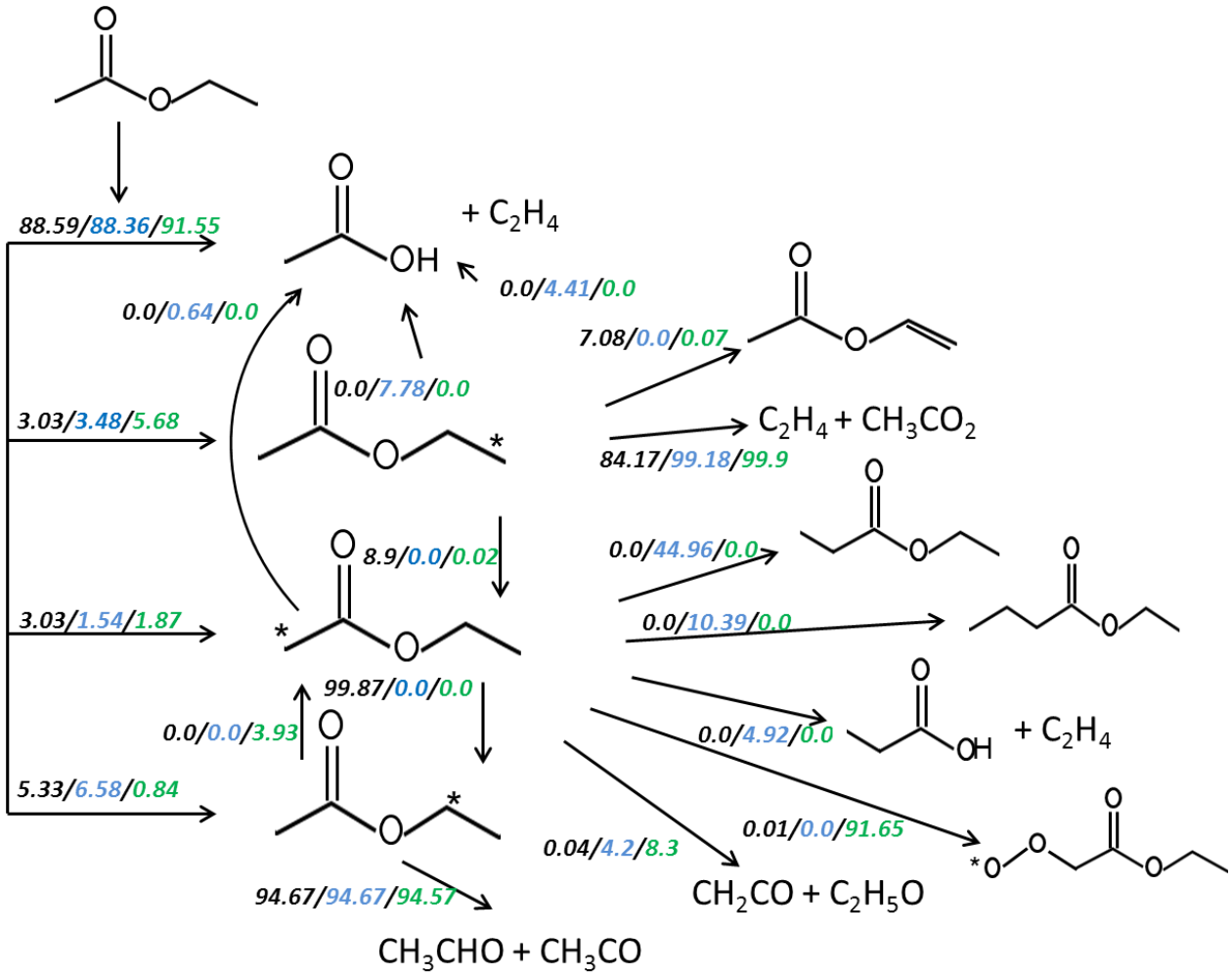

Figure S1 Primary reaction pathways of AcOEt decomposition in the fuel-rich flame. Numbers are derived from the analysis of the Dayma, Sun and Ahmed mechanisms (first/second/third, respectively)

Measured and calculated mole fraction profiles of selected species

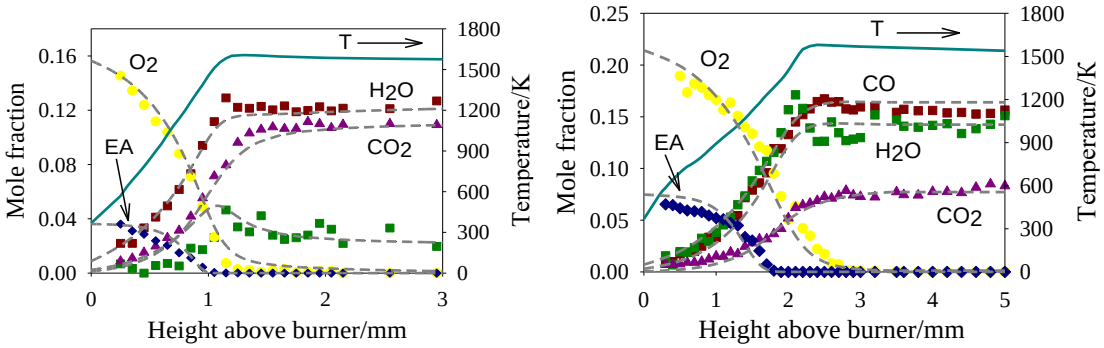

Figure S2 Temperature profiles and mole fraction profiles of reactants and major flame products in the near-stoichiometric (left) and fuel-rich (right) flames. Symbols: experiment, dashed lines: modeling, solid line: temperature.

