Supplementary Material

Contents

1. Thermochemistry

The heats of formation at 298 K ($H_{f\ 298}$), entropies of formation (S_{298}) and heat capacities (C_P) at 300, 400, 500, 600, 800, 1000 and 1500 K contained in the thermochemistry file are included in Table 1.

SPECIES	$H_{f\ 298}$	$S_{\ 298}$	C_p300	C_p400	C_p500	C_p600	C_p800	C_p1000	C_p1500
H	52.10	27.42	4.97	4.97	4.97	4.97	4.97	4.97	4.97
H_2	0.00	31.23	6.89	7.00	7.00	6.99	7.08	7.21	7.73
O	59.55	38.49	5.23	5.13	5.08	5.05	5.02	5.00	4.98
O_2	0.00	49.03	7.02	7.20	7.43	7.67	8.07	8.34	8.72
OH	8.91	43.91	7.14	7.07	7.05	7.06	7.15	7.34	7.88
OH*	101.55	43.88	7.15	7.10	7.07	7.06	7.13	7.33	7.87
H_2O	-57.80	45.13	8.03	8.19	8.42	8.68	9.26	9.87	11.31
N_2	0.00	45.80	6.96	7.00	7.07	7.19	7.51	7.81	8.31
HO_2	2.94	54.76	8.35	8.89	9.46	9.99	10.77	11.38	12.48
H_2O_2	-32.48	56.06	10.15	11.09	11.99	12.79	13.99	14.95	16.59
Ar	0.00	37.01	4.97	4.97	4.97	4.97	4.97	4.97	4.97
CH_2O	-26.09	52.28	8.47	9.36	10.44	11.52	13.37	14.82	16.93
CO	-26.42	47.24	6.96	7.02	7.12	7.27	7.62	7.93	8.40
CO_2	-94.05	51.10	8.89	9.86	10.66	11.32	12.29	12.98	13.91
HCO	10.11	53.60	8.29	8.75	9.29	9.84	10.85	11.66	12.94
HO_2CHO	-67.41	73.87	15.22	17.67	19.71	21.39	23.91	25.57	27.64
O_2CHO	-31.30	74.09	13.30	14.75	16.04	17.18	19.05	20.45	22.47
HOCHO	-90.48	59.07	9.90	11.50	13.09	14.50	16.57	18.12	20.39
HOCO	-43.34	60.17	10.45	11.81	12.99	13.98	15.39	16.39	17.81
OCHO	-31.00	60.93	10.05	11.04	12.10	13.09	14.71	15.98	17.92
$HOCH_2O_2H$	-76.03	75.92	18.70	22.12	24.94	27.23	30.62	32.86	35.98
$HOCH_2O_2$	-42.22	74.79	16.64	19.21	21.35	23.14	25.89	27.84	30.90
OCH_2O_2H	-24.06	74.46	17.71	20.81	23.33	25.36	28.26	30.09	32.45
$HOCH_2O$	-42.16	66.11	13.07	14.75	16.38	17.92	20.66	22.84	26.03

CH_3OH	-48.04	57.52	10.28	12.07	14.07	15.98	19.00	21.38	25.07
CH_2OH	-4.06	58.36	11.35	12.79	14.16	15.36	17.08	18.44	20.59
CH_3O	5.02	55.99	10.20	12.05	13.86	15.47	17.86	19.70	22.25
CH_3O_2H	-30.29	65.94	16.01	18.83	21.17	23.02	25.52	27.50	30.65
CH_3O_2	2.92	64.50	11.99	14.07	16.08	17.90	20.79	22.91	26.13
CH_2O_2H	15.00	67.42	15.81	17.67	19.33	20.79	23.18	24.92	27.24
CH_4	-17.83	44.54	8.55	9.69	11.11	12.60	15.31	17.62	21.62
CH_3	35.06	46.37	9.20	9.98	10.75	11.50	12.86	14.09	16.25
CH_2	93.50	46.47	8.37	8.73	9.07	9.39	9.97	10.59	11.77
CH_2(S)	102.48	45.22	8.08	8.33	8.66	9.04	9.83	10.57	11.91
CH	142.40	43.75	6.97	6.99	7.03	7.11	7.37	7.71	8.57
CH*	208.55	43.72	6.95	7.00	7.05	7.11	7.37	7.78	8.75
C	171.28	37.79	4.98	4.97	4.97	4.97	4.97	4.97	4.97
C_2H_6	-20.04	54.78	12.60	15.57	18.58	21.36	25.80	29.32	34.71
C_2H_5	28.92	59.09	12.06	14.71	17.11	19.28	22.95	25.79	30.18
C_2H_4	12.55	52.42	10.29	12.58	14.88	16.95	20.05	22.49	26.19
C_2H_3	70.88	55.85	10.09	11.81	13.46	14.90	17.06	18.78	21.50
C_2H_2	54.54	48.02	10.55	12.01	13.08	13.89	15.16	16.23	18.14
C_2H	135.77	50.98	10.05	10.54	10.88	11.19	11.90	12.56	13.88
CH_3CHO	-39.72	63.09	13.26	15.78	18.29	20.58	24.16	26.91	30.96
CH_3CO	-2.46	63.92	12.17	14.27	16.30	18.13	20.99	23.19	26.34
CH_2CHO	3.05	63.15	13.03	15.49	17.66	19.45	21.97	23.83	26.59
CH_2CO	-11.52	57.66	12.22	14.02	15.48	16.69	18.59	20.04	22.35
HCCO	42.61	58.89	11.97	13.27	14.21	14.93	16.08	16.93	18.27
HCCOH	22.30	59.64	13.80	15.44	16.67	17.64	19.19	20.40	22.43
CH_3CO_3H	-80.49	77.24	20.55	24.40	27.64	30.35	34.52	37.42	41.51
CH_3CO_3	-42.35	77.37	19.97	23.01	25.58	27.74	31.09	33.48	37.05
CH_3CO_2	-51.38	64.94	14.78	17.74	20.26	22.41	25.78	28.20	31.77
C_2H_5OH	-56.15	67.06	15.67	19.31	22.84	25.96	30.59	34.15	39.53
PC_2H_4OH	-5.70	69.72	16.47	19.38	22.06	24.40	27.94	30.70	35.00

SC_2H_4OH	-12.91	69.07	15.36	18.30	21.07	23.48	27.16	30.02	34.52
C_2H_5O	-3.25	66.36	15.91	18.93	21.79	24.34	28.35	31.44	36.01
$O_2C_2H_4OH$	-41.29	86.96	21.80	25.33	28.43	31.17	35.67	39.14	44.68
$C_2H_5O_2H$	-39.14	74.47	20.09	24.22	27.75	30.75	35.47	38.90	44.17
$C_2H_5O_2$	-6.86	73.85	18.27	22.14	25.71	28.75	33.14	36.37	41.03
$C_2H_4O_2H$	11.86	82.15	19.77	22.84	25.42	27.61	30.99	33.42	37.14
CH_3CHO_2H	4.76	78.29	20.22	23.37	26.09	28.46	32.27	35.12	39.56
$C_2H_4O1\text{-}2$	-12.58	58.05	11.44	14.71	17.92	20.71	24.62	27.54	31.71
$C_2H_3O1\text{-}2$	39.31	60.35	10.98	13.71	16.33	18.56	21.59	23.83	27.04
CH_3COCH_3	-51.34	70.66	17.81	21.78	25.69	29.21	34.63	38.76	44.84
CH_3COCH_2	-7.97	73.50	17.47	20.98	24.28	27.17	31.57	34.91	39.98
$CH_3COCH_2O_2$	-35.38	92.65	25.67	29.37	32.69	35.64	40.59	44.46	50.54
$CH_3COCH_2O_2$	-71.49	92.43	27.71	32.27	36.25	39.71	45.29	49.45	55.63
CH_3COCH_2O	-33.71	80.46	21.23	25.02	28.43	31.48	36.55	40.42	46.11
C_2H_3CHO	-20.32	67.40	17.08	20.88	24.03	26.64	30.59	33.34	37.42
C_2H_3CO	11.58	66.01	16.88	19.96	22.44	24.44	27.37	29.42	32.78
C_2H_5CHO	-44.25	69.03	18.07	22.25	26.21	29.73	35.18	39.32	45.51
C_2H_5CO	-7.85	75.12	16.27	19.59	22.94	25.99	30.70	34.31	39.70
CH_2CH_2CHO	3.64	76.16	19.37	21.83	24.66	27.68	33.64	38.74	45.39
CH_3CHCHO	-5.56	70.38	13.99	19.16	23.77	27.85	34.61	39.73	46.16
CH_3OCH_3	-44.00	63.90	15.51	18.77	21.82	24.64	29.54	33.43	39.34
CH_3OCH_2	0.10	67.78	14.50	17.35	19.95	22.30	26.31	29.46	34.44
$CH_3OCH_2O_2$	-36.90	83.11	21.38	25.65	29.26	32.30	37.00	40.37	45.46
$CH_2OCH_2O_2H$	-26.10	86.76	22.66	27.44	31.36	34.56	39.24	42.28	46.27
$CH_3OCH_2O_2H$	-70.21	84.26	23.43	28.55	32.81	36.35	41.68	45.32	50.51
CH_3OCH_2O	-34.47	73.95	18.32	21.65	24.67	27.40	32.01	35.56	40.81
$O_2CH_2OCH_2O$	-63.11	102.09	29.23	35.42	40.27	44.05	49.20	52.33	56.66
HO_2CH_2OCHO	-111.88	87.08	23.54	28.80	33.15	36.70	41.84	45.01	48.38
OCH_2OCHO	-76.96	75.61	18.47	21.67	24.62	27.27	31.63	34.71	38.17
$HOCH_2OCO$	-82.59	81.62	19.83	22.28	24.60	26.74	30.41	33.18	36.77

CH_3OCHO	-86.90	68.42	14.97	17.94	20.97	23.75	28.02	31.22	35.90
CH_3OCO	-39.05	69.02	15.86	18.23	20.45	22.44	25.63	28.01	31.56
CH_2OCHO	-37.42	70.63	14.64	17.57	20.24	22.62	26.52	29.28	32.46
He	0.00	30.15	4.97	4.97	4.97	4.97	4.97	4.97	4.97
C_3H_8	-25.02	64.61	17.67	22.34	26.84	30.85	37.01	41.78	48.99
NC_3H_7	24.22	69.42	17.12	21.14	24.95	28.33	33.53	37.59	43.91
IC_3H_7	21.56	69.34	15.73	19.52	23.37	26.91	32.52	36.89	43.58
C_3H_6	4.78	63.73	15.47	19.17	22.71	25.88	30.78	34.56	40.26
C_3H_5-A	40.91	61.88	15.22	18.99	22.28	25.03	29.06	32.12	36.75
C_3H_5-T	60.60	65.26	15.57	18.94	21.93	24.54	28.73	31.88	36.81
C_3H_5-S	64.10	64.66	15.39	18.93	22.01	24.64	28.79	31.90	36.79
C_3H_4-A	45.63	58.18	14.13	17.11	19.77	22.04	25.40	27.99	31.90
C_3H_4-P	44.32	59.34	14.57	17.28	19.70	21.80	25.12	27.71	31.71
C_3H_3	84.01	61.34	15.56	17.83	19.55	20.92	23.11	24.81	27.54
C_3H_5O	22.15	73.00	17.62	21.52	24.92	27.87	32.59	36.03	41.06
C_3H_6OOH1-3	4.17	87.41	25.05	30.29	34.77	38.60	44.65	49.04	55.50
C_3H_6OOH1-2	3.07	91.34	24.20	28.89	32.97	36.51	42.25	46.55	53.30
$C_3H_6OOH_2$-1	1.00	88.11	26.02	31.08	35.29	38.78	44.14	47.97	54.08
$C_3H_6OOH_2$-2	1.00	88.11	26.02	31.08	35.29	38.78	44.14	47.97	54.08
C_3H_6OOH1-2	-35.60	100.30	32.12	38.36	43.55	47.88	54.48	59.15	66.08
C_3H_6OOH1-3	-30.93	100.96	31.61	37.66	42.78	47.10	53.83	58.68	65.85
$C_3H_6OOH_2$-1	-35.60	100.30	32.12	38.36	43.55	47.88	54.48	59.15	66.08
NC_3H_7O	-8.48	72.19	19.61	24.48	29.05	33.06	39.10	43.68	50.50
IC_3H_7O	-13.14	71.01	20.42	25.58	29.90	33.50	39.00	42.87	48.63
$NC_3H_7O_2H$	-43.41	87.86	23.36	28.81	34.06	38.65	45.35	50.39	57.95
$IC_3H_7O_2H$	-49.50	81.96	26.34	32.38	37.49	41.79	48.48	53.28	60.40
$NC_3H_7O_2$	-10.15	77.64	21.61	26.69	31.71	36.21	43.00	48.08	55.56
$IC_3H_7O_2$	-16.10	80.81	24.29	29.48	33.93	37.73	43.79	48.29	55.29
C_3H_6O1-3	-19.38	65.65	14.86	19.73	24.60	28.89	35.04	39.60	46.14
C_3H_6O1-2	-22.17	67.28	17.45	22.12	26.48	30.25	35.79	39.93	45.95

C_3KET12	-67.64	90.75	26.84	32.54	37.27	41.18	47.07	51.11	56.80
C_3KET13	-64.01	90.85	27.31	32.28	36.54	40.18	45.93	50.11	56.22
C_3KET21	-71.32	90.94	27.10	31.82	35.98	39.62	45.54	49.93	56.20
$C_3H_5$1-2,3O	-20.00	104.98	33.45	39.90	45.21	49.55	56.01	60.37	66.48
$C_3H_5$2-1,3O	-17.98	103.80	33.05	39.02	44.08	48.35	54.95	59.59	66.07
C_3H_6OH	-14.78	80.97	19.36	23.88	27.91	31.46	37.33	41.75	48.38
$HOC_3H_6O_2$	-49.60	94.95	27.46	32.69	37.17	41.01	47.14	51.72	59.00
CH_3CHCO	-19.61	67.80	17.93	21.39	24.26	26.64	30.28	32.88	36.95
AC_3H_5OOH	-14.23	82.92	24.12	28.78	32.74	36.10	41.37	45.17	50.89
C_2H_3OOH	-7.59	72.50	18.43	22.06	25.07	27.55	31.25	33.75	37.25
C_4H_{10}	-30.04	73.71	23.34	29.68	35.27	40.17	48.21	54.27	63.52
PC_4H_9	18.96	78.50	22.57	28.30	33.36	37.79	45.05	50.53	58.86
SC_4H_9	16.31	79.52	21.81	27.37	32.37	36.84	44.27	49.92	58.31
C_4H_8-1	-0.01	72.98	20.55	25.40	30.13	34.46	41.39	46.61	54.37
C_4H_8-2	-2.67	70.82	21.04	25.86	30.55	34.80	41.54	46.70	54.44
$C_4H_7$1-1	58.76	74.40	20.09	24.63	28.85	32.55	38.25	42.65	49.39
$C_4H_7$1-2	55.25	71.86	20.16	24.83	29.15	32.95	38.85	43.37	50.26
$C_4H_7$1-3	32.53	73.16	19.39	24.17	28.70	32.67	38.65	43.21	50.12
$C_4H_7$1-4	48.90	75.85	20.35	24.99	29.37	33.21	39.00	43.44	50.22
$C_4H_7$2-2	53.50	74.87	19.96	23.86	27.86	31.58	37.53	42.14	49.15
C_4H_6	26.33	66.41	18.33	23.15	27.34	30.90	36.41	40.48	46.76
$PC_4H_9O_2H$	-49.76	93.42	31.28	38.65	44.97	50.37	58.93	65.17	74.47
$SC_4H_9O_2H$	-54.43	92.75	31.85	39.36	45.73	51.13	59.55	65.63	74.68
$PC_4H_9O_2$	-16.36	92.27	29.30	35.75	41.37	46.25	54.18	60.15	69.34
$SC_4H_9O_2$	-21.03	91.60	29.80	36.46	42.17	47.06	54.86	60.64	69.57
PC_4H_9O	-14.23	84.75	25.43	32.06	37.79	42.72	50.54	56.22	64.57
SC_4H_9O	-18.12	81.80	25.75	32.44	38.22	43.19	51.05	56.68	64.66
C_4H_7O	12.92	80.33	23.19	29.39	34.57	38.88	45.40	49.86	56.18
C_4H_8O1-2	-27.60	76.22	22.88	29.54	35.18	39.95	47.37	52.67	60.58
C_4H_8O1-3	-27.66	73.66	21.77	28.51	34.32	39.31	47.15	52.71	60.18

C_4H_8O1-4	-43.63	73.89	19.26	26.07	32.06	37.30	45.71	51.76	59.70
$C_4H_8O_2$-3	-31.18	72.36	23.60	30.44	36.12	40.83	47.98	52.95	60.12
PC_4H_8OH	-19.33	90.65	25.00	31.04	36.38	41.09	48.76	54.45	62.80
SC_4H_8OH	-21.85	87.70	25.04	31.48	36.90	41.46	48.51	53.55	61.22
C_4H_8OH-$1O_2$	-54.61	104.37	32.97	39.67	45.41	50.35	58.21	64.07	73.27
C_4H_8OH-$2O_2$	-58.98	102.37	33.46	40.44	46.34	51.32	59.10	64.78	73.67
C_4H_8OOH1-1	-7.55	98.76	31.59	37.71	43.14	47.92	55.72	61.49	69.72
C_4H_8OOH1-2	-1.86	98.94	29.36	35.83	41.40	46.17	53.78	59.43	68.24
C_4H_8OOH1-3	-3.41	97.86	29.68	36.28	42.02	46.99	54.95	60.75	69.08
C_4H_8OOH1-4	-0.76	96.83	30.52	37.28	43.06	47.99	55.76	61.42	69.80
$C_4H_8OOH_2$-1	-5.43	96.17	31.04	37.97	43.82	48.75	56.40	61.88	70.02
$C_4H_8OOH_2$-2	-13.41	99.48	30.81	36.70	41.93	46.56	54.21	60.00	68.71
$C_4H_8OOH_2$-3	-8.08	97.19	30.28	37.04	42.85	47.81	55.64	61.30	69.56
$C_4H_8OOH_2$-4	-5.43	96.17	31.04	37.97	43.82	48.75	56.40	61.88	70.02
C_4H_8OOH1-2	-40.53	109.72	37.54	45.29	51.79	57.22	65.57	71.51	80.39
C_4H_8OOH1-3	-40.53	109.72	37.54	45.29	51.79	57.22	65.57	71.51	80.39
C_4H_8OOH1-4	-35.86	110.38	37.17	44.65	51.01	56.41	64.88	71.03	80.15
$C_4H_8OOH_2$-1	-40.53	109.72	37.54	45.29	51.79	57.22	65.57	71.51	80.39
$C_4H_8OOH_2$-3	-45.20	109.05	38.52	46.36	52.84	58.20	66.33	72.05	80.65
$C_4H_8OOH_2$-4	-40.53	109.72	37.54	45.29	51.79	57.22	65.57	71.51	80.39
NC_4KET12	-72.57	100.17	32.31	39.50	45.52	50.53	58.17	63.49	71.12
NC_4KET13	-73.61	99.61	33.34	39.99	45.60	50.34	57.69	62.96	70.76
NC_4KET14	-68.94	100.27	32.84	39.27	44.79	49.51	56.99	62.46	70.51
NC_4KET21	-76.64	100.54	33.24	39.31	44.59	49.18	56.60	62.15	70.42
NC_4KET23	-80.02	99.08	31.59	38.84	44.93	50.02	57.82	63.27	71.04
NC_4KET24	-76.39	99.19	32.09	38.61	44.22	49.03	56.68	62.27	70.46
$C_2H_5COCH_3$	-57.31	81.27	24.23	29.04	33.71	37.97	44.88	50.15	58.11
$C_2H_5COCH_2$	-14.58	80.72	24.49	29.81	34.39	38.33	44.59	49.18	55.97
CH_2CH_2COCH	-7.88	85.86	23.40	28.31	32.66	36.50	42.82	47.64	54.95
$CH_3CHCOCH_3$	-17.08	78.70	22.83	28.21	32.88	36.93	43.43	48.24	55.35

$C_2H_3COCH_3$	-30.40	78.20	21.23	26.36	30.77	34.55	40.53	44.88	51.30
$CH_3CHOOCOC$	-45.08	100.17	30.13	36.44	41.73	46.15	52.98	57.88	65.44
$CH_2CHOOHCO$	-32.18	103.37	31.41	37.94	43.34	47.81	54.53	59.17	65.91
NC_3H_7CHO	-49.27	78.24	22.94	28.79	34.36	39.29	46.74	52.23	60.11
NC_3H_7CO	-12.53	83.28	24.02	28.91	33.21	36.99	43.16	47.81	54.82
C_3H_6CHO-1	-0.43	85.57	24.08	28.96	33.25	37.02	43.16	47.79	54.78
C_3H_6CHO-2	-3.08	86.60	23.28	28.03	32.30	36.10	42.42	47.24	54.35
C_3H_6CHO-3	-9.63	79.79	23.58	28.85	33.43	37.39	43.73	48.40	55.34
C_2H_5CHCO	-24.37	77.60	23.04	28.23	32.54	36.11	41.56	45.40	51.31
SC_3H_5CHO	-28.19	75.99	22.27	27.41	31.76	35.44	41.16	45.26	51.38
SC_3H_5CO	2.71	74.60	22.12	26.49	30.15	33.22	37.96	41.37	46.61
IC_4H_{10}	-32.26	70.62	23.21	29.58	35.58	40.82	48.69	54.67	63.54
IC_4H_9	17.63	72.82	23.56	29.24	34.39	38.84	45.65	50.90	59.03
TC_4H_9	13.15	77.05	19.79	24.96	30.19	35.01	42.62	48.49	57.37
IC_4H_8	-4.20	68.70	20.66	26.18	31.26	35.66	42.24	47.22	54.65
IC_4H_7	32.89	71.89	19.74	24.74	29.23	33.09	38.90	43.33	50.13
$IC_4H_9O_2$	-18.60	89.58	29.05	35.69	41.43	46.39	54.36	60.30	69.42
$TC_4H_9O_2$	-25.43	87.93	29.34	36.03	42.00	47.06	54.54	60.14	68.60
$TC_4H_8O_2H$-I	-7.50	92.81	31.54	38.20	43.77	48.42	55.58	60.67	68.57
$IC_4H_8O_2H$-I	-3.00	94.15	30.32	37.21	43.08	48.07	55.90	61.54	69.86
$IC_4H_8O_2H$-T	-6.10	97.79	30.09	35.94	41.07	45.58	52.94	58.53	67.30
IC_4H_8O	-31.48	71.25	23.39	30.23	35.94	40.69	47.96	53.08	60.80
CC_4H_8O	-25.53	69.91	20.47	27.82	34.00	39.18	47.14	52.73	60.95
TC_4H_9O	-20.77	73.90	25.48	32.29	38.46	43.79	51.77	57.43	65.39
IC_4H_9O	-15.55	76.25	24.45	31.18	37.46	42.95	51.24	57.21	65.67
$IC_4H_9O_2H$	-52.00	90.73	31.10	38.59	45.00	50.46	59.06	65.29	74.52
$TC_4H_9O_2H$	-57.62	84.67	32.78	40.17	46.63	52.06	60.07	66.05	75.20
IC_4H_7O	13.91	80.56	23.77	28.96	33.49	37.42	43.74	48.41	55.37
IC_4H_8OH	-24.10	88.50	25.35	30.72	35.64	40.09	47.66	53.56	62.54
$IO_2C_4H_8OH$	-60.19	100.05	33.58	40.34	46.11	51.03	58.83	64.60	73.67

IC_3H_7CHO	-51.20	79.66	23.57	29.64	34.90	39.43	46.67	51.96	59.79
TC_3H_6CHO	-13.50	76.58	24.14	29.29	33.76	37.63	43.86	48.51	55.61
IC_3H_6CHO	-2.20	83.08	22.80	28.26	32.98	37.04	43.51	48.22	55.15
IC_3H_7CO	-14.30	81.59	22.74	28.21	32.94	37.02	43.50	48.23	55.16
TC_4H_8OOH-I	-44.10	103.72	37.89	45.69	52.19	57.61	65.91	71.79	80.59
IC_4H_8OOH-I	-38.10	107.70	36.91	44.59	51.08	56.55	65.06	71.18	80.24
IC_4H_8OOH-T	-44.10	103.72	37.89	45.69	52.19	57.61	65.91	71.79	80.59
IC_4KETII	-70.71	99.15	31.52	38.56	44.53	49.56	57.35	62.86	70.73
IC_4KETIT	-75.84	93.28	32.50	39.72	45.81	50.91	58.71	64.10	71.51
IC_4H_7OH	-38.26	82.02	24.73	30.24	35.07	39.28	46.10	51.20	58.91
IC_4H_6OH	-2.16	80.26	24.19	29.63	34.25	38.18	44.32	48.76	55.43
IC_3H_5CHO	-27.34	74.65	23.18	28.32	32.61	36.20	41.71	45.61	51.52
IC_3H_5CO	4.56	73.26	23.00	27.39	31.02	34.00	38.52	41.71	46.70
TC_3H_6OCHO	-39.04	84.25	26.68	32.97	38.31	42.82	49.75	54.58	61.28
IC_3H_6CO	-28.06	75.35	24.27	28.96	32.92	36.26	41.48	45.29	51.24
IC_4H_7OOH	-24.38	91.48	30.26	36.22	41.32	45.67	52.56	57.59	65.20
TC_3H_6OHCHO	-91.01	85.71	27.63	34.26	39.92	44.71	52.15	57.40	64.91
TC_3H_6OH	-24.40	76.94	20.50	24.97	28.79	32.06	37.24	41.06	47.12
IC_3H_5OH	-38.81	72.63	19.11	23.28	26.94	30.15	35.36	39.24	45.00
$TC_3H_6O_2CHO$	-39.73	93.50	30.47	36.84	42.27	46.88	54.07	59.18	66.46
$TC_3H_6O_2HCO$	-38.93	94.40	31.74	38.35	43.91	48.56	55.63	60.46	66.91
$IC_3H_5O_2HCH$	-26.83	96.70	31.82	38.41	43.96	48.59	55.63	60.44	66.90
CH_2CCH_2OH	27.09	76.27	18.24	21.60	24.59	27.24	31.61	34.92	39.88
TC_4H_8CHO	-9.30	89.66	28.85	36.26	42.53	47.82	56.00	61.77	70.11
$O_2C_4H_8CHO$	-43.39	104.72	35.90	43.69	50.31	55.93	64.69	70.94	80.10
$O_2HC_4H_8CO$	-42.59	105.62	37.02	45.11	51.97	57.74	66.59	72.69	80.95
C_3H_5OH	-29.55	72.84	18.45	23.03	27.21	30.79	36.06	39.95	45.60
TIC_4H_7Q2-I	-31.87	110.84	40.01	47.29	53.37	58.44	66.17	71.58	79.58
IIC_4H_7Q2-I	-25.88	115.30	39.10	46.27	52.38	57.57	65.68	71.43	79.66
IIC_4H_7Q2-T	-30.68	117.13	38.99	45.23	50.83	55.80	64.01	70.15	78.92

IIC_4H_7Q2-T	-35.02	83.13	28.44	36.52	43.55	49.66	59.49	66.78	77.82
CC_3H_4	66.20	58.22	12.73	16.22	19.20	21.69	25.34	27.98	31.86
C_4H_4	68.00	66.58	17.50	21.46	24.54	27.01	30.88	33.71	37.98
C_4H_3-I	119.20	70.19	19.86	22.54	24.55	26.15	28.72	30.62	33.56
$C_4H_6$12	39.34	69.72	19.30	23.66	27.46	30.75	36.04	39.99	45.59
C_4H_2	111.01	61.20	21.26	22.17	23.04	23.85	25.32	26.59	29.00
C_4H_3-N	127.10	67.99	17.74	20.93	23.31	25.16	28.00	30.12	33.36
C_4H_5-N	85.40	69.47	18.76	22.97	26.46	29.35	33.80	37.10	42.26
C_4H_5-I	77.40	68.47	18.11	22.42	26.01	29.00	33.57	36.98	42.24
$CH_3CHCHCO$	9.40	73.04	16.88	22.01	26.54	30.47	36.50	40.11	45.97
$CH_2CHCHCHO$	9.40	73.04	16.88	22.01	26.54	30.47	36.50	40.11	45.97
C_4H_6O25	-26.00	67.94	18.18	24.03	29.42	33.95	40.17	44.65	50.94
$C_2H_3CHOCH_2$	2.00	71.82	19.87	24.97	29.58	33.69	40.43	45.19	51.87
C_4H_5-2	74.31	71.22	18.84	22.43	25.65	28.51	33.15	36.34	41.55
C_4H_6-2	34.67	65.98	18.42	22.42	26.06	29.35	34.83	38.88	45.46
C_4H_6O23	-17.30	67.94	18.18	24.03	29.42	33.95	40.17	44.65	50.94
$CH_3CHCHCHO$	-25.70	79.62	18.29	24.07	29.17	33.59	40.42	44.55	50.64
C_4H_4O	-8.29	63.87	15.73	21.02	25.69	29.48	34.46	37.98	42.80
H_2CC	99.13	52.82	10.20	11.20	12.09	12.86	14.14	15.19	16.95
H_2C_4O	54.60	66.44	17.27	19.62	21.79	23.73	26.81	28.73	31.51
C_2H_2OH	31.79	62	13.28	15.99	18.2	19.97	22.56	24.35	26.96
$O_2CCHOOJ$	-61.7	88.69	22.8	24.4	25.93	27.35	29.84	31.82	34.65
HCOH	23.33	55.43	9.83	12.88	15.17	16.85	18.89	19.84	20.65
C_2H_3OH	-29.38	61.76	14.84	18.07	20.65	22.7	25.68	27.71	31.13
O_2CH_2CHO	-21.01	79.98	17.37	21.66	25.1	27.84	31.78	34.4	38.4
HO_2CH_2CO	-19.64	81.79	20.6	24.15	27	29.27	32.5	34.54	37.2

[1]

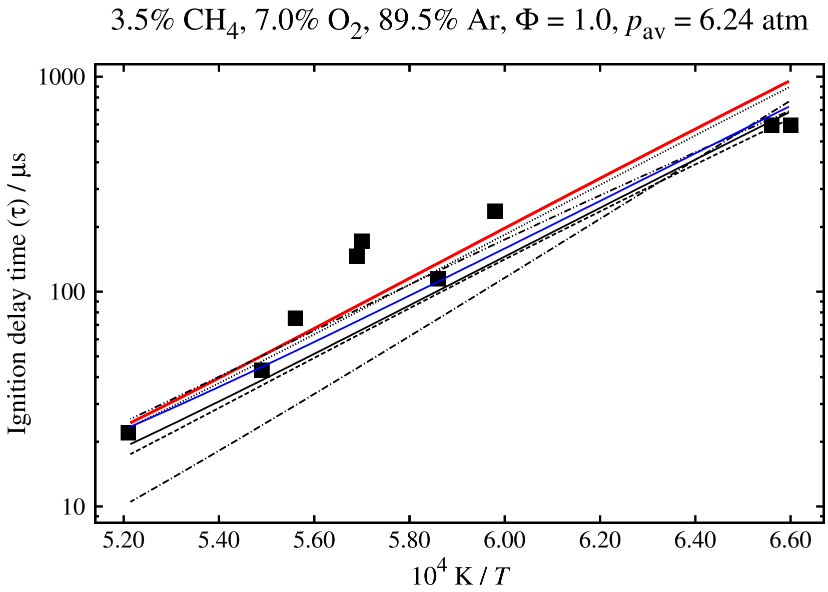
[1]Units are H_f kcal mol^{-1}, S cal K^{-1} mol^{-1}, C_p cal K^{-1} mol^{-1}

2. Mechanism Performance

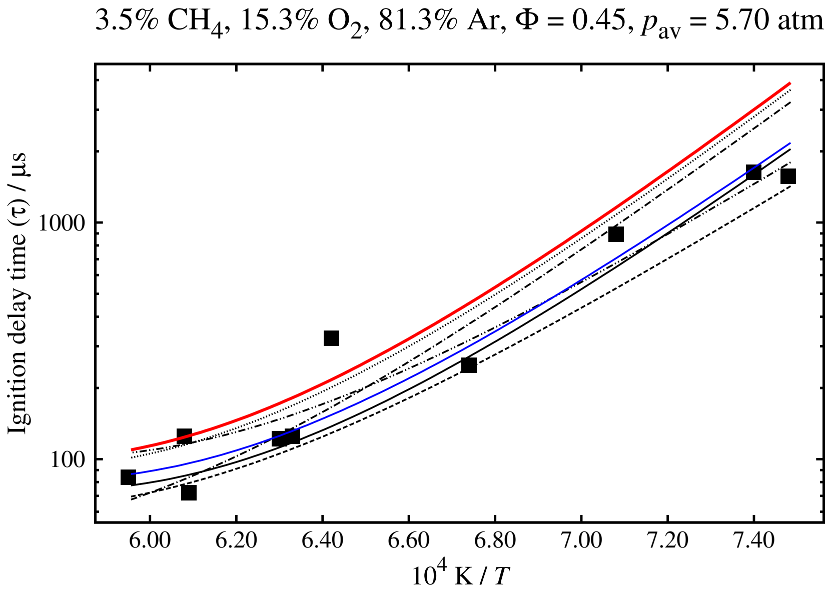
Throughout the supplementary material symbols represent experimental data and lines represent model predictions. The lines are set out as follows: — AramcoMech 1.3 as presented in this work, — GRI-Mech 3.0 [1], - - - Leeds Mech [2], · · · MFC [3], – · – Ranzi [4], – · · San Diego Mech [5], — USC II [6]. Not all of these mechanisms are validated against all of the species contained in this document and are included for comparative purposes.

2.1. Methane

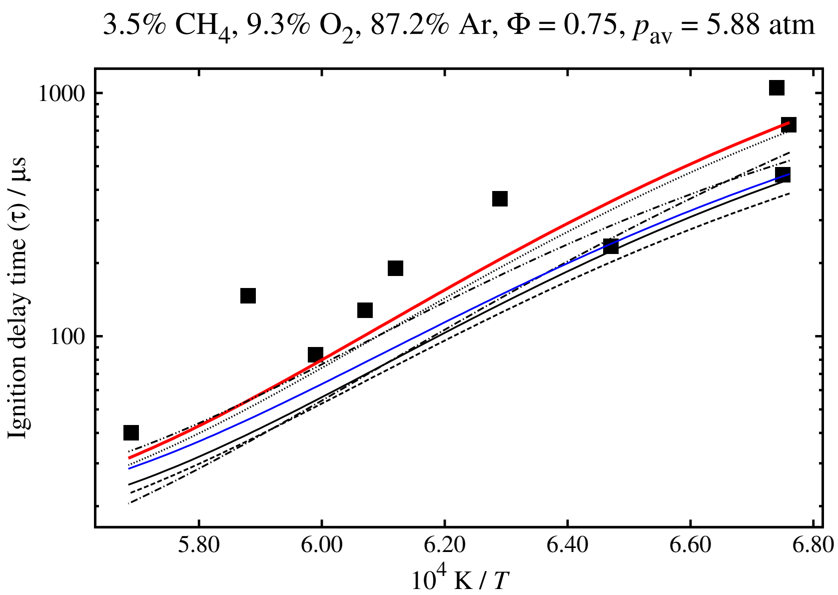
2.1.1. Shock Tube



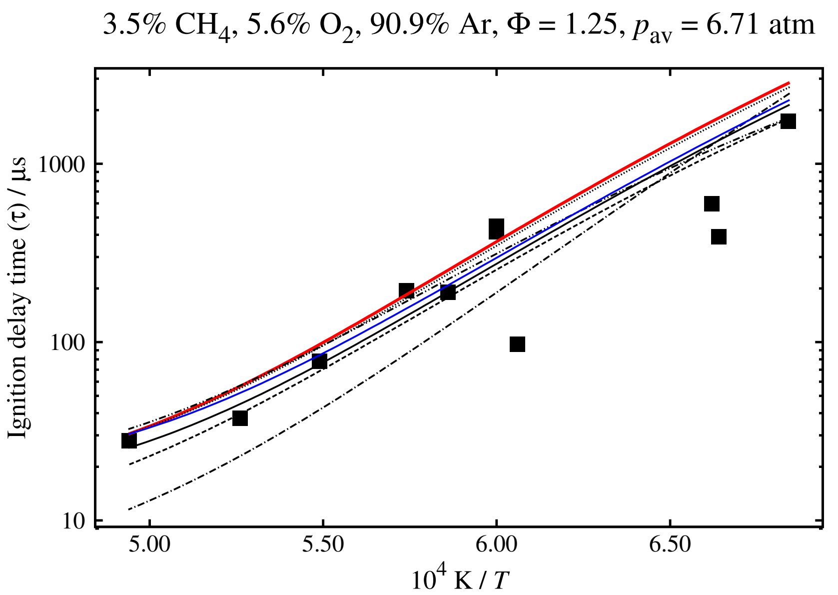
(a)



(b)

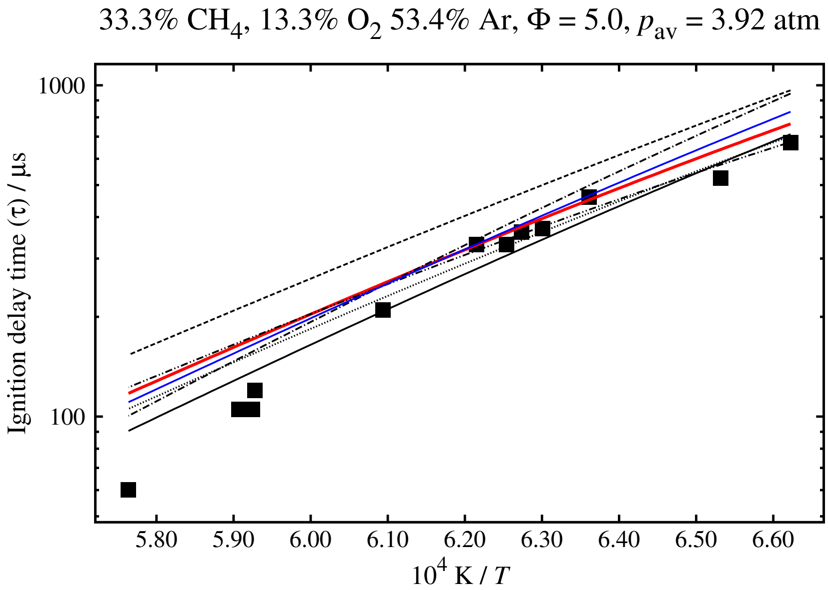


(c)