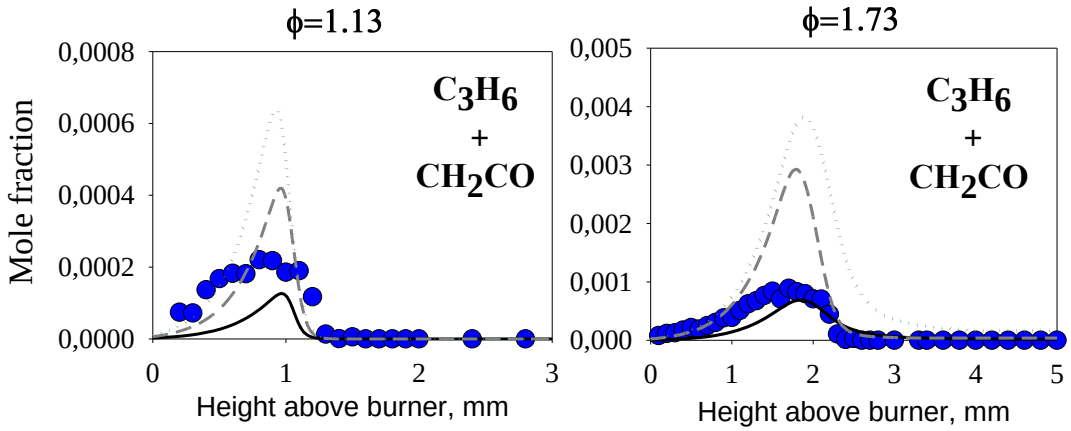

Figure S3 Profiles of combined mole fraction of propene and ketene in near-stoichiometric (left) and fuel-rich (right) flames of EA. Symbols correspond to the experiment, and lines represent the modeling (solid, dashed and dotted lines for the Dayma, Sun and Ahmed mechanisms, respectively).

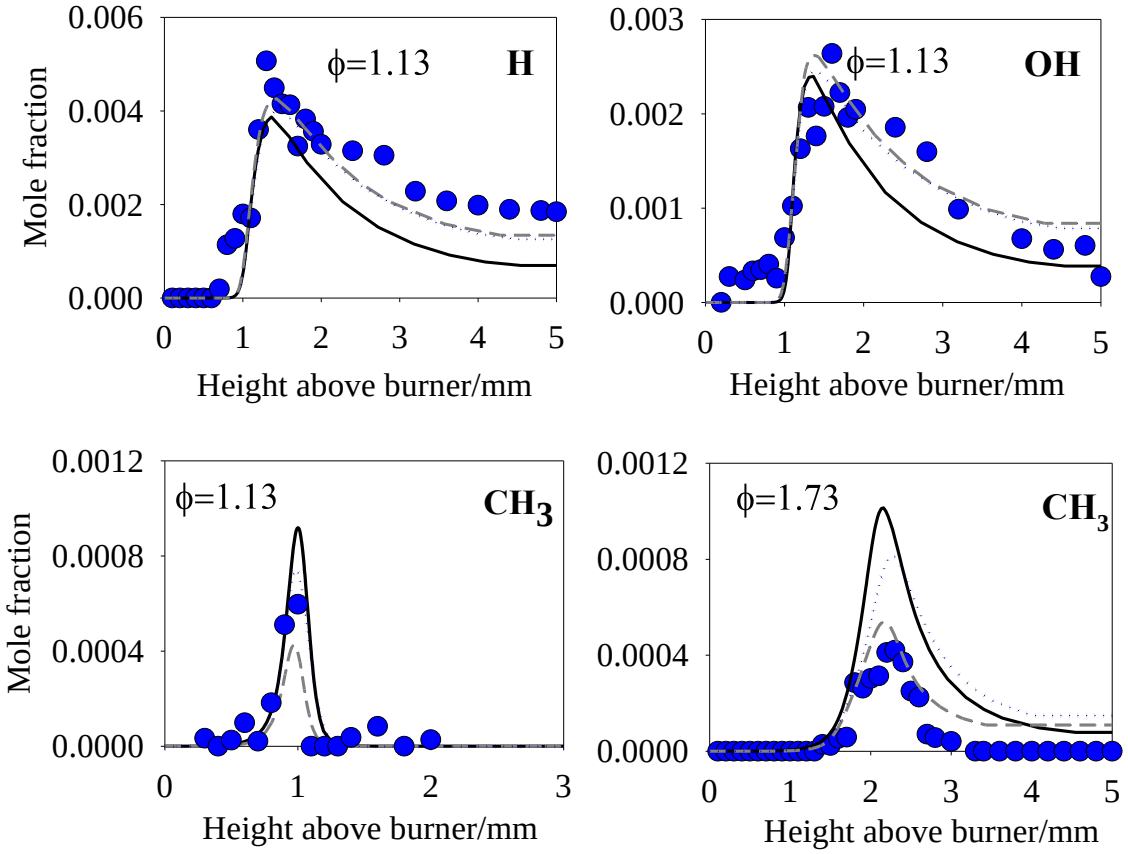

Figure S4 Mole fraction profiles of radicals in the near-stoichiometric and fuel-rich flames. Symbols correspond to the experiment, and lines represent the modeling (solid, dashed and dotted lines for the Dayma, Sun and Ahmed mechanisms, respectively).