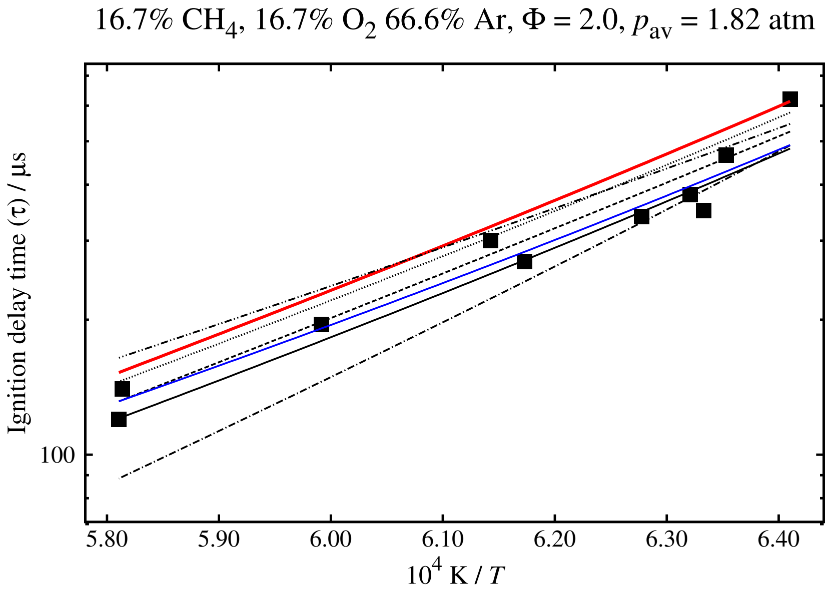


(d)

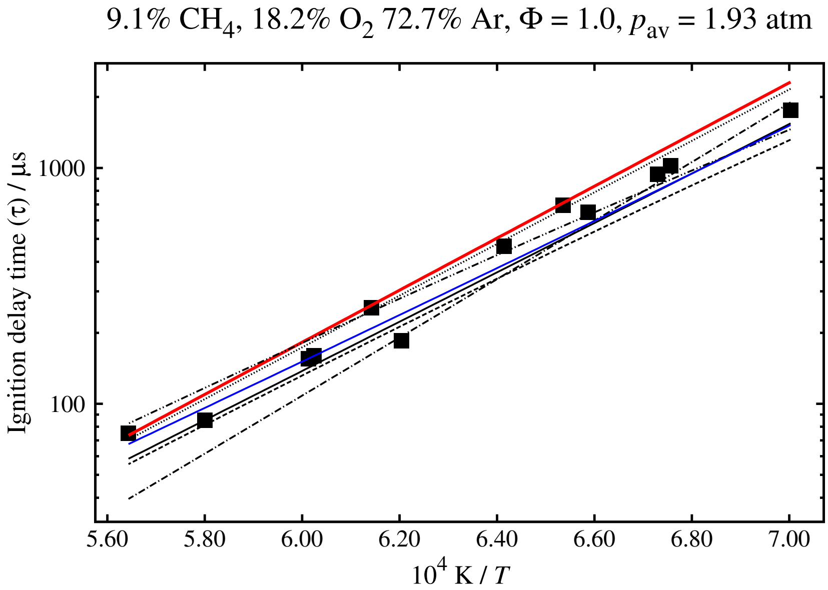
S1 Shock tube ignition delay times of methane/oxygen/argon mixtures. Symbols are experimental data [7] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


33.3% CH4, 13.3% O2 53.4% Ar, Φ = 5.0, pav = 3.92 atm
1000
100
Ignition delay time (τ) / μs
5.80
5.90
6.00
6.10
6.20
6.30
6.40
6.50
6.60
10^4 K / T

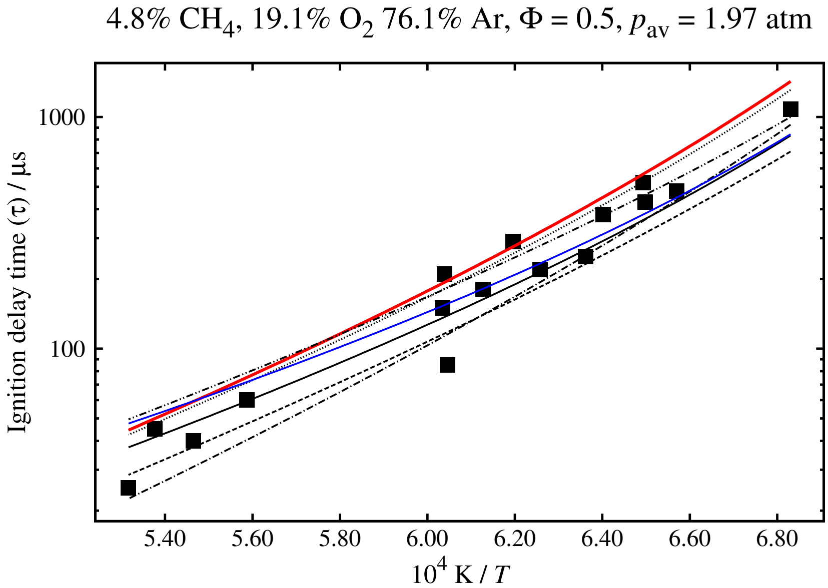
(a)


16.7% CH4, 16.7% O2 66.6% Ar, Φ = 2.0, pav = 1.82 atm
100
Ignition delay time (τ) / μs
5.80
5.90
6.00
6.10
6.20
6.30
6.40
10^4 K / T

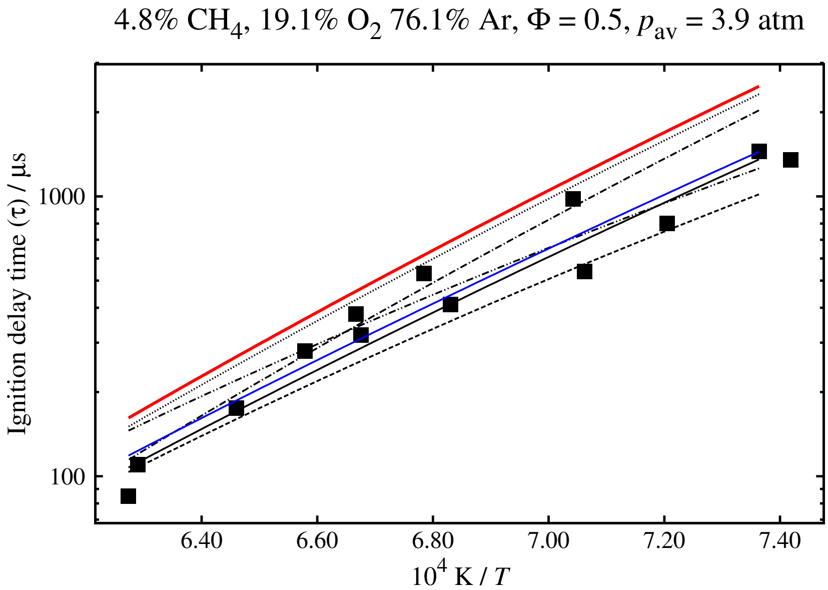
(b)


9.1% CH4, 18.2% O2 72.7% Ar, Φ = 1.0, pav = 1.93 atm
Ignition delay time (τ) / µs
1000
100
5.60
5.80
6.00
6.20
6.40
6.60
6.80
7.00
10^4 K / T

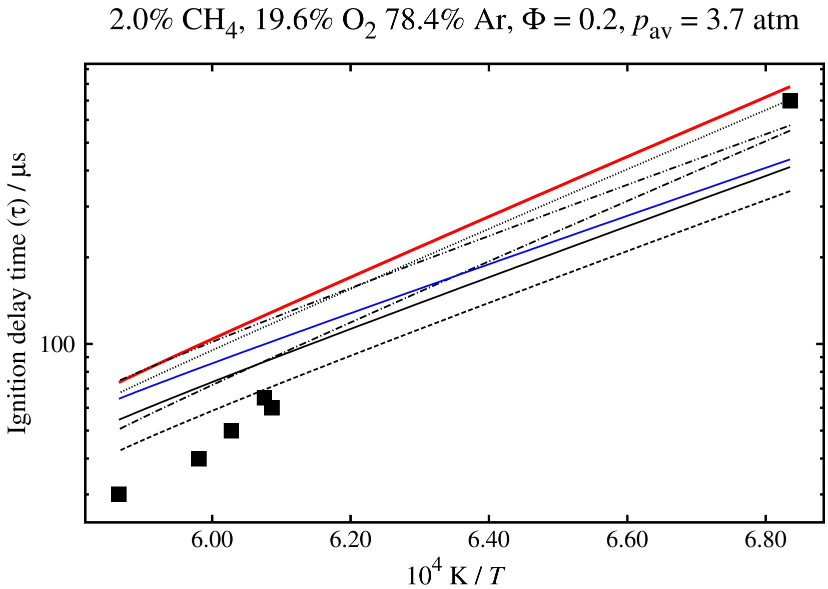
(c)


4.8% CH4, 19.1% O2 76.1% Ar, Φ = 0.5, pav = 1.97 atm
Ignition delay time (τ) / µs
1000
100
5.40
5.60
5.80
6.00
6.20
6.40
6.60
6.80
10^4 K / T

(d)

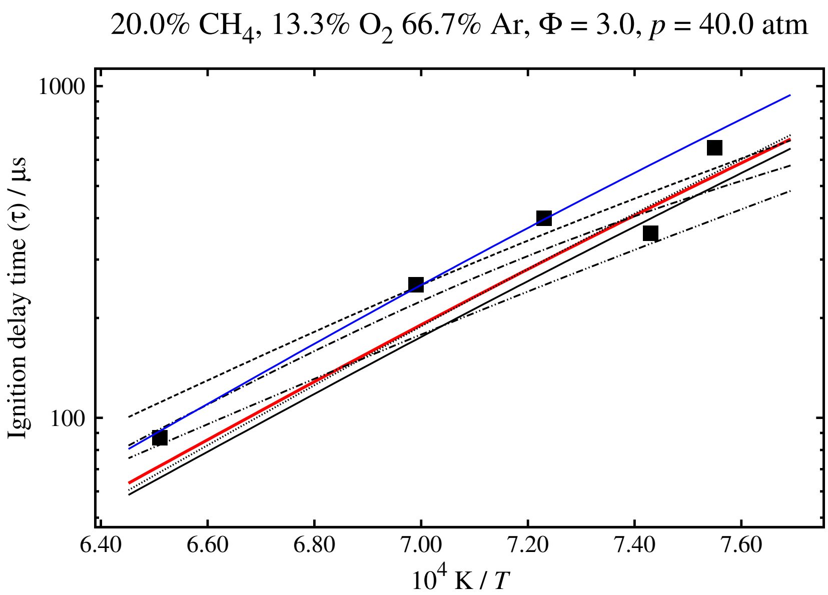


(e)

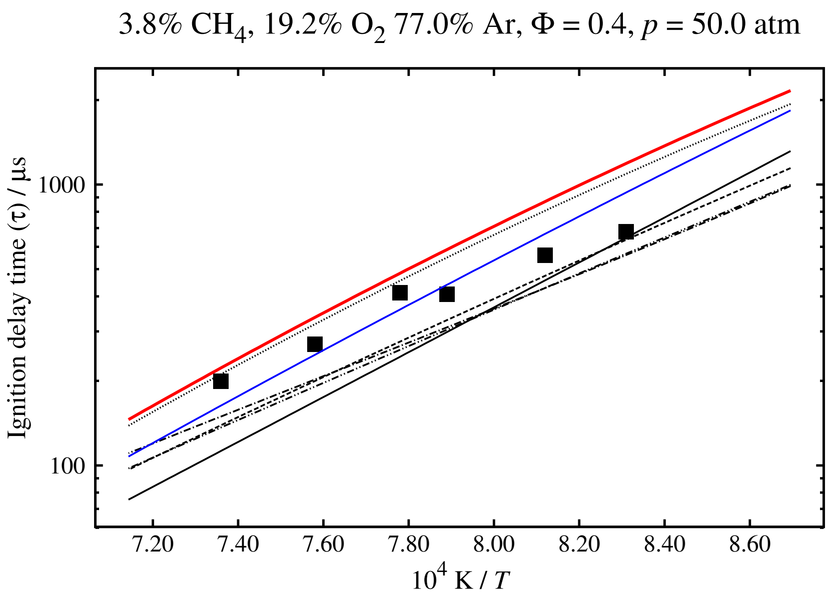


(f)

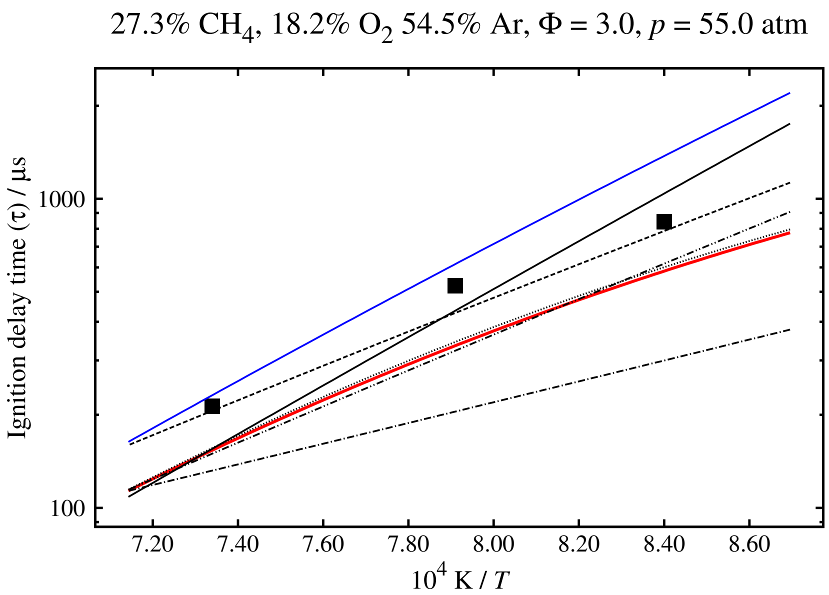
S2 Shock tube ignition delay times of methane/oxygen/argon mixtures Symbols are experimental data [9] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


20.0% CH4, 13.3% O2 66.7% Ar, Φ = 3.0, p = 40.0 atm
Ignition delay time (τ) / µs
1000
100
6.40
6.60
6.80
7.00
7.20
7.40
7.60
10^4 K / T

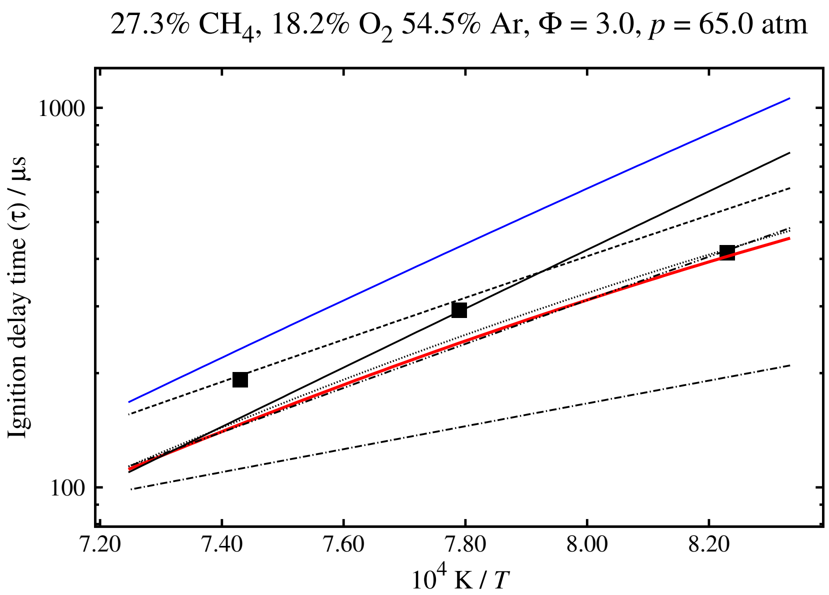
(a)


3.8% CH4, 19.2% O2 77.0% Ar, Φ = 0.4, p = 50.0 atm
Ignition delay time (τ) / µs
1000
100
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
10^4 K / T

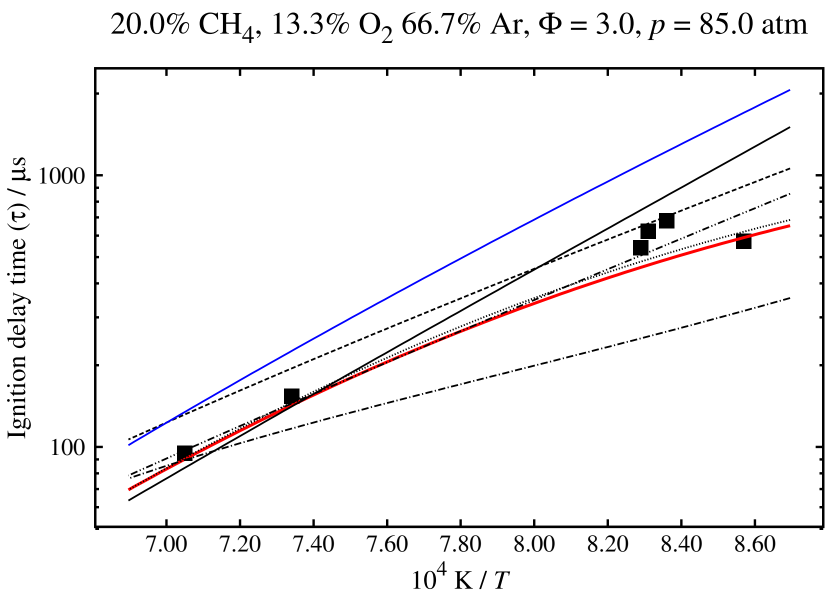
(b)


27.3% CH4, 18.2% O2 54.5% Ar, Φ = 3.0, p = 55.0 atm
Ignition delay time (τ) / μs
1000
100
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
10^4 K / T

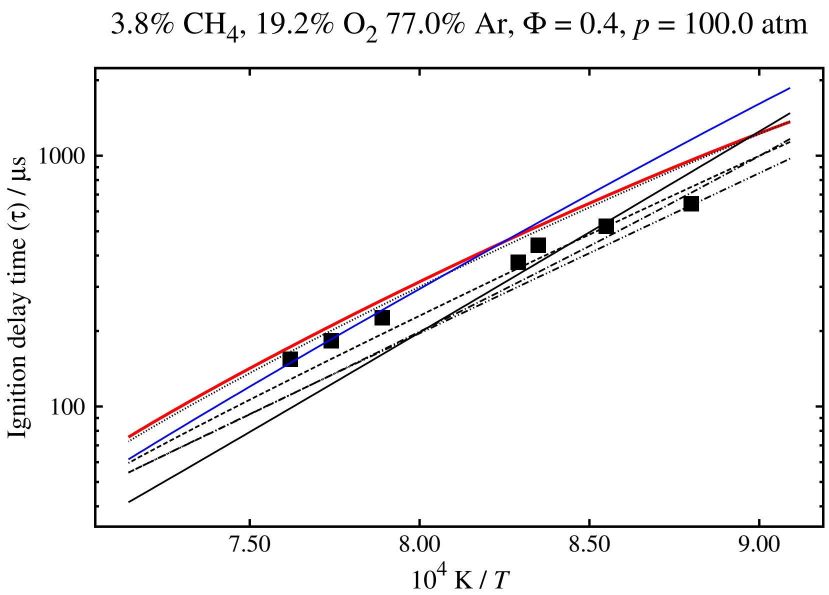
(c)


27.3% CH4, 18.2% O2 54.5% Ar, Φ = 3.0, p = 65.0 atm
Ignition delay time (τ) / μs
1000
100
7.20
7.40
7.60
7.80
8.00
8.20
10^4 K / T

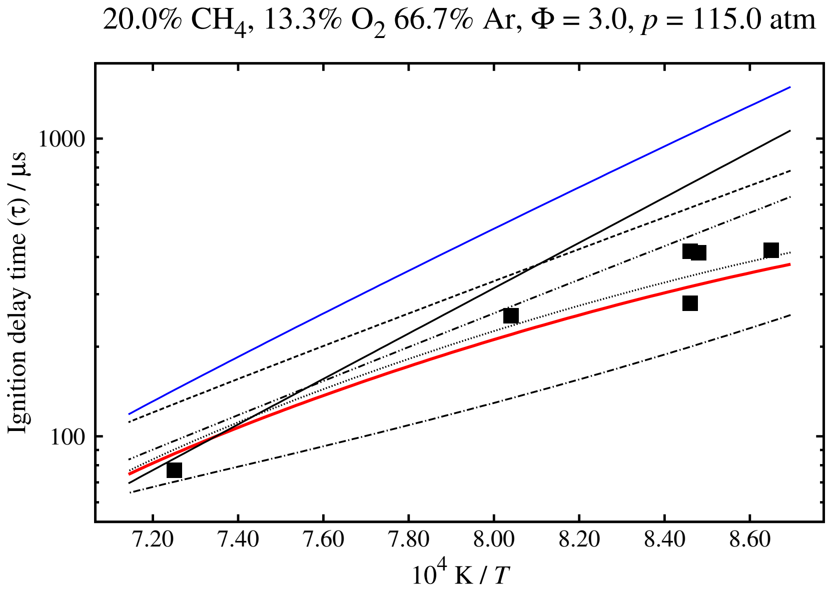
(d)


20.0% CH_4, 13.3% O_2 66.7% Ar, Φ = 3.0, p = 85.0 atm
Ignition delay time (τ) / μs
1000
100
7.00
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
10^4 K / T

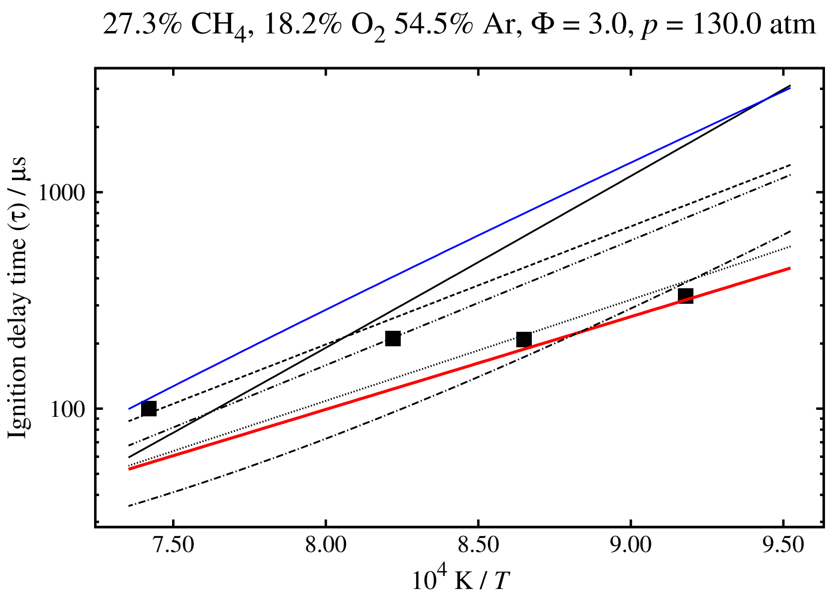
(e)


3.8% CH_4, 19.2% O_2 77.0% Ar, Φ = 0.4, p = 100.0 atm
Ignition delay time (τ) / μs
1000
100
7.50
8.00
8.50
9.00
10^4 K / T

(f)

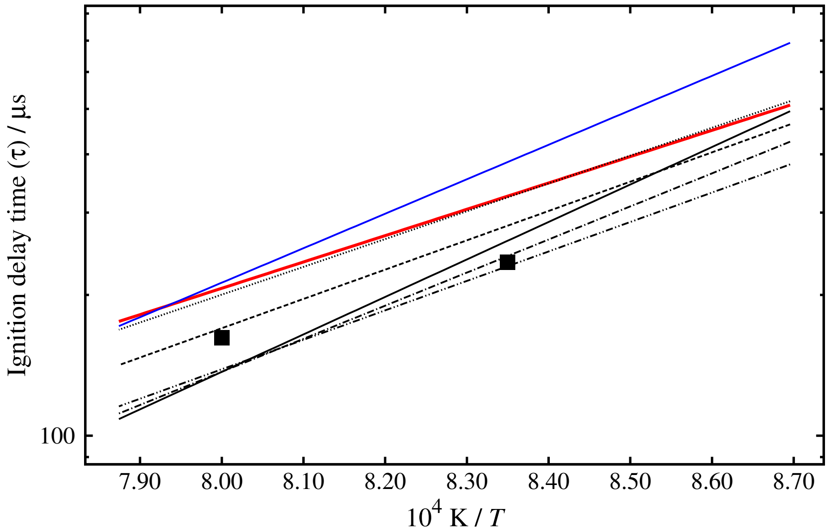

20.0% CH4, 13.3% O2 66.7% Ar, Φ = 3.0, p = 115.0 atm
Ignition delay time (τ) / µs
1000
100
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
10^4 K / T

(g)


27.3% CH4, 18.2% O2 54.5% Ar, Φ = 3.0, p = 130.0 atm
Ignition delay time (τ) / µs
1000
100
7.50
8.00
8.50
9.00
9.50
10^4 K / T

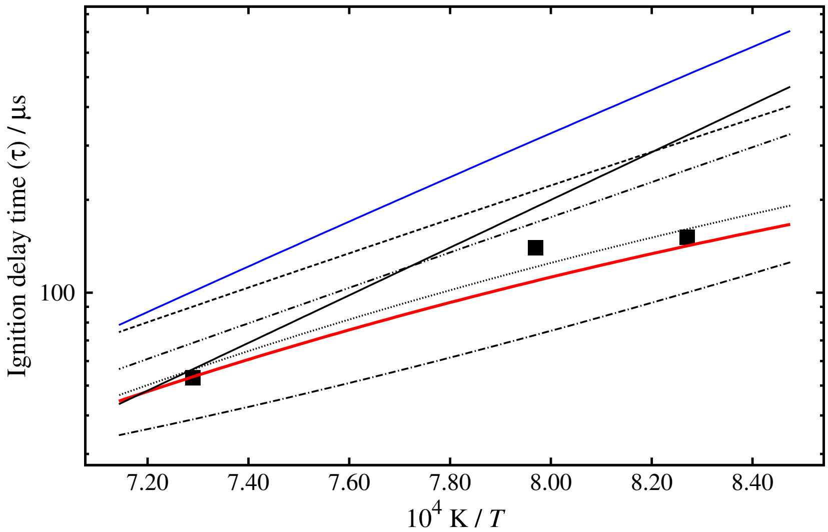
(h)

3.8% CH_4, 19.2% O_2 77.0% Ar, $\Phi = 0.4$, $p = 150.0$ atm

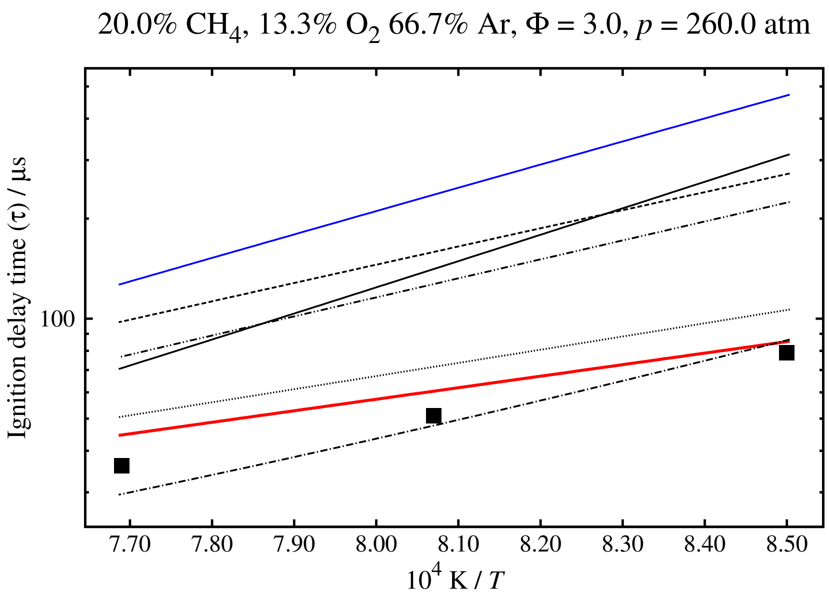


(i)

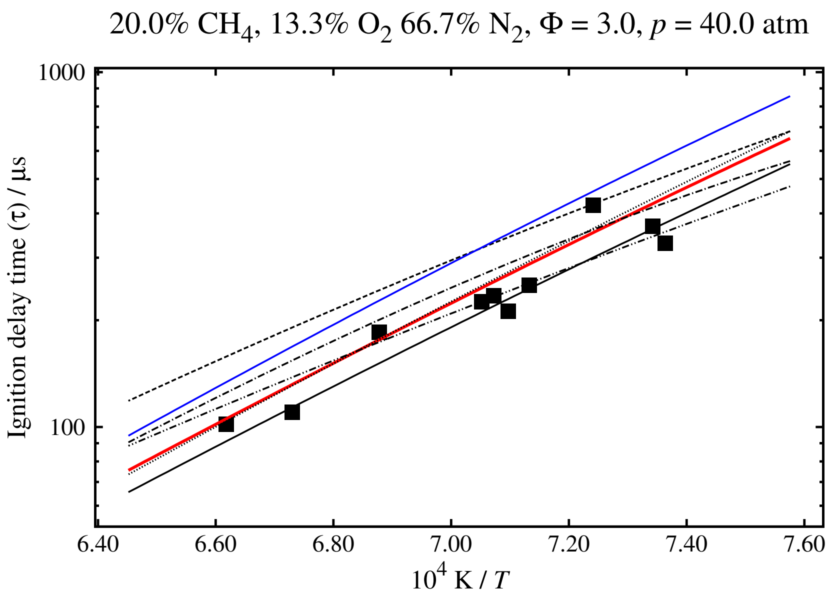
20.0% CH_4, 13.3% O_2 66.7% Ar, $\Phi = 3.0$, $p = 170.0$ atm



(j)

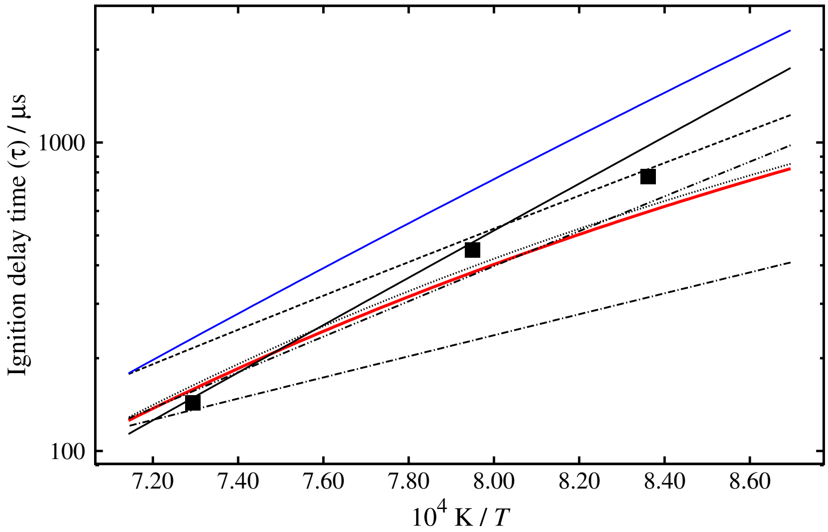

20.0% CH4, 13.3% O2 66.7% Ar, Φ = 3.0, p = 260.0 atm
Ignition delay time (τ) / μs
100
7.70
7.80
7.90
8.00
8.10
8.20
8.30
8.40
8.50
10^4 K / T

(k)


20.0% CH4, 13.3% O2 66.7% N2, Φ = 3.0, p = 40.0 atm
Ignition delay time (τ) / μs
1000
100
6.40
6.60
6.80
7.00
7.20
7.40
7.60
10^4 K / T

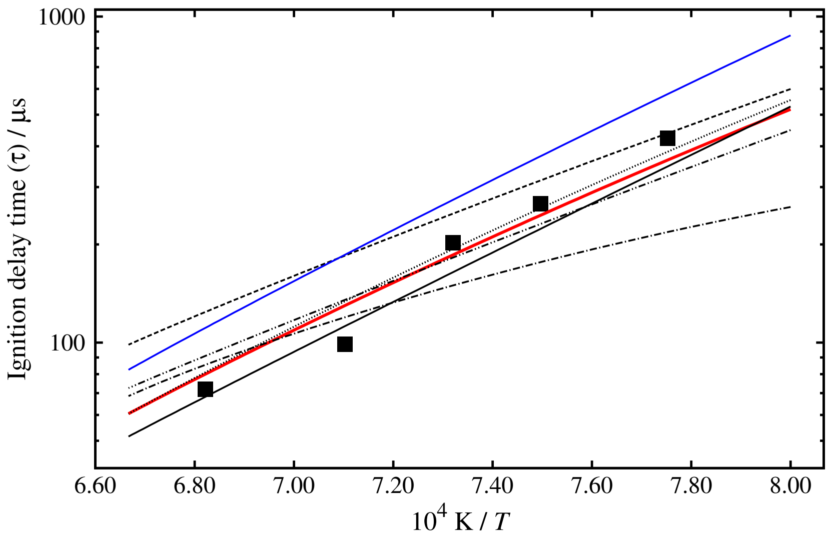
(l)

27.3% CH_4, 18.2% O_2 54.5% N_2, Φ = 3.0, p = 55.0 atm



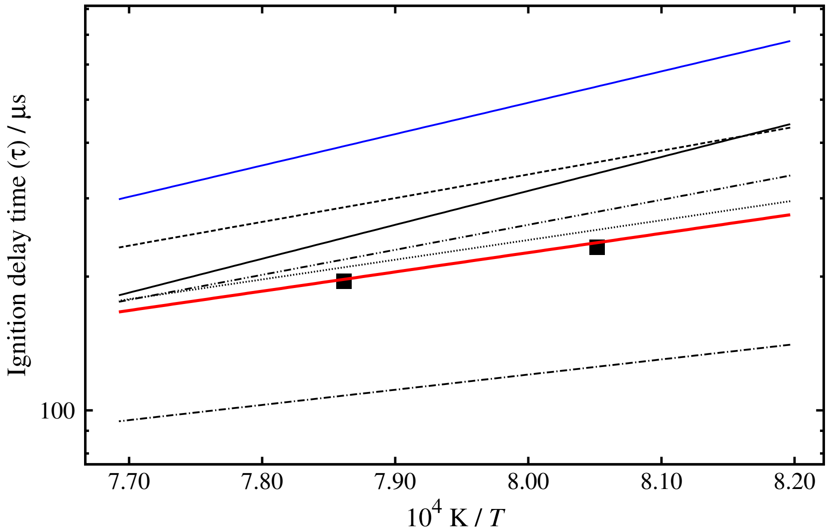
(m)

20.0% CH_4, 13.3% O_2 66.7% N_2, Φ = 3.0, p = 75.0 atm



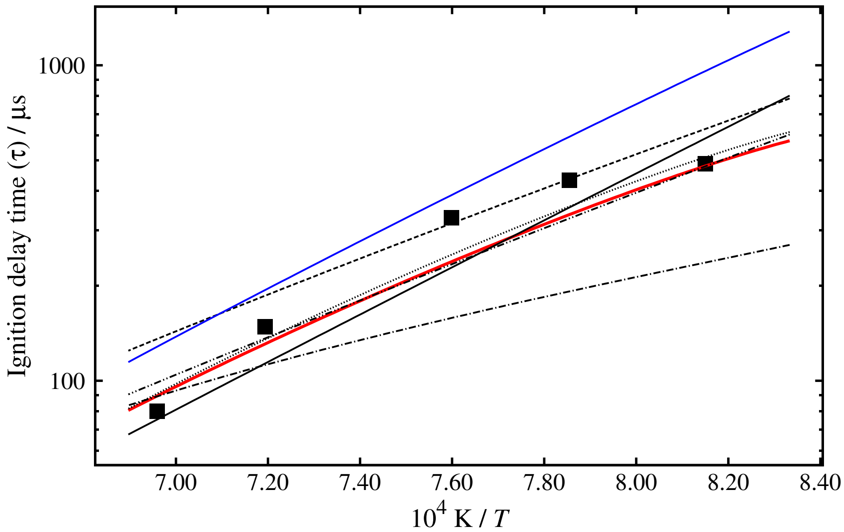
(n)

27.3% CH_4, 18.2% O_2 54.5% N_2, Φ = 3.0, p = 85.0 atm

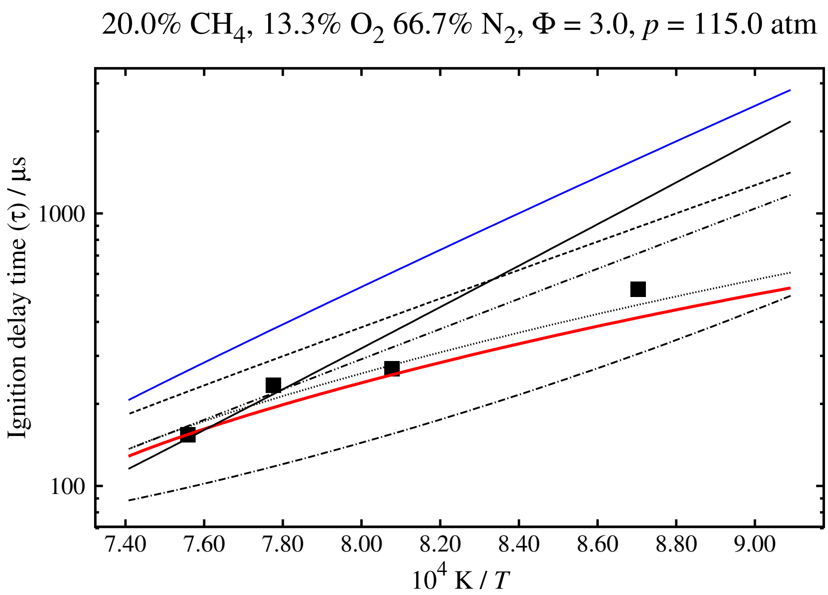


(o)