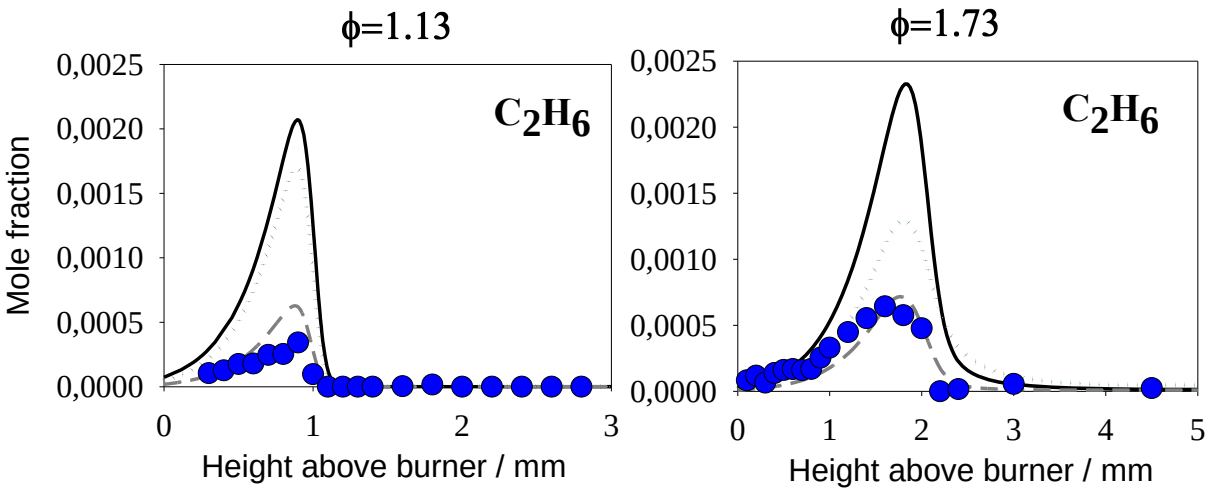

Figure S5 Mole fraction profiles of ethane in the near-stoichiometric (left) and fuel-rich (right) flames of AcOEt. Symbols correspond to the experiment, and lines represent the modeling (solid, dashed and dotted lines for the Dayma, Sun and Ahmed mechanisms, respectively).

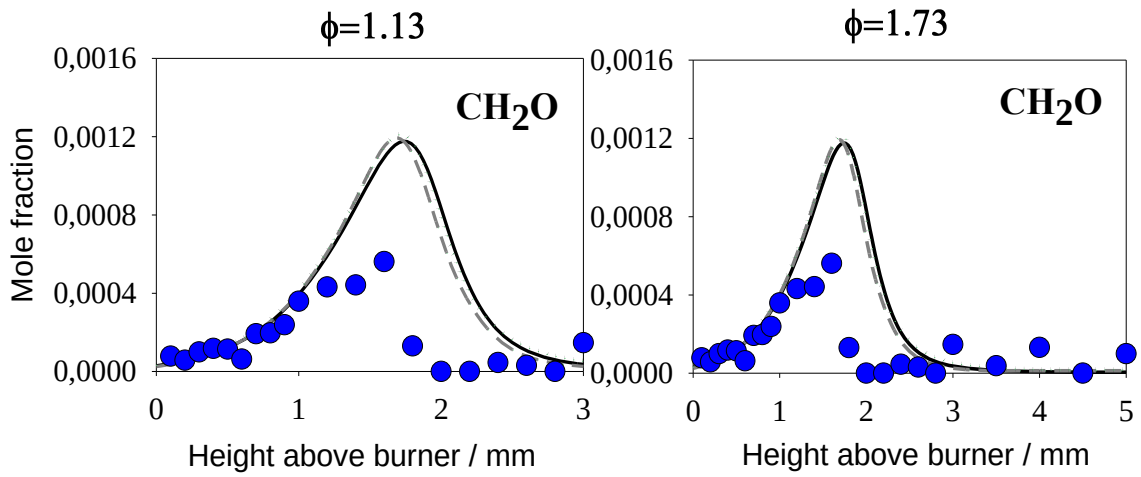

Figure S6 Mole fraction profiles of formaldehyde in the near-stoichiometric (left) and fuel-rich (right) flames of AcOEt. Symbols correspond to the experiment, and lines represent the modeling (solid, dashed and dotted lines for the Dayma, Sun and Ahmed mechanisms, respectively).