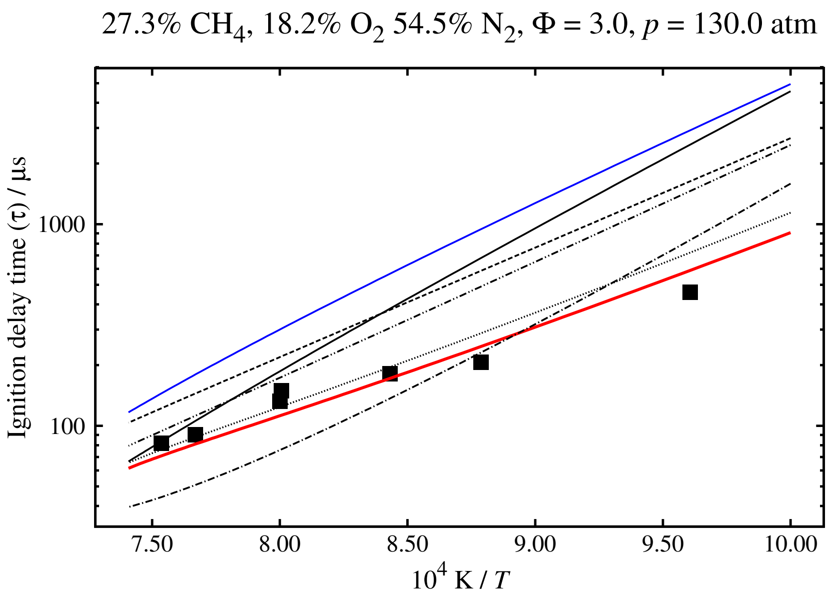
20.0% CH_4, 13.3% O_2 66.7% N_2, Φ = 3.0, p = 85.0 atm



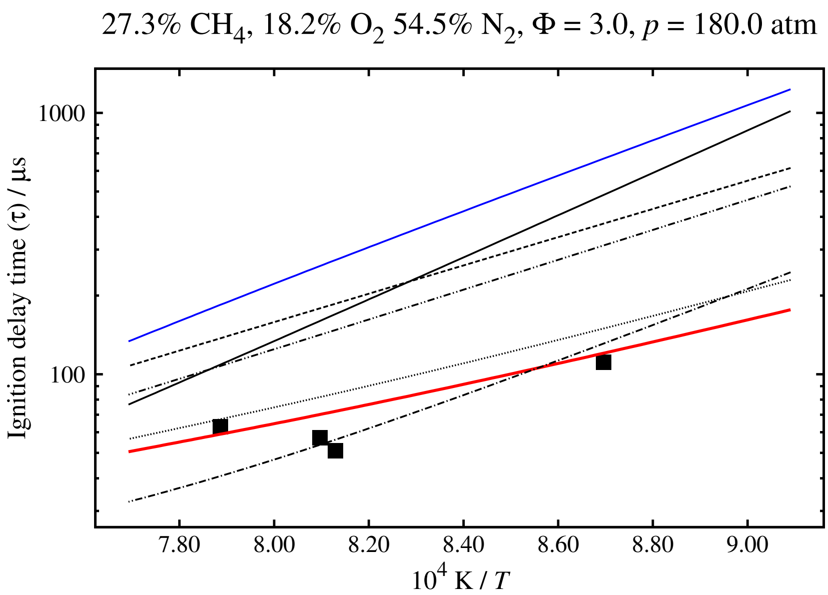
(p)


20.0% CH_4, 13.3% O_2 66.7% N_2, Φ = 3.0, p = 115.0 atm
Ignition delay time (τ) / μs
1000
100
7.40
7.60
7.80
8.00
8.20
8.40
8.60
8.80
9.00
10^4 K / T

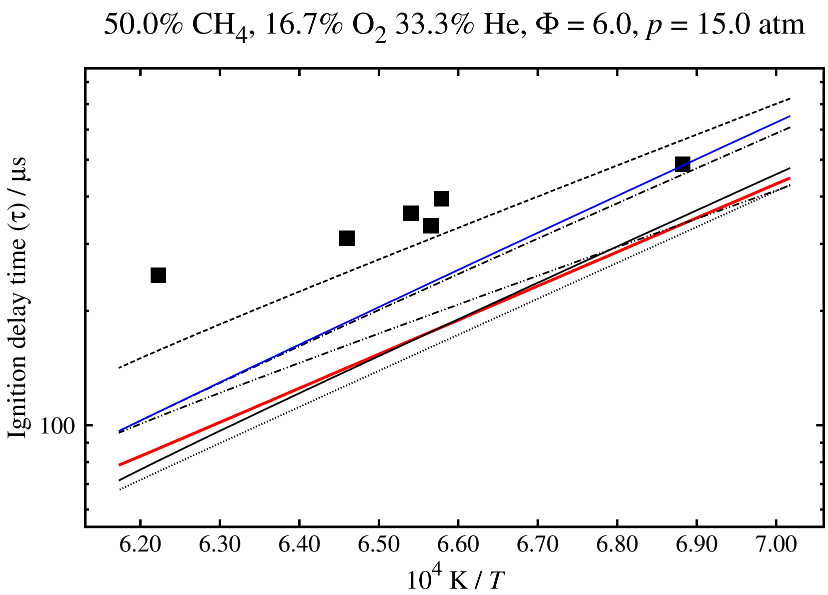
(q)


27.3% CH_4, 18.2% O_2 54.5% N_2, Φ = 3.0, p = 130.0 atm
Ignition delay time (τ) / μs
1000
100
7.50
8.00
8.50
9.00
9.50
10.00
10^4 K / T

(r)

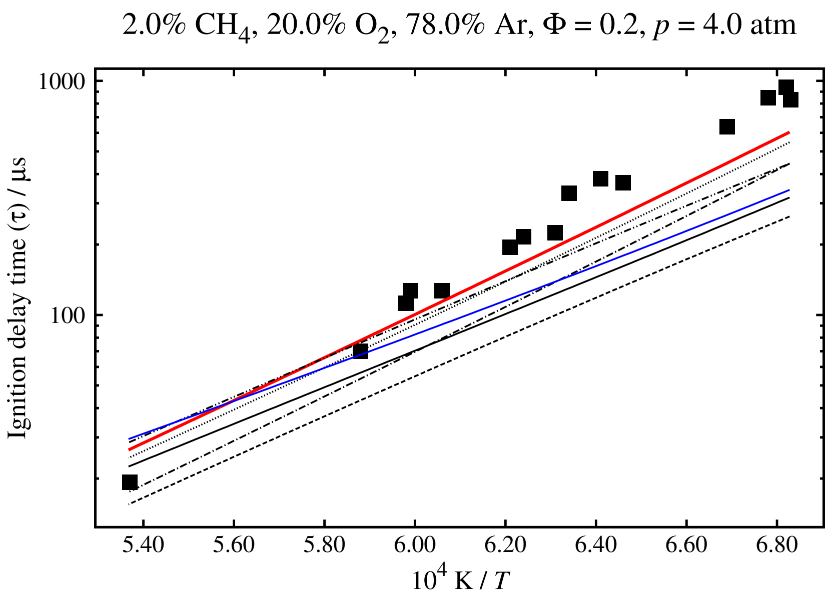


(s)

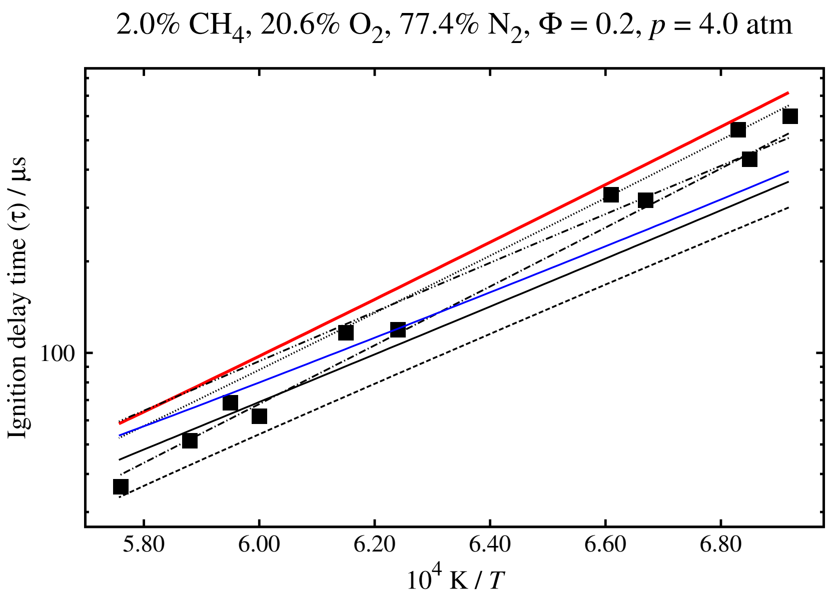


(t)

S3 Shock tube ignition delay times of methane/air mixtures. Symbols are experimental data [8] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

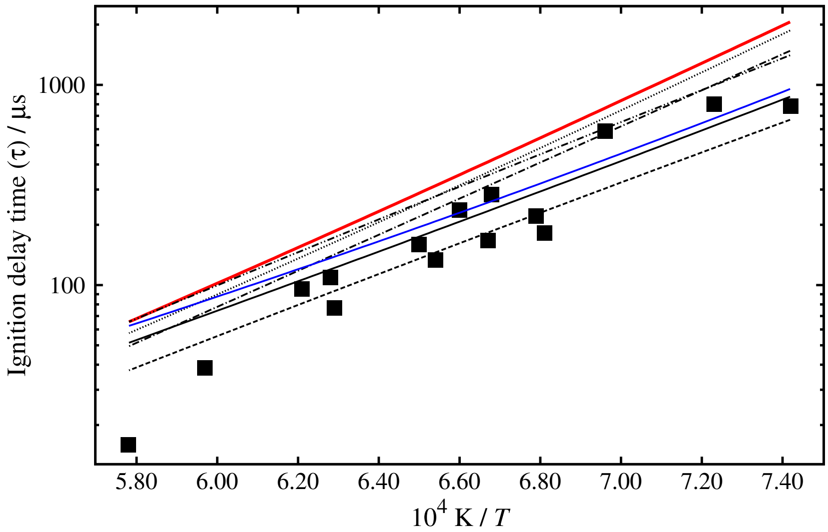

2.0% CH4, 20.0% O2, 78.0% Ar, Φ = 0.2, p = 4.0 atm
Ignition delay time (τ) / µs
1000
100
5.40
5.60
5.80
6.00
6.20
6.40
6.60
6.80
10^4 K / T

(a)


2.0% CH4, 20.6% O2, 77.4% N2, Φ = 0.2, p = 4.0 atm
Ignition delay time (τ) / µs
100
5.80
6.00
6.20
6.40
6.60
6.80
10^4 K / T

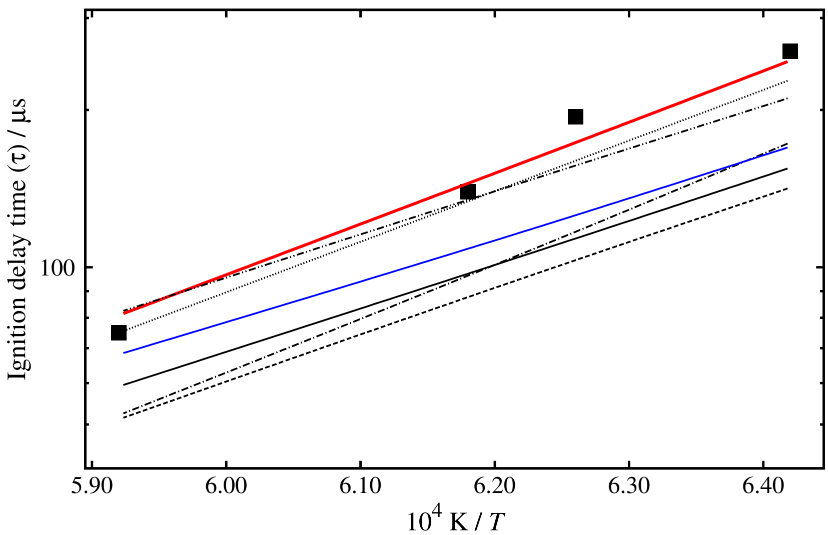
(b)

1.0% CH_4, 20.8% O_2, 78.2% N_2, $\Phi = 0.1$, $p = 4.0$ atm



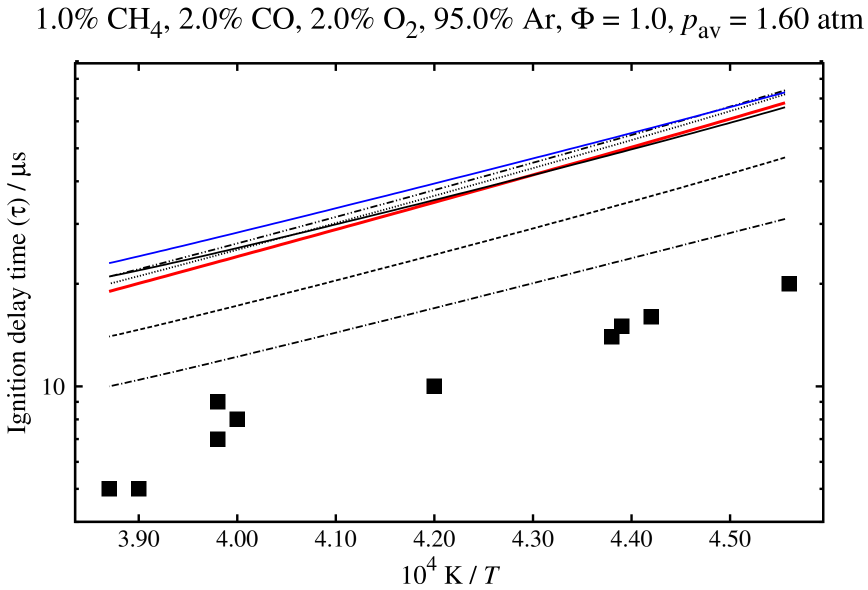
(c)

4.0% CH_4, 20.2% O_2, 75.81% N_2, $\Phi = 0.4$, $p = 4.0$ atm

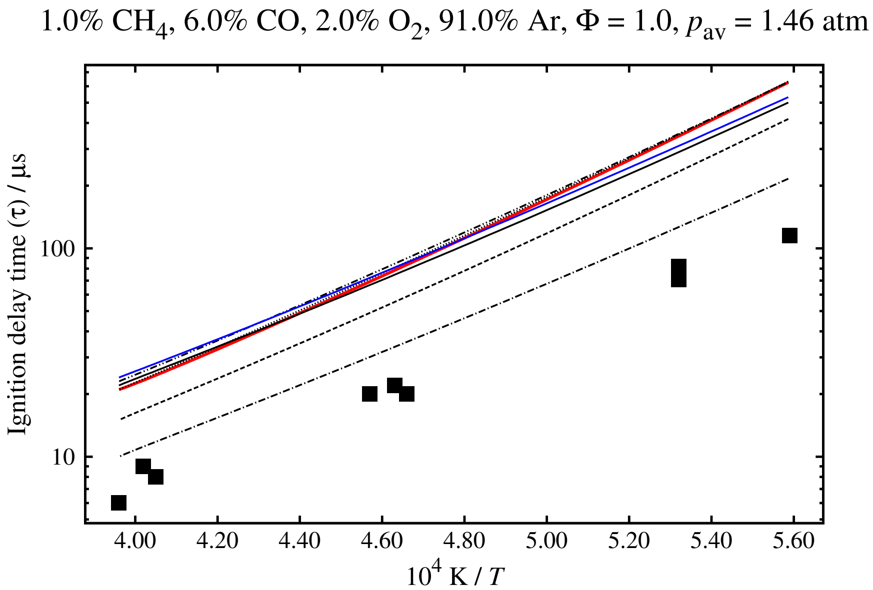


(d)

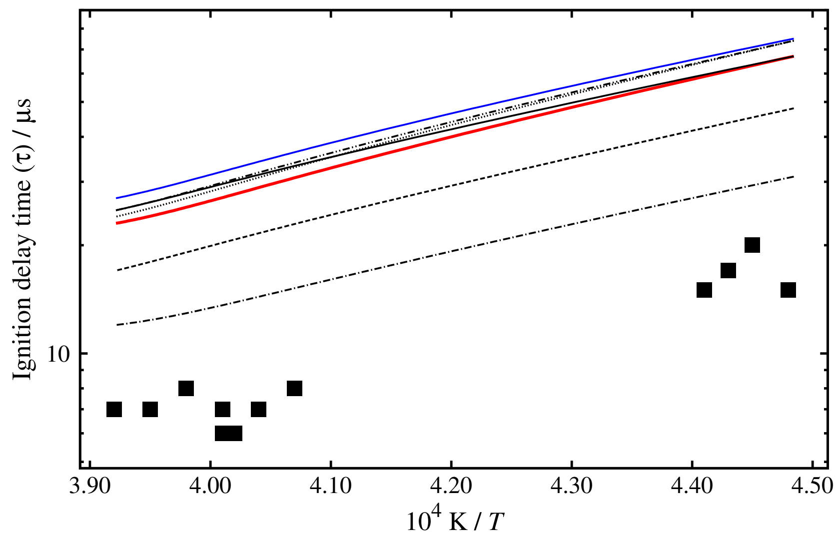
S4 Shock tube ignition delay times of methane/oxygen/argon mixtures. Symbols are experimental data [10] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


1.0% CH_4, 2.0% CO, 2.0% O_2, 95.0% Ar, Φ = 1.0, p_{av} = 1.60 atm
Ignition delay time (τ) / µs
10
3.90
4.00
4.10
4.20
4.30
4.40
4.50
10^4 K / T

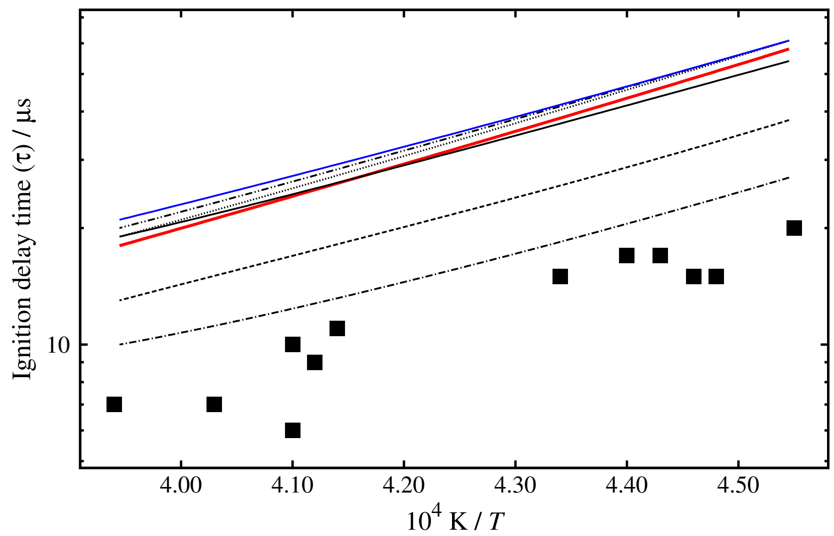
(a)


1.0% CH_4, 6.0% CO, 2.0% O_2, 91.0% Ar, Φ = 1.0, p_{av} = 1.46 atm
Ignition delay time (τ) / µs
100
10
4.00
4.20
4.40
4.60
4.80
5.00
5.20
5.40
5.60
10^4 K / T

(b)



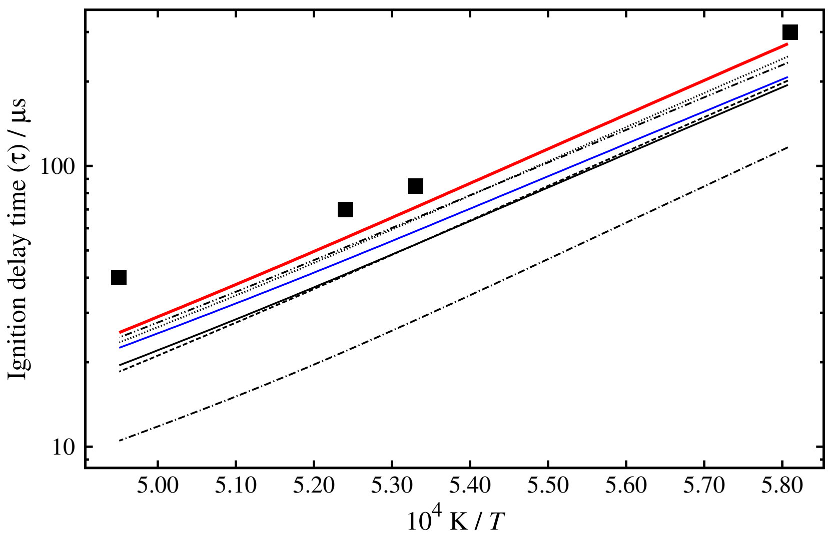
(c)



(d)

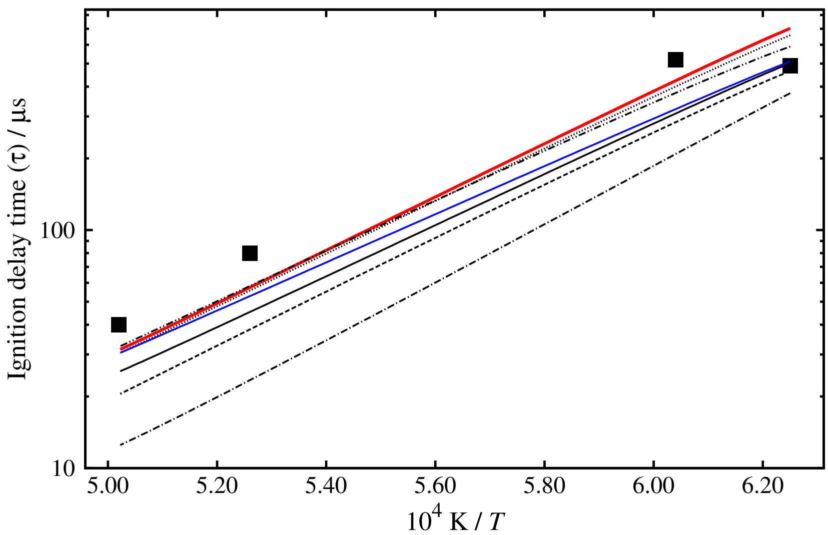
S5 Shock tube ignition delay times of methane/air mixtures. Symbols are experimental data [11] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, − − − Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, — USC II.