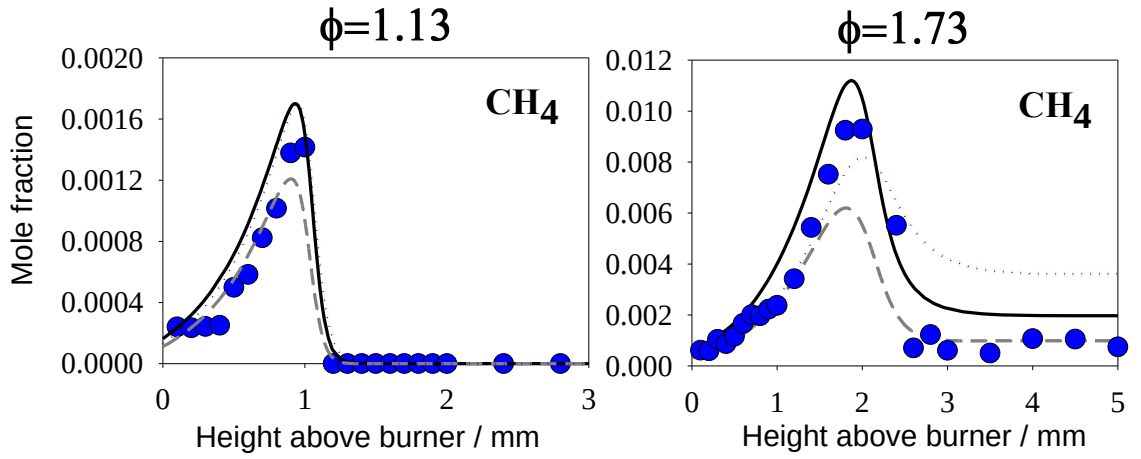

Figure S7 Mole fraction profiles of methane in near-stoichiometric (left) and fuel-rich (right) flames of AcOEt. Symbols correspond to the experiment, and lines represent the modeling (solid, dashed and dotted lines for the Dayma, Sun and Ahmed mechanisms, respectively).

Table S1 Species mole fractions measured in the near-stoichiometric AcOEt/O_2/Ar flame (ϕ = 1.13) at different heights above the burner (HAB).

HAB/mm	H	HAB/mm	CH_3	HAB/mm	CH_4
0,1000	0,0000	0,3000	3,3238e-5	0,1000	2,4064e-4
0,2000	0,0000	0,4000	0,0000	0,2000	2,3443e-4
0,3000	0,0000	0,5000	2,5191e-5	0,3000	2,4305e-4
0,4000	0,0000	0,6000	9,8563e-5	0,4000	2,5063e-4
0,5000	0,0000	0,7000	2,0788e-5	0,5000	4,9884e-4
0,6000	0,0000	0,8000	1,8255e-4	0,6000	5,8300e-4
0,7000	1,9519e-4	0,9000	5,1068e-4	0,7000	8,2355e-4
0,8000	1,1384e-3	1,0000	5,9695e-4	0,8000	1,0159e-3
0,9000	1,2743e-3	1,1000	0,0000	0,9000	1,3779e-3
1,0000	1,7955e-3	1,2000	0,0000	1,0000	1,4155e-3
1,1000	1,7125e-3	1,3000	0,0000	1,1000	0,0000
1,2000	3,6017e-3	1,4000	3,7013e-5		
1,3000	5,0689e-3	1,6000	8,3532e-5		
1,4000	4,4936e-3	1,8000	0,0000		
1,5000	4,1494e-3	2,0000	2,7328e-5		
1,6000	4,1303e-3				
1,7000	3,2458e-3				
1,8000	3,8272e-3				
1,9000	3,5622e-3				
2,0000	3,2847e-3				
2,4000	3,1472e-3				
2,8000	3,0513e-3				
3,2000	2,2821e-3				
3,6000	2,0756e-3				
4,0000	1,9853e-3				
4,4000	1,8949e-3				
4,8000	1,8701e-3				
5,0000	1,8453e-3				
HAB/mm	OH	HAB/mm	H_2O	HAB/mm	C_2H_2
0,1000		0,2500	0,0219	0,1000	5,6817e-5
0,2000	0,0000	0,3500	0,0219	0,2000	9,0252e-5
0,3000	2,7398e-4	0,4500	0,0333	0,3000	8,2324e-5
0,4000		0,5500	0,0412	0,4000	1,1952e-4
0,5000	2,3748e-4	0,6500	0,0495	0,5000	1,3783e-4
0,6000	3,3348e-4	0,7500	0,0616	0,6000	1,7150e-4
0,7000	3,4792e-4	0,8500	0,0732	0,7000	2,7067e-4
0,8000	4,0520e-4	0,9500	0,0941	0,8000	3,8295e-4
0,9000	2,5693e-4	1,0500	0,1117	0,9000	5,9055e-4
1,0000	6,8752e-4	1,1500	0,1291	1,0000	7,7883e-4
1,1000	1,0230e-3	1,2500	0,1222	1,1000	1,6439e-4
1,2000	1,6289e-3	1,3500	0,1215	1,2000	3,5891e-5
1,3000	2,0664e-3	1,4500	0,1229	1,3000	1,5657e-5
1,4000	1,7637e-3	1,5500	0,1203	1,4000	0,0000
1,5000	2,0779e-3	1,6500	0,1232		
1,6000	2,6389e-3	1,7500	0,1189		
1,7000	2,2242e-3	1,8500	0,1199		
1,8000	1,9604e-3	1,9500	0,1226		
1,9000	2,0465e-3	2,0500	0,1196		
2,0000		2,1500	0,1215		