1.0% CH_4, 2.0% O_2, 97% Ar, Φ = 1.0, p_{av} = 10.43 atm



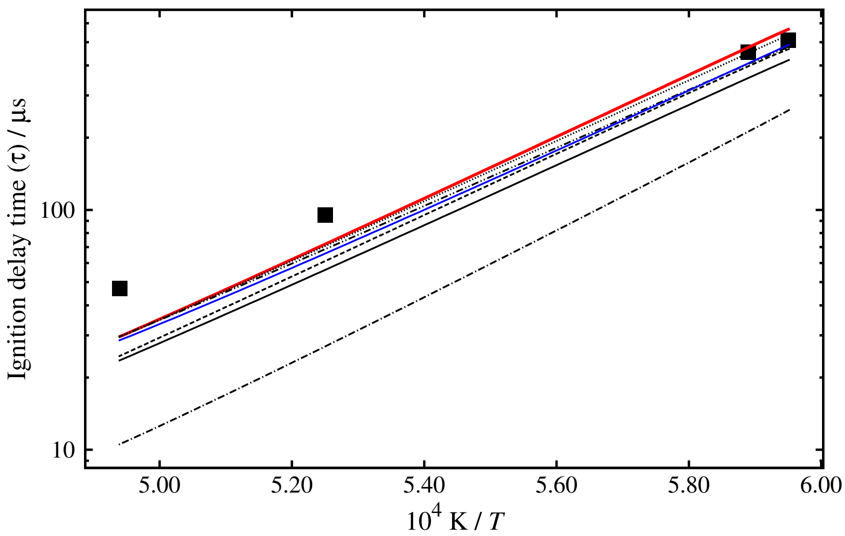
(a)

3.5% CH_4, 7.0% O_2, 89.5% Ar, Φ = 1.0, p_{av} = 3.04 atm



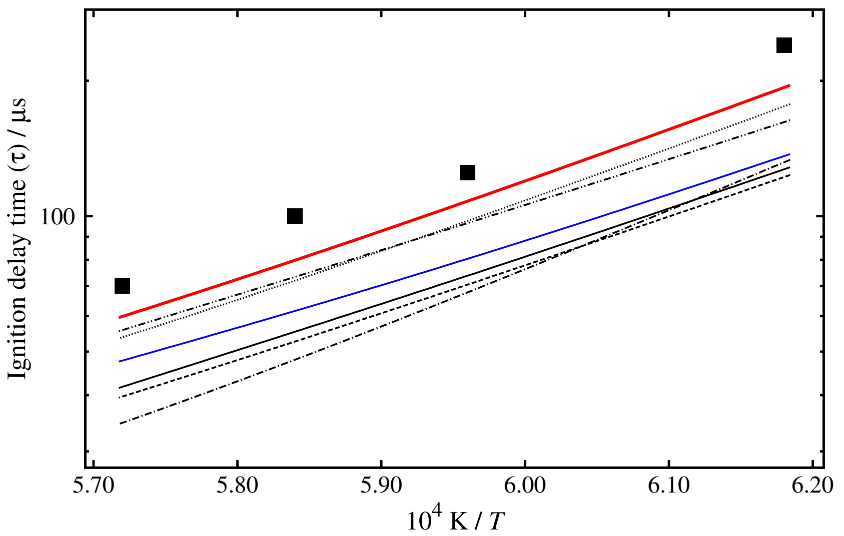
(b)

2.1% CH_4, 2.1% O_2, 95.8% Ar, Φ = 2.0, p_{av} = 9.42 atm

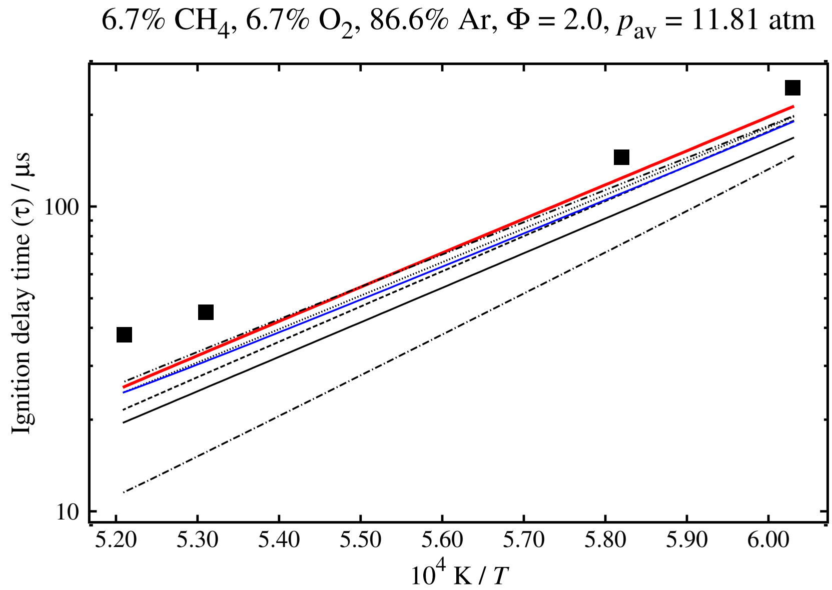


(c)

2.0% CH_4, 8.0% O_2, 90.0% Ar, Φ = 0.5, p_{av} = 9.21 atm

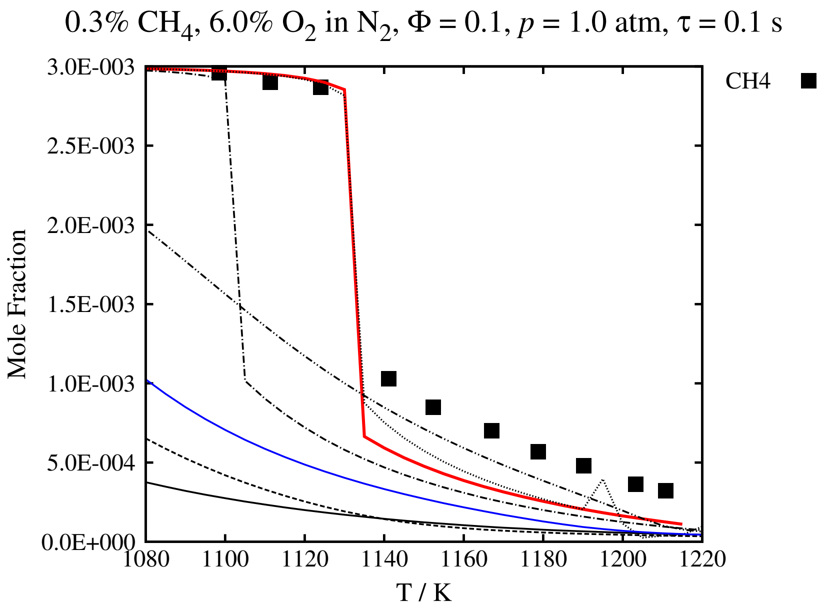


(d)

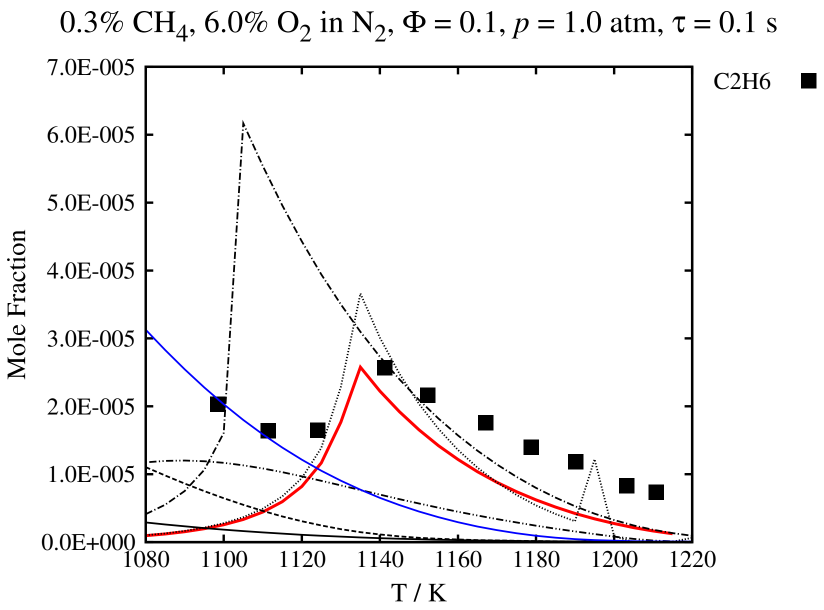


(e)

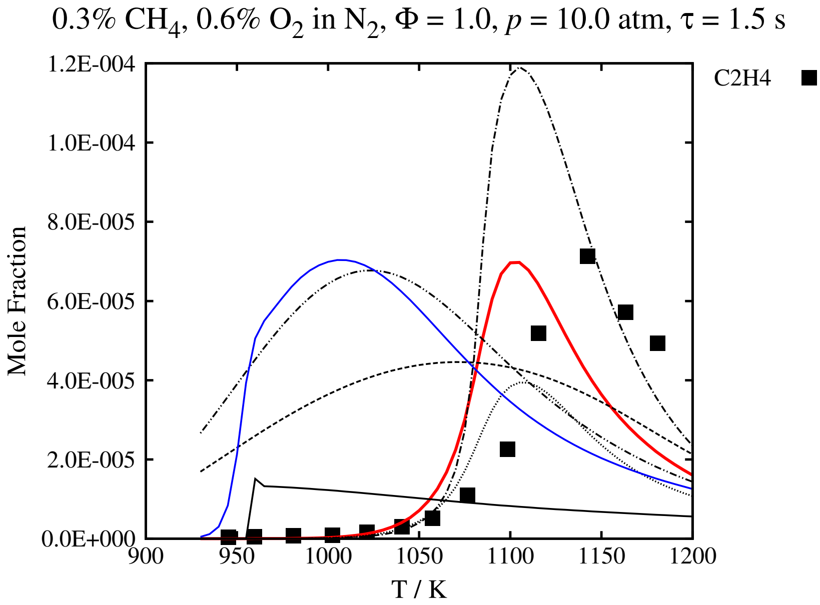
S6 Shock tube ignition delay times of methane/oxygen/argon mixtures. Symbols are experimental data [12] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.3% CH_4, 6.0% O_2 in N_2, Φ = 0.1, *p* = 1.0 atm, τ = 0.1 s
CH4
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
1080
1100
1120
1140
1160
1180
1200
1220
T / K

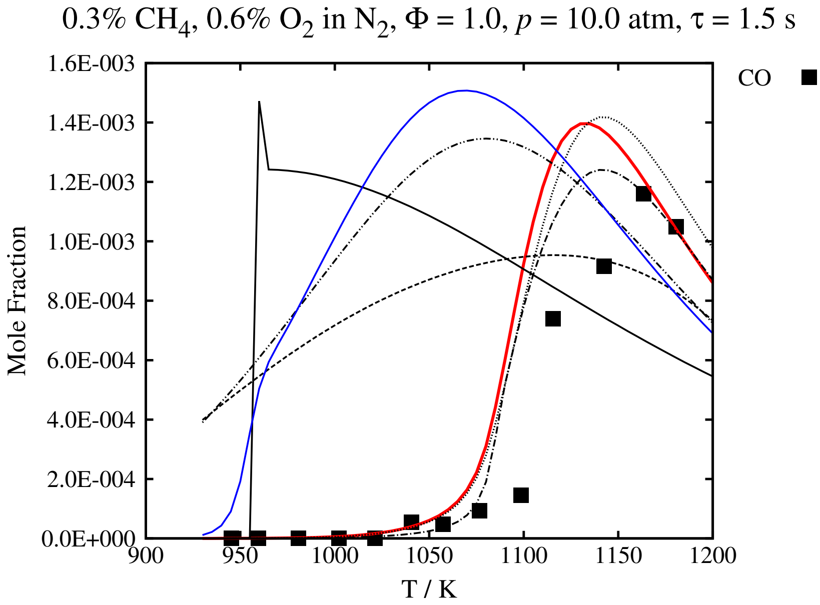
(a)


0.3% CH_4, 6.0% O_2 in N_2, Φ = 0.1, *p* = 1.0 atm, τ = 0.1 s
C2H6
Mole Fraction
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
1080
1100
1120
1140
1160
1180
1200
1220
T / K

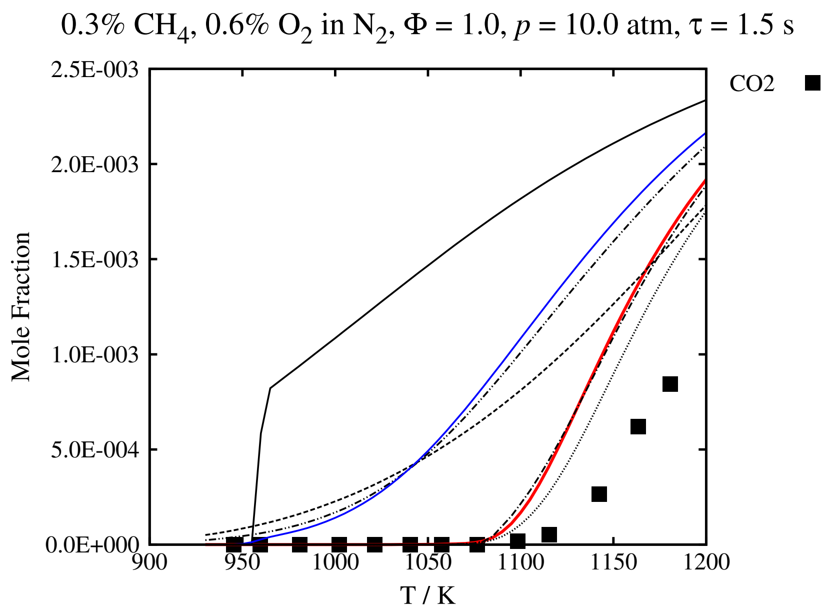
(b)


0.3% CH4, 0.6% O2 in N2, Φ = 1.0, p = 10.0 atm, τ = 1.5 s
C2H4
Mole Fraction
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
900
950
1000
1050
1100
1150
1200
T / K

(c)

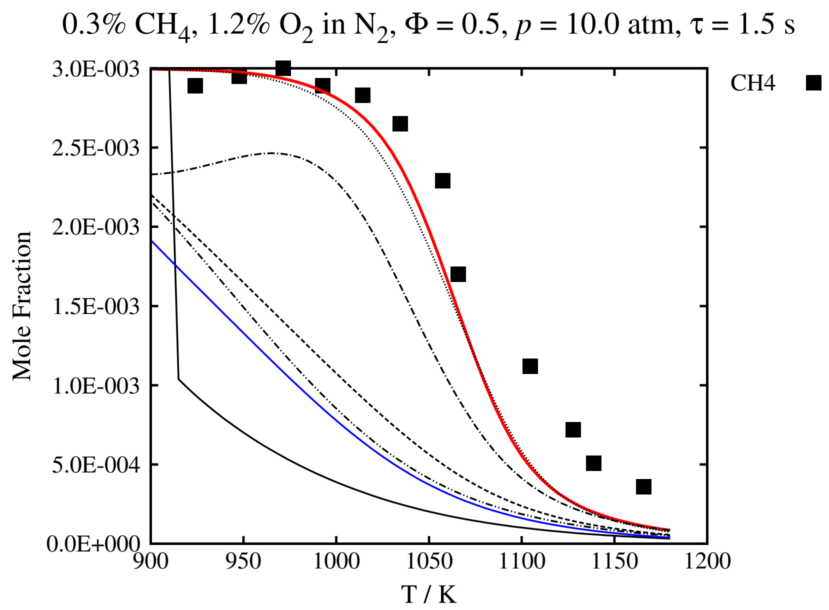

0.3% CH4, 0.6% O2 in N2, Φ = 1.0, p = 10.0 atm, τ = 1.5 s
CO
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
900
950
1000
1050
1100
1150
1200
T / K

(d)

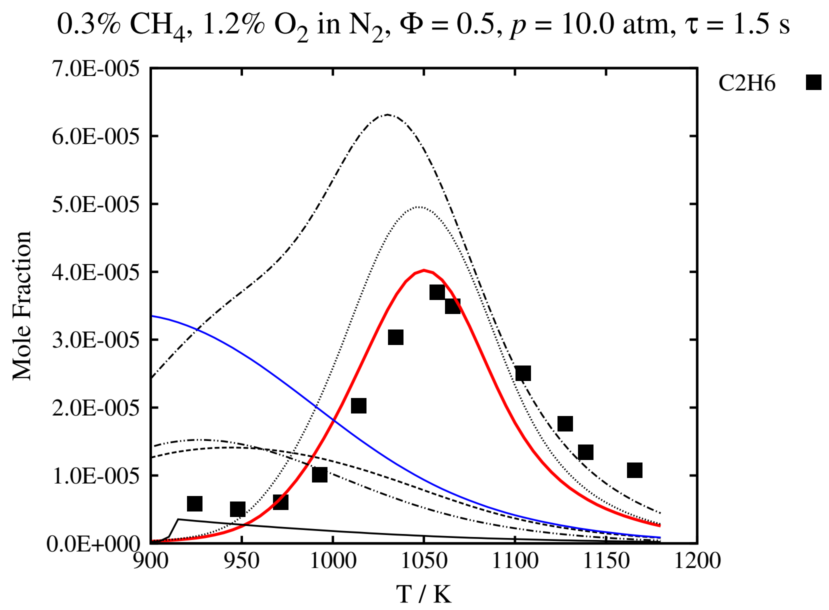


(e)