2,4000	1,8554e-3	2,5500	0,1212		
2,8000	1,5970e-3	2,9500	0,1269		
3,2000	9,8736e-4	3,3500	0,1205		
4,0000	6,7643e-4	3,7500	0,1266		
4,4000	5,6272e-4	4,1500	0,1262		
4,8000	6,0331e-4	4,5500	0,1258		
5,0000	2,7398e-4	4,9500	0,1217		
HAB/mm	C_2H_4	HAB/mm	CO	HAB/mm	CH_2O
0,1000		0,2500	6,7943e-3	0,1000	7,8348e-5
0,2000	1,1716e-3	0,3500	3,4567e-3	0,2000	5,7836e-5
0,3000	1,3559e-3	0,4500	0,0000	0,3000	9,9698e-5
0,4000	1,7487e-3	0,5500	5,6218e-3	0,4000	1,1824e-4
0,5000	1,9657e-3	0,6500	7,1246e-3	0,5000	1,1444e-4
0,6000	2,0825e-3	0,7500	5,2376e-3	0,6000	6,3355e-5
0,7000	2,5568e-3	0,8500	0,0184	0,7000	1,9281e-4
0,8000	3,0011e-3	0,9500	0,0173	0,8000	1,9724e-4
0,9000	3,7483e-3	1,0500	0,0262	0,9000	2,3864e-4
1,0000	2,6185e-3	1,1500	0,0465	1,0000	3,5914e-4
1,1000	1,6212e-4	1,2500	0,0340	1,2000	4,3189e-4
1,2000	1,1217e-4	1,3500	0,0304	1,4000	4,4219e-4
1,3000	0,0000	1,4500	0,0422	1,6000	5,6175e-4
		1,5500	0,0279	1,8000	1,3025e-4
		1,6500	0,0248	2,0000	0,0000
		1,7500	0,0260	2,2000	0,0000
		1,8500	0,0280	2,4000	4,5682e-5
		1,9500	0,0367	2,6000	3,1443e-5
		2,0500	0,0323	2,8000	0,0000
		2,1500	0,0219	3,0000	1,4704e-4
		2,5500	0,0332	3,5000	3,8070e-5
		2,9500	0,0196	4,0000	1,3151e-4
		3,3500	0,0252	4,5000	0,0000
		3,7500	0,0209	5,0000	9,9957e-5
		4,1500	0,0237		
		4,5500	0,0264		
		4,9500	0,0213		
		5,1500	0,0232		

HAB/mm	C_2H_6	HAB/mm	O_2	HAB/mm	C_3H_6+CH_2CO
0,3000	1,0457e-4	0,2500	0,1455	0,1000	
0,4000	1,2643e-4	0,3500	0,1345	0,2000	7,4481e-5
0,5000	1,7559e-4	0,4500	0,1239	0,3000	7,2331e-5
0,6000	1,7988e-4	0,5500	0,1118	0,4000	1,3707e-4
0,7000	2,4642e-4	0,6500	0,1039	0,5000	1,6791e-4
0,8000	2,5328e-4	0,7500	0,0880	0,6000	1,8273e-4
0,9000	3,4265e-4	0,8500	0,0709	0,7000	1,8169e-4
1,0000	9,6438e-5	0,9500	0,0489	0,8000	2,2072e-4
1,1000	0,0000	1,0500	0,0265	0,9000	2,1766e-4
1,2000	0,0000	1,1500	7,3920e-3	1,0000	1,8587e-4
1,3000	0,0000	1,2500	2,9419e-3	1,1000	1,9004e-4
1,4000	0,0000	1,3500	2,1996e-3	1,2000	1,1737e-4
1,6000	3,7963e-6	1,4500	8,0916e-4	1,3000	1,3575e-5

1,8000	1,5919e-5	1,5500	1,8575e-3	1,4000	9,1974e-7
2,0000	0,0000	1,6500	2,9059e-3	1,5000	5,8678e-6
		1,7500	5,5073e-4	1,6000	0,0000
		1,8500	1,1091e-3		
		1,9500	1,3253e-3		
		2,0500	1,5546e-3		
HAB/mm	CH_3CHO	HAB/mm	CO_2	HAB/mm	CH_3COOH
0,3000	3,2029e-4	0,2500	8,8280e-3	0,1000	5,3672e-4
0,4000	9,7971e-4	0,3500	0,0110	0,2000	7,7862e-4
0,5000	9,5461e-4	0,4500	0,0152	0,3000	3,6178e-4
0,6000	1,7045e-3	0,5500	0,0197	0,4000	8,6706e-4
0,7000	2,0347e-3	0,6500	0,0260	0,5000	7,0862e-4
0,8000	1,2652e-3	0,7500	0,0314	0,6000	1,1052e-3
0,9000	1,3891e-3	0,8500	0,0418	0,7000	1,5018e-3
1,0000	0,0000	0,9500	0,0553	0,8000	1,5216e-3
1,1000	0,0000	1,0500	0,0714	0,9000	2,1558e-3
1,2000	3,2029e-4	1,1500	0,0796	1,0000	2,3583e-3
1,3000	4,6013e-4	1,2500	0,0962	1,1000	1,1523e-3
1,4000	0,0000	1,3500	0,1031	1,2000	0,0000
1,6000	3,8515e-4	1,4500	0,1059	1,3000	0,0000
1,8000	0,0000	1,5500	0,1076	1,4000	0,0000
2,0000	0,0000	1,6500	0,1065	1,5000	0,0000
2,2000	0,0000	1,7500	0,1065	1,6000	0,0000
2,4000	0,0000	1,8500	0,1115	1,7000	0,0000
2,6000	0,0000	1,9500	0,1100	1,8000	0,0000
2,8000	0,0000	2,0500	0,1071	1,9000	0,0000
		2,1500	0,1095	2,0000	0,0000
		2,5500	0,1101	2,4000	0,0000
		2,9500	0,1092	2,8000	0,0000
		3,3500	0,1075	3,2000	0,0000
		3,7500	0,1065	3,6000	0,0000
		4,1500	0,1075	4,0000	0,0000
		4,5500	0,1084	4,4000	0,0000
		4,9500	0,1097	4,8000	0,0000
		5,1500	0,1097	5,0000	0,0000

HAB/mm	AcOEt
0,2500	0,0361
0,3500	0,0310
0,4500	0,0286
0,5500	0,0238
0,6500	0,0204
0,7500	0,0149
0,8500	0,0112
0,9500	4,3301e-3
1,0500	4,4387e-4
1,1500	6,8240e-5
1,2500	1,3498e-4
1,3500	0,0000
1,4500	0,0000

Table S2 Species mole fractions measured in the fuel-rich AcOEt/O_2/Ar flame (ϕ = 1.73) at different heights above burner (HAB).