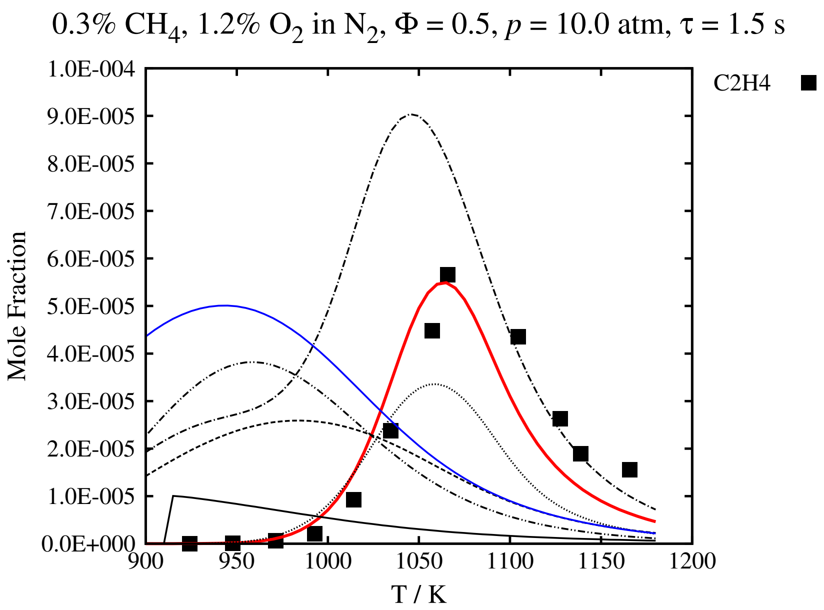
S7 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [13] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.3% CH_4, 1.2% O_2 in N_2, Φ = 0.5, p = 10.0 atm, τ = 1.5 s
CH4
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
900
950
1000
1050
1100
1150
1200
T / K

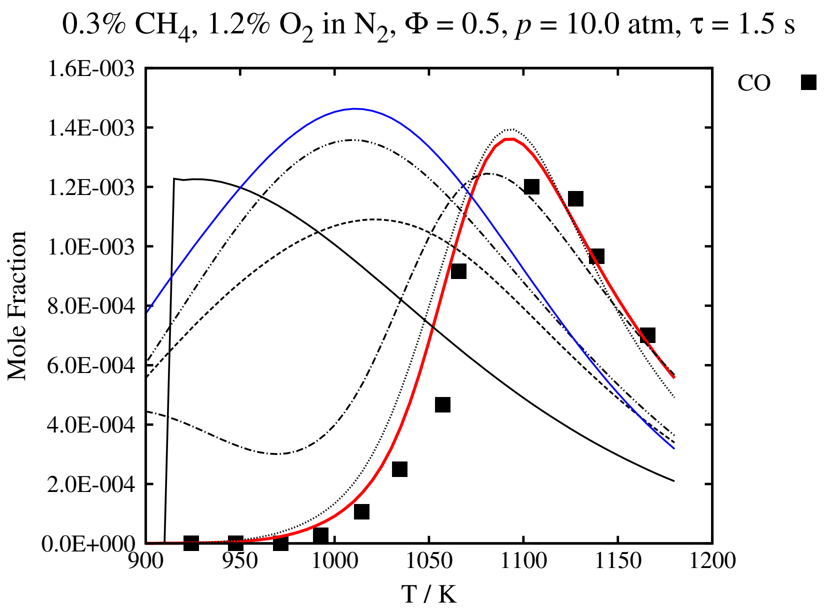
(a)


0.3% CH_4, 1.2% O_2 in N_2, Φ = 0.5, p = 10.0 atm, τ = 1.5 s
C2H6
Mole Fraction
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
900
950
1000
1050
1100
1150
1200
T / K

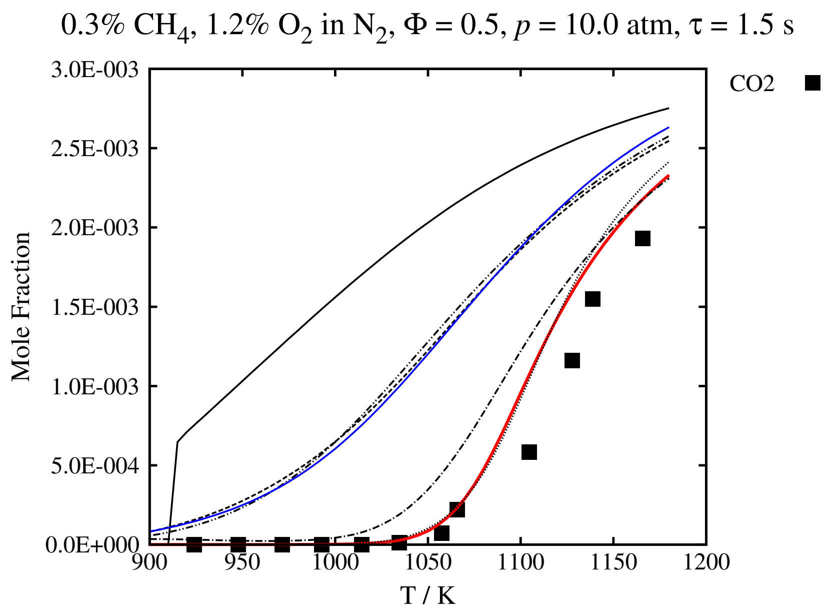
(b)


0.3% CH4, 1.2% O2 in N2, Φ = 0.5, p = 10.0 atm, τ = 1.5 s
C2H4
Mole Fraction
T / K
1.0E-004
9.0E-005
8.0E-005
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
900
950
1000
1050
1100
1150
1200

(c)


0.3% CH4, 1.2% O2 in N2, Φ = 0.5, p = 10.0 atm, τ = 1.5 s
CO
Mole Fraction
T / K
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
900
950
1000
1050
1100
1150
1200

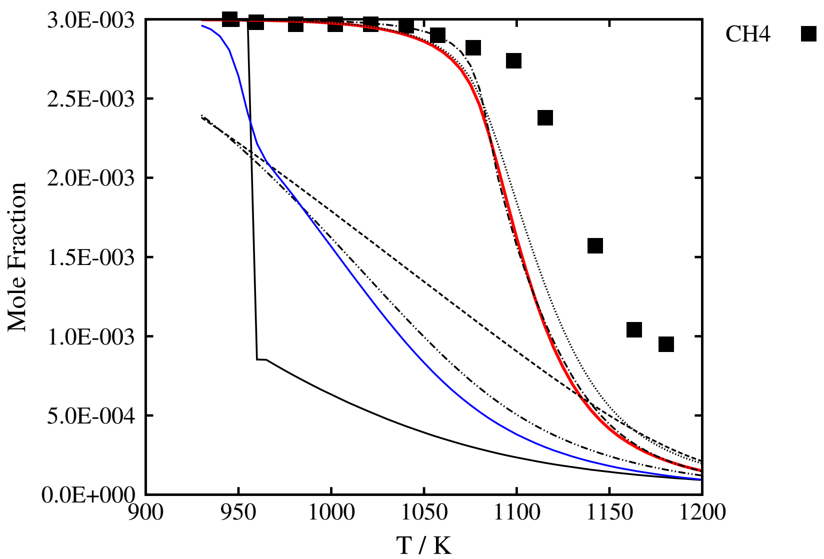
(d)



(e)

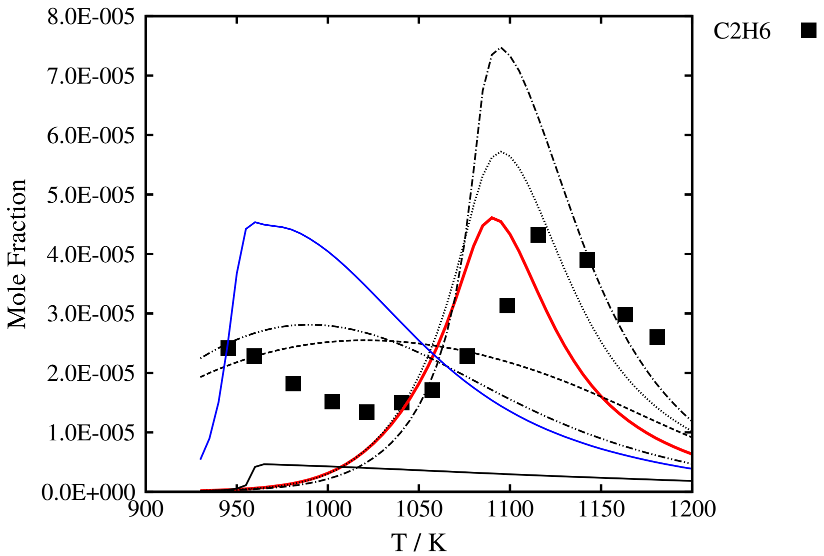
S8 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [13] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

0.3% CH_4, 0.6% O_2 in N_2, Φ = 1.0, p = 10.0 atm, τ = 1.5 s

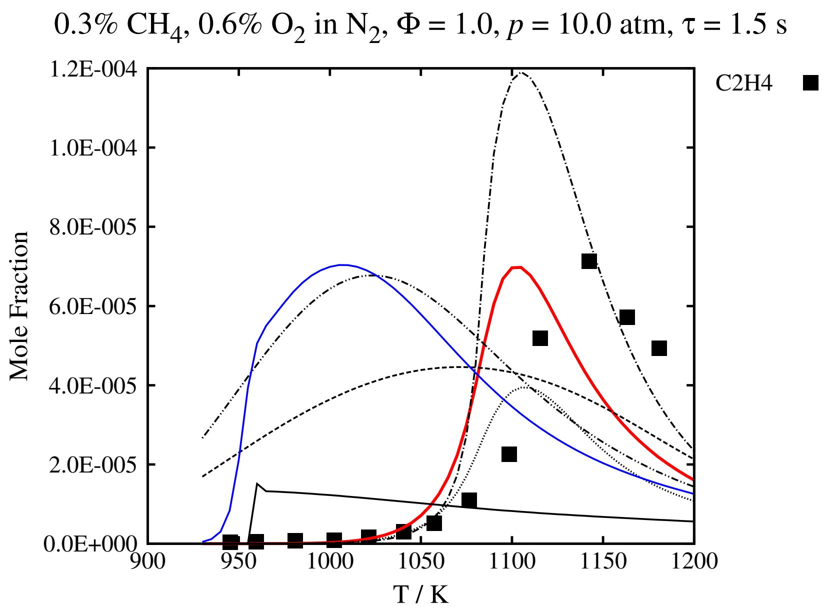


(a)

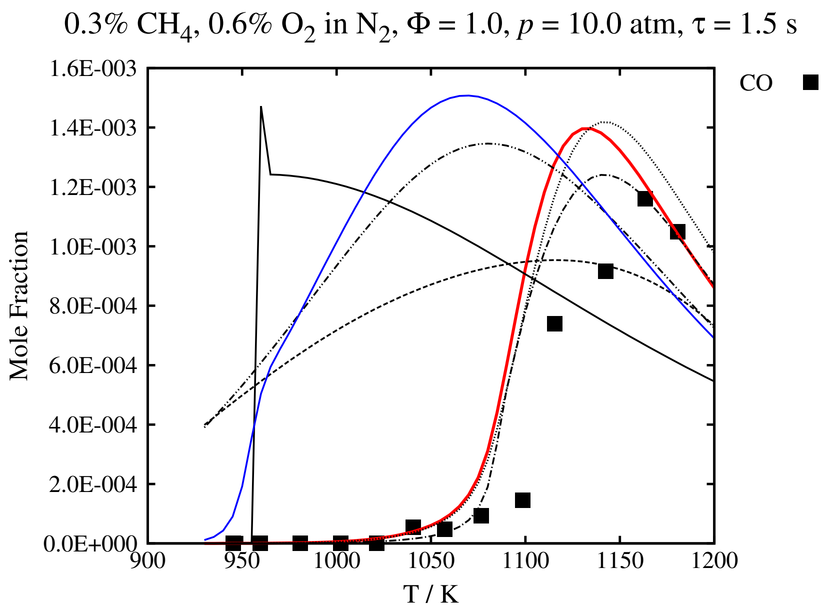
0.3% CH_4, 0.6% O_2 in N_2, Φ = 1.0, p = 10.0 atm, τ = 1.5 s



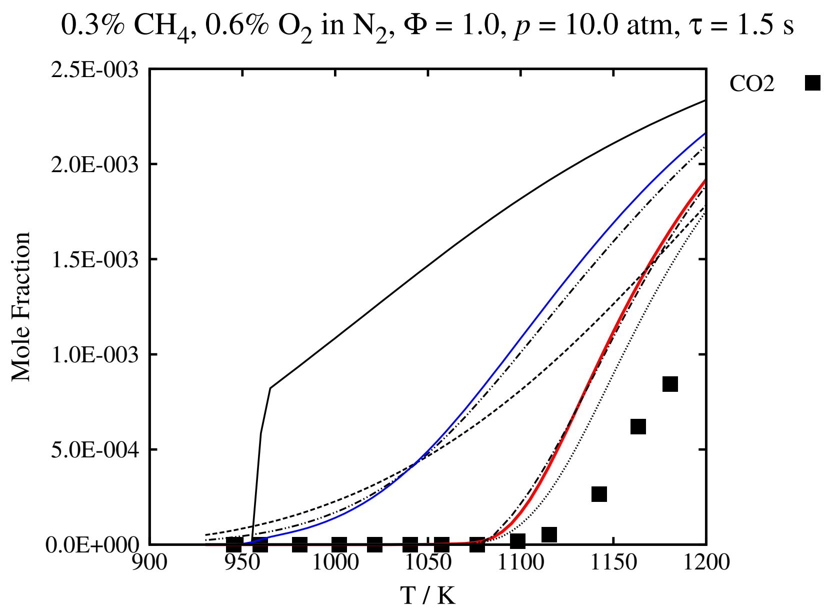
(b)


0.3% CH4, 0.6% O2 in N2, Φ = 1.0, p = 10.0 atm, τ = 1.5 s
C2H4
Mole Fraction
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
900
950
1000
1050
1100
1150
1200
T / K

(c)

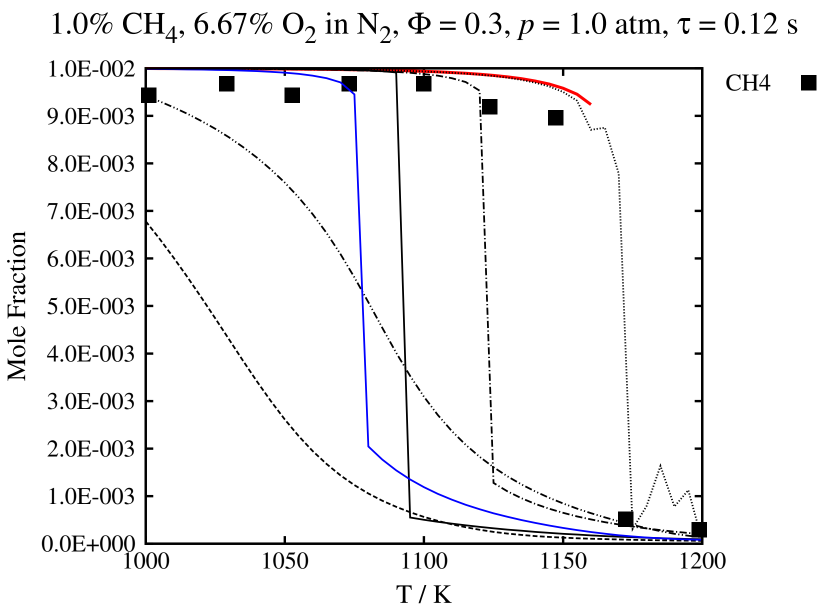

0.3% CH4, 0.6% O2 in N2, Φ = 1.0, p = 10.0 atm, τ = 1.5 s
CO
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
900
950
1000
1050
1100
1150
1200
T / K

(d)

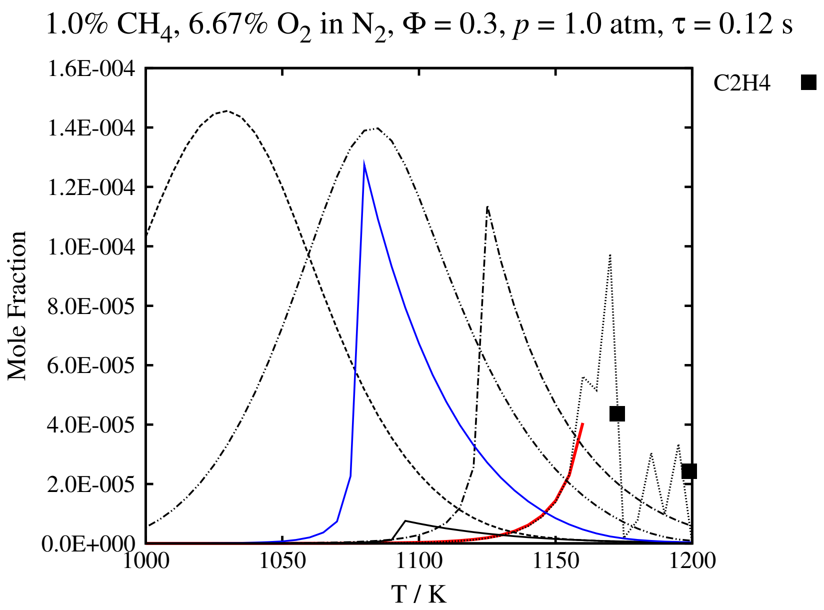


(e)

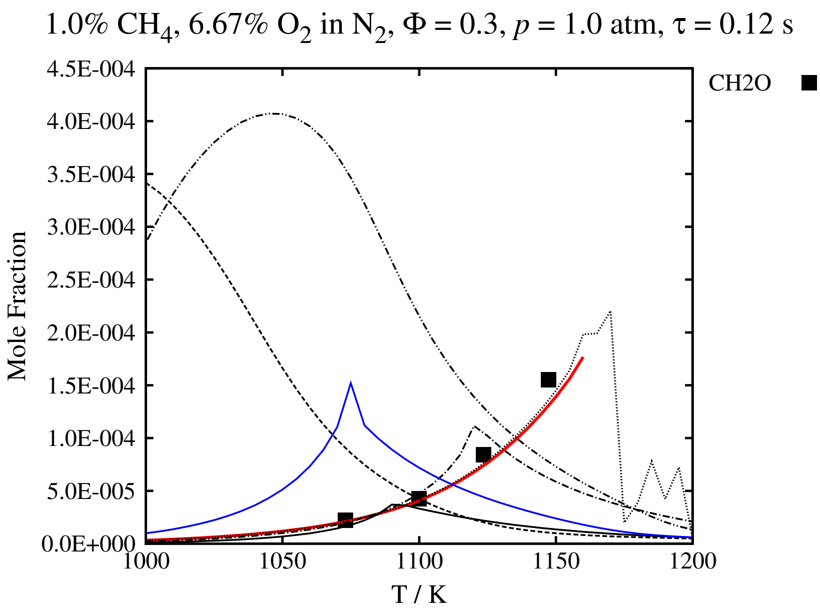
S9 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [13] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