HAB/mm	CH_3	HAB/mm	CH_4	HAB/mm	H_2O
0,1000	0,0000	0,1000	6,1511e-4	0,3000	8,3152e-3
0,2000	0,0000	0,2000	5,9404e-4	0,4000	9,9159e-3
0,3000	0,0000	0,3000	1,0417e-3	0,5000	0,0175
0,4000	0,0000	0,4000	8,7365e-4	0,6000	0,0190
0,5000	0,0000	0,5000	1,1642e-3	0,7000	0,0199
0,6000	0,0000	0,6000	1,6704e-3	0,8000	0,0249
0,7000	0,0000	0,7000	2,0118e-3	0,9000	0,0334
0,8000	0,0000	0,8000	1,9662e-3	1,0000	0,0332
0,9000	0,0000	0,9000	2,2268e-3	1,1000	0,0457
1,0000	0,0000	1,0000	2,3770e-3	1,2000	0,0469
1,1000	0,0000	1,2000	3,4208e-3	1,3000	0,0544
1,2000	0,0000	1,4000	5,4316e-3	1,4000	0,0718
1,3000	0,0000	1,6000	7,5175e-3	1,5000	0,0791
1,4000	2,8258e-5	1,8000	9,2453e-3	1,6000	0,0859
1,5000	2,3351e-5	2,0000	9,2930e-3	1,7000	0,0958
1,6000	5,3156e-5	2,2000		1,8000	0,1192
1,7000	5,8335e-5	2,4000	5,5156e-3	1,9000	0,1191
1,8000	2,8535e-4	2,6000	7,0523e-4	2,0000	0,1327
1,9000	2,6220e-4	2,8000	1,2283e-3	2,1000	0,1451
2,0000	3,0299e-4	3,0000	6,0995e-4	2,2000	0,1521
2,1000	3,1373e-4	3,5000	5,0434e-4	2,3000	0,1577
2,2000	4,1108e-4	4,0000	1,0703e-3	2,4000	0,1647
2,3000	4,2066e-4	4,5000	1,0502e-3	2,5000	0,1673
2,4000	3,7134e-4	5,0000	7,4785e-4	2,6000	0,1642
2,5000	2,5002e-4			2,7000	0,1646
2,6000	2,2520e-4			2,8000	0,1576
2,7000	7,0773e-5			2,9000	0,1567
2,8000	5,6408e-5			3,0000	0,1596
3,0000	4,0331e-5			3,2000	0,1599
3,3000	0,0000			3,5000	0,1543
				3,6000	0,1573
				3,8000	0,1558
				4,0000	0,1561
				4,2000	0,1538
				4,4000	0,1542
				4,6000	0,1526
				4,8000	0,1533
				5,0000	0,1565
				5,2000	0,1580

HAB/mm	C_2H_2	HAB/mm	C_2H_4	HAB/mm	CO
0,1000	2,9405e-4	0,1000	1,1731e-3	0,3000	0,0155
0,2000	1,9195e-4	0,2000	2,1340e-3	0,4000	6,8364e-3
0,3000	2,5257e-4	0,3000	2,5545e-3	0,5000	0,0195
0,4000	4,4317e-4	0,4000	2,7601e-3	0,6000	0,0188
0,5000	5,5266e-4	0,5000	3,0681e-3	0,7000	0,0233
0,6000	4,5346e-4	0,6000	3,4858e-3	0,8000	0,0325
0,7000	5,8875e-4	0,7000	5,2039e-3	0,9000	0,0293
0,8000	7,9497e-4	0,8000	5,6954e-3	1,0000	0,0382
0,9000	7,9493e-4	0,9000	7,7371e-3	1,1000	0,0457
1,0000	1,3463e-3	1,0000	8,6942e-3	1,2000	0,0529

1,1000	1,5783e-3	1,1000	9,4174e-3	1,3000	0,0649
1,2000	2,0360e-3	1,2000	0,0117	1,4000	0,0734
1,3000	2,2135e-3	1,3000	0,0137	1,5000	0,0880
1,4000	2,3634e-3	1,4000	0,0152	1,6000	0,0981
1,5000	3,5033e-3	1,5000	0,0159	1,7000	0,1068
1,6000	3,6212e-3	1,6000	0,0178	1,8000	0,1156
1,7000	4,5461e-3	1,7000	0,0197	1,9000	0,1346
1,8000	5,2811e-3	1,8000	0,0129	2,0000	0,1568
1,9000	5,7328e-3	1,9000	2,5086e-3	2,1000	0,1712
2,0000	7,0060e-3	2,0000	6,2505e-4	2,2000	0,1581
2,1000	7,7679e-3	2,1000	1,9810e-4	2,3000	0,1391
2,2000	8,3018e-3	2,2000	9,2542e-5	2,4000	0,1261
2,3000	8,1052e-3	2,3000	1,2765e-4	2,5000	0,1264
2,4000	5,3522e-3	2,4000	8,7198e-5	2,6000	0,1450
2,5000	5,5267e-3	2,5000	6,2702e-5	2,7000	0,1346
2,6000	4,5258e-3	2,6000	1,6455e-4	2,8000	0,1270
2,7000	3,4717e-3	2,7000	9,1085e-5	2,9000	0,1284
2,8000		2,8000	0,0000	3,0000	0,1299
3,0000	2,9437e-3	3,0000	0,0000	3,2000	0,1518
3,3000	2,6433e-3	3,3000	0,0000	3,5000	0,1469
3,4000	2,5192e-3	3,4000	0,0000	3,6000	0,1409
3,6000	2,3950e-3	3,6000	0,0000	3,8000	0,1400
3,8000	2,0535e-3	3,8000	0,0000	4,0000	0,1417
4,0000	1,7119e-3	4,0000	0,0000	4,2000	0,1433
4,2000	1,6021e-3	4,2000	0,0000	4,4000	0,1339
4,4000	1,4922e-3	4,4000	0,0000	4,6000	0,1385
4,6000	1,4123e-3	4,6000	0,0000	4,8000	0,1427
4,8000	1,3324e-3	4,8000	0,0000	5,0000	0,1511
5,0000	9,5799e-4	5,0000	0,0000	5,2000	0,1350
5,2000	5,8354e-4	5,2000	0,0000	5,4000	0,1453

HAB/mm	CH_2O	HAB/mm	C_2H_6	HAB/mm	O_2
0,1000	7,8348e-5	0,1000	8,2220e-5	0,5000	0,1895
0,2000	5,7836e-5	0,2000	1,1782e-4	0,6000	0,1736
0,3000	9,9698e-5	0,3000	6,5095e-5	0,7000	0,1819
0,4000	1,1824e-4	0,4000	1,3799e-4	0,8000	0,1783
0,5000	1,1444e-4	0,5000	1,6060e-4	0,9000	0,1709
0,6000	6,3355e-5	0,6000	1,6730e-4	1,0000	0,1665
0,7000	1,9281e-4	0,7000	1,6002e-4	1,1000	0,1567
0,8000	1,9724e-4	0,8000	1,6866e-4	1,2000	0,1637
0,9000	2,3864e-4	0,9000	2,5352e-4	1,3000	0,1508
1,0000	3,5914e-4	1,0000	3,2948e-4	1,4000	0,1398
1,2000	4,3189e-4	1,2000	4,4776e-4	1,5000	0,1337
1,4000	4,4219e-4	1,4000	5,5298e-4	1,6000	0,1211
1,6000	5,6175e-4	1,6000	6,4244e-4	1,7000	0,1175
1,8000	1,3025e-4	1,8000	5,7488e-4	1,8000	0,0951
2,0000	0,0000	2,0000	4,7633e-4	1,9000	0,0731
2,2000	0,0000	2,4000	1,5510e-5	2,0000	0,0505
2,4000	4,5682e-5	2,6000	0,0000	2,1000	0,0632
2,6000	3,1443e-5	2,8000	0,0000	2,2000	0,0422
2,8000	0,0000	3,0000	0,0000	2,3000	0,0350
3,0000	1,4704e-4	3,5000	0,0000	2,4000	0,0222
3,5000	3,8070e-5	4,0000	0,0000	2,5000	0,0173
4,0000	1,3151e-4	4,5000	0,0000	2,6000	8,1469e-3
4,5000	0,0000	5,0000	0,0000	2,7000	7,1434e-3

5,0000	9,9957e-5			2,8000 2,9000	1,4038e-3 1,1876e-3

HAB/mm	C_3H_6+CH_2CO	HAB/mm	CH_3CHO	HAB/mm	CO_2
0,1000	8,1038e-5	0,1000	0,0000	0,3000	7,0820e-3
0,2000	1,1677e-4	0,2000	0,0000	0,4000	7,1320e-3
0,3000	1,2854e-4	0,3000	0,0000	0,5000	7,5692e-3
0,4000	1,7365e-4	0,4000	1,9196e-4	0,6000	9,1973e-3
0,5000	2,1771e-4	0,5000	7,3709e-4	0,7000	9,1313e-3
0,6000	1,9161e-4	0,6000	9,3949e-4	0,8000	0,0101
0,7000	2,5173e-4	0,7000	7,6259e-4	0,9000	0,0123
0,8000	3,0546e-4	0,8000	9,0690e-4	1,0000	0,0151
0,9000	3,8332e-4	0,9000	1,4116e-3	1,1000	0,0149
1,0000	3,9063e-4	1,0000	1,3619e-3	1,2000	0,0190
1,1000	5,1096e-4	1,1000	1,6267e-3	1,3000	0,0174
1,2000	6,2308e-4	1,2000	1,4837e-3	1,4000	0,0246
1,3000	6,7752e-4	1,3000	1,2881e-3	1,5000	0,0279
1,4000	7,6778e-4	1,4000	1,5282e-3	1,6000	0,0316
1,5000	8,3985e-4	1,5000	1,4566e-3	1,7000	0,0318
1,6000	7,0615e-4	1,6000	1,3654e-3	1,8000	0,0368
1,7000	8,8913e-4	1,7000	1,2401e-3	1,9000	0,0417
1,8000	8,3140e-4	1,8000	7,7270e-4	2,0000	0,0519
1,9000	7,9926e-4	1,9000	5,6210e-4	2,1000	0,0621
2,0000	7,0916e-4	2,0000	4,8739e-4	2,2000	0,0646
2,1000	7,0473e-4	2,1000	2,8898e-4	2,3000	0,0662
2,2000	4,4681e-4	2,2000	3,6566e-4	2,4000	0,0688
2,3000	1,0668e-4	2,3000	3,1489e-4	2,5000	0,0727
2,4000	1,4901e-5	2,4000	1,9196e-4	2,6000	0,0711
2,5000	3,0623e-5	2,5000	2,3423e-4	2,7000	0,0737
2,6000	0,0000	2,6000	0,0000	2,8000	0,0786
2,7000	0,0000	2,7000	0,0000	2,9000	0,0742
2,8000	0,0000	2,8000	0,0000	3,0000	0,0728
3,0000	0,0000	3,0000	0,0000	3,2000	0,0723
3,3000	0,0000	3,3000	0,0000	3,5000	0,0773
3,4000	0,0000	3,4000	0,0000	3,6000	0,0745
3,6000	0,0000	3,6000	0,0000	3,8000	0,0741
3,8000	0,0000	3,8000	0,0000	4,0000	0,0776
4,0000	0,0000	4,0000	0,0000	4,2000	0,0776
4,2000	0,0000	4,2000	0,0000	4,4000	0,0764
4,4000	0,0000	4,4000	0,0000	4,6000	0,0817
4,6000	0,0000	4,6000	0,0000	4,8000	0,0849
4,8000	0,0000	4,8000	0,0000	5,0000	0,0831
5,0000	0,0000	5,0000	0,0000	5,2000	0,0850
5,2000	0,0000	5,2000	0,0000	5,4000	0,0861

HAB/mm	CH_3COOH	HAB/mm	AcOEt
0,1000	2,3270e-3	0,3000	0,0653
0,2000	2,9349e-3	0,4000	0,0645
0,3000	2,9484e-3	0,5000	0,0615
0,4000	3,2047e-3	0,6000	0,0594
0,5000	3,2458e-3	0,7000	0,0586
0,6000	3,7828e-3	0,8000	0,0578
0,7000	4,3156e-3	0,9000	0,0545
0,8000	5,9181e-3	1,0000	0,0520
0,9000	5,6741e-3	1,1000	0,0509

1,0000	6,1935e-3	1,2000	0,0472
1,1000	7,5092e-3	1,3000	0,0449
1,2000	7,9964e-3	1,4000	0,0336
1,3000	9,2420e-3	1,5000	0,0303
1,4000	0,0101	1,6000	0,0203
1,5000	0,0102	1,7000	7,2000e-3
1,6000	0,0112	1,8000	1,2374e-3
1,7000	8,9716e-3	1,9000	0,0000
1,8000	3,8899e-3		
1,9000	4,3782e-3		
2,0000	1,9612e-3		
2,1000	3,0686e-4		
2,2000	2,4371e-5		
2,3000	2,8309e-5		
2,4000	5,6887e-5		
2,5000	5,7616e-5		
2,6000	5,8345e-5		
2,7000	0,0000		

Table S3 Temperature measured in the near-stoichiometric (ϕ = 1.13) and fuel-rich (ϕ = 1.73) AcOEt/O_2/Ar flames at different heights above burner (HAB)**.**

ϕ = 1.13			ϕ = 1.73	
HAB/mm	*T*/K		HAB/mm	*T*/K
0,0000	368,0000		0,0000	368,0000
0,2000	529,0000		0,2000	524,0000
0,2500	568,0000		0,2500	560,0000
0,3000	631,6000		0,3000	586,2000
0,3500	683,9400		0,3500	615,2000
0,4000	733,1600		0,4000	641,3000
0,4500	784,5600		0,4500	666,1800
0,5000	840,3600		0,5000	691,1200
0,5500	898,1600		0,5500	713,7000
0,6000	954,0200		0,6000	732,7000
0,6500	1020,8000		0,6500	746,7400
0,7000	1083,2000		0,7000	762,8600
0,7500	1138,4000		0,7500	781,0200
0,8000	1197,4000		0,8000	801,1800
0,8500	1263,4000		0,8500	823,3400
0,9000	1327,0000		0,9000	847,5000
0,9500	1387,2000		0,9500	870,5000
1,0000	1454,4400		1,0000	893,3200
1,0500	1511,7400		1,0500	914,9800
1,1000	1554,0800		1,1000	936,5000
1,1500	1582,6000		1,1500	956,9200
1,2000	1601,4800		1,2000	977,2800
1,3000	1606,5000		1,2500	997,5400
1,4000	1604,6400		1,3000	1019,7200
1,5000	1601,3200		1,3500	1043,8000
1,6000	1596,5600		1,4000	1067,8200
1,8000	1591,4000		1,4500	1094,7400
2,0000	1586,2400		1,5000	1122,5800
2,5000	1580,1500		1,5500	1149,3400
3,0000	1575,5000		1,6000	1175,0400

			1,6500	1205,6400
			1,7000	1233,2600
			1,7500	1258,8800
			1,8000	1284,5000
			1,8500	1311,1200
			1,9000	1336,8000
			2,0000	1402,2800
			2,2000	1550,2200
			2,3000	1571,5600
			2,4000	1580,7200
			2,5000	1578,6600
			3,0000	1568,4000
			4,0000	1555,0500
			5,0000	1539,7000

References

S1. A. M. Dmitriev, D. A. Knyazkov, T. A. Bolshova, A. G. Shmakov and O. P. Korobeinichev, *Combust. Flame*, 2015, **162**, 1964.

S2. I. E. Gerasimov, D. A. Knyazkov, S. A. Yakimov, T. A. Bolshova, A. G. Shmakov and O. P. Korobeinichev, *Combust. Flame*, 2012, **159**, 1840.

S3. T. A. Cool, K. Nakajima, C. A. Taatjes, A. McIlroy, P. R. Westmoreland, M. E. Law and A. Morel, *Proc. Combust. Inst.*, 2005, **30**, 1681.