1.0% CH4, 6.67% O2 in N2, Φ = 0.3, p = 1.0 atm, τ = 0.12 s
Mole Fraction
T / K
CH4
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
1000
1050
1100
1150
1200

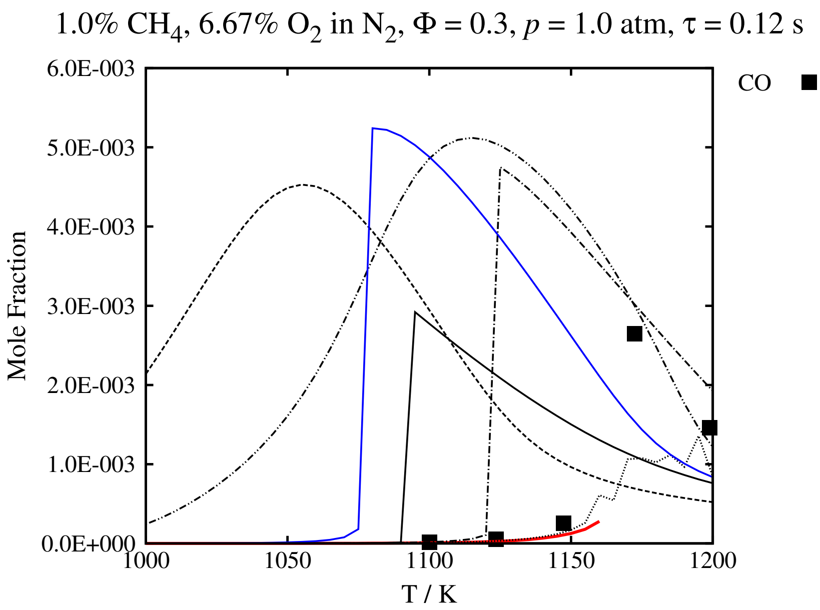
(a)


1.0% CH4, 6.67% O2 in N2, Φ = 0.3, p = 1.0 atm, τ = 0.12 s
Mole Fraction
T / K
C2H4
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
1000
1050
1100
1150
1200

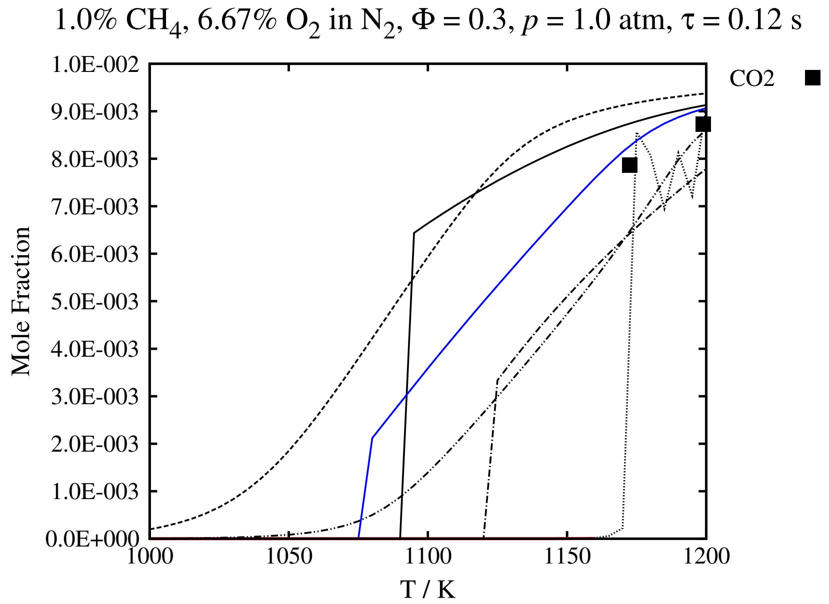
(b)


1.0% CH4, 6.67% O2 in N2, Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH2O
Mole Fraction
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
1000
1050
1100
1150
1200
T / K

(c)

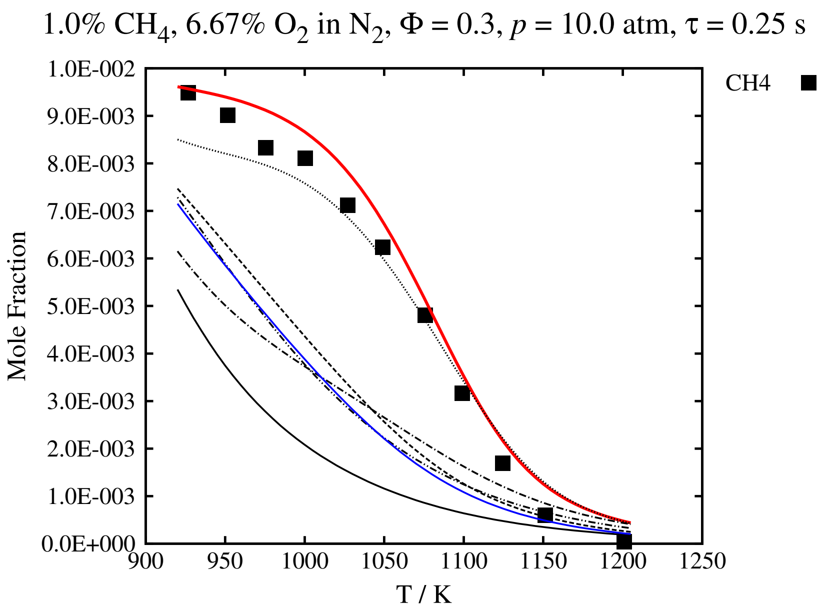

1.0% CH4, 6.67% O2 in N2, Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CO
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
1000
1050
1100
1150
1200
T / K

(d)

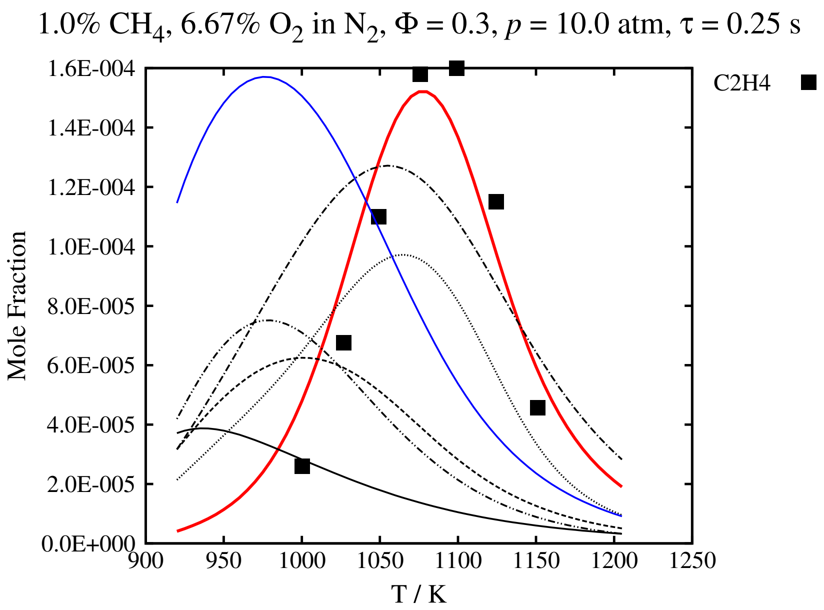


(e)

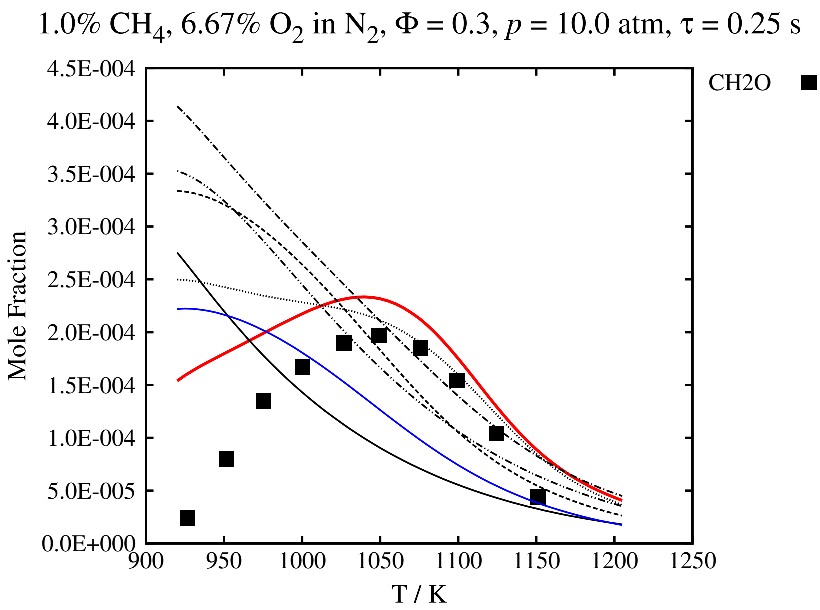
S10 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


1.0% CH_4, 6.67% O_2 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
T / K
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
900
950
1000
1050
1100
1150
1200
1250

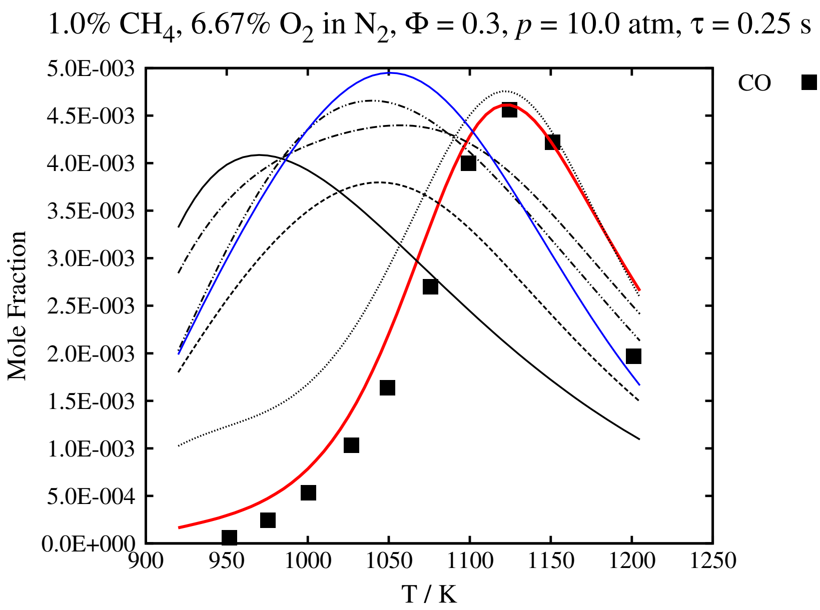
(a)


1.0% CH_4, 6.67% O_2 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
C2H4
Mole Fraction
T / K
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
900
950
1000
1050
1100
1150
1200
1250

(b)

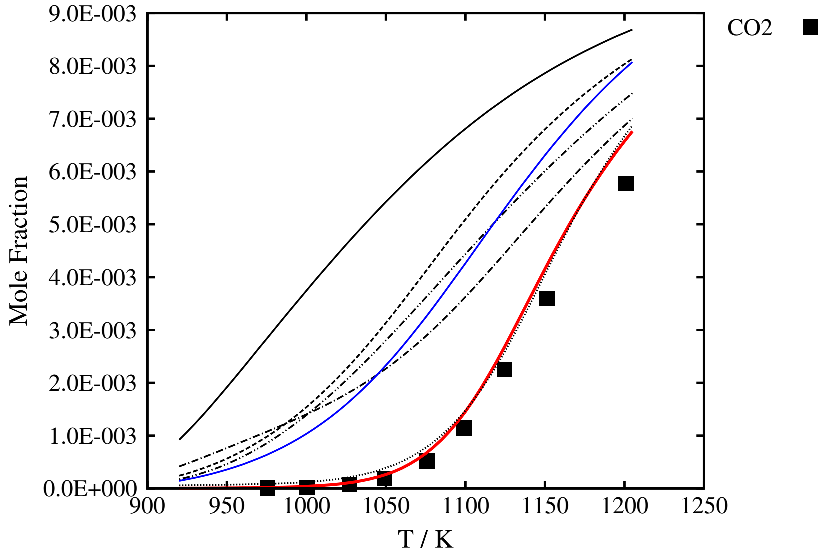

1.0% CH_4, 6.67% O_2 in N_2, $\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s
CH2O
Mole Fraction
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
900
950
1000
1050
1100
1150
1200
1250
T / K

(c)


1.0% CH_4, 6.67% O_2 in N_2, $\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s
CO
Mole Fraction
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
900
950
1000
1050
1100
1150
1200
1250
T / K

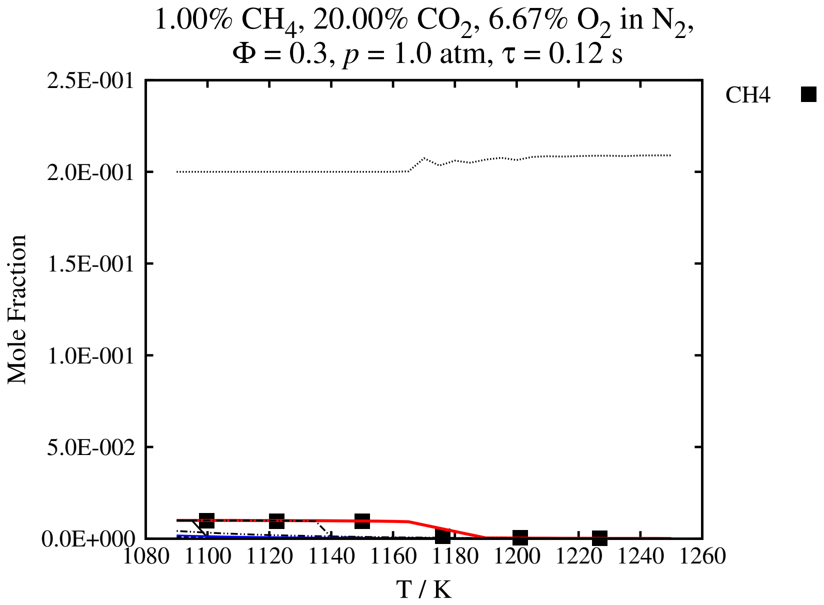
(d)

1.0% CH_4, 6.67% O_2 in N_2, $\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s

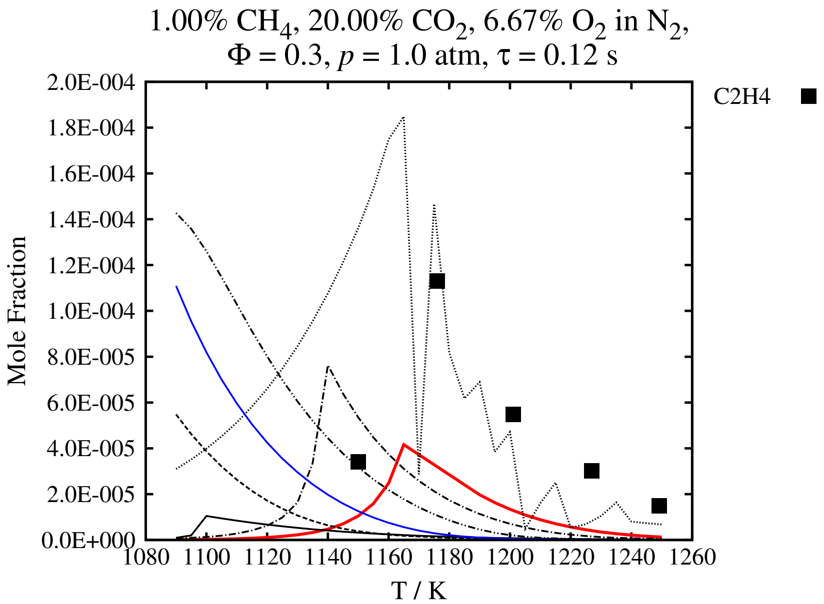


(e)

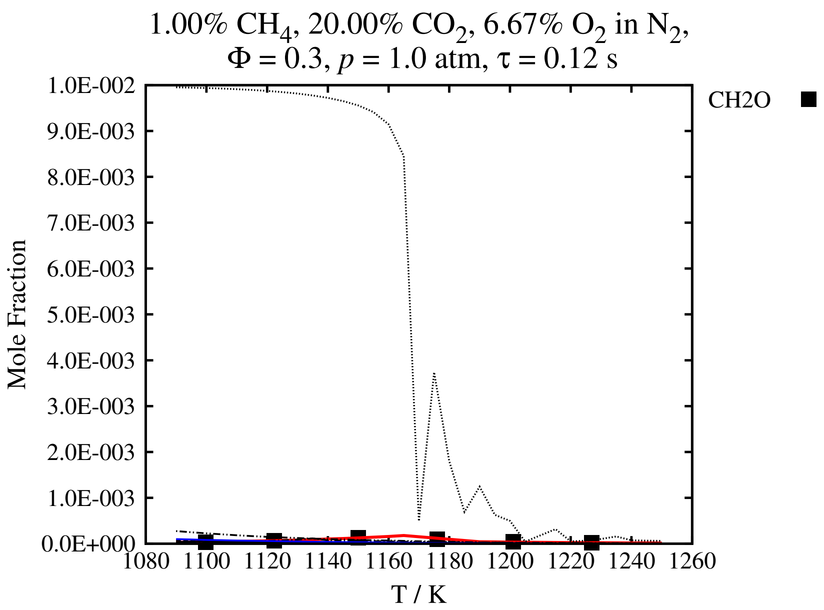
S11 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


1.00% CH_4, 20.00% CO_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH4
Mole Fraction
2.5E-001
2.0E-001
1.5E-001
1.0E-001
5.0E-002
0.0E+000
1080 1100 1120 1140 1160 1180 1200 1220 1240 1260
T / K

(a)

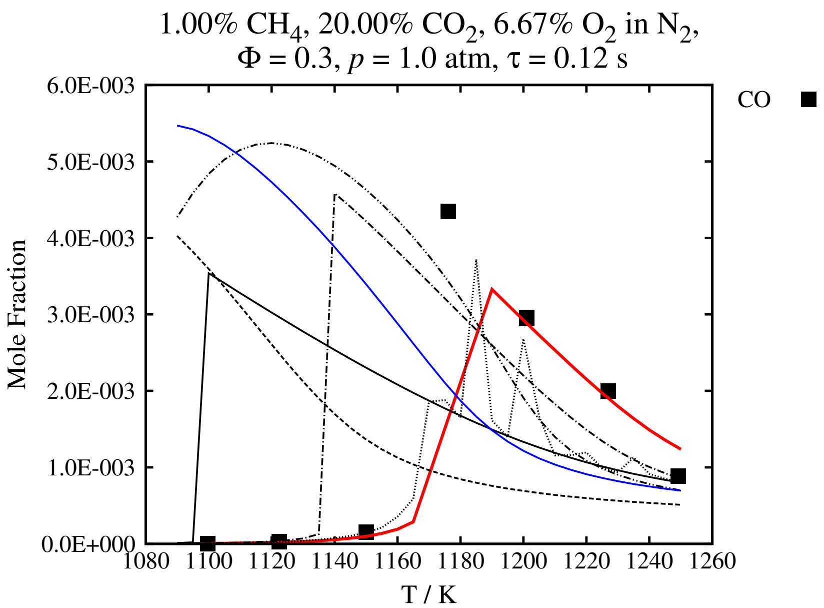

1.00% CH_4, 20.00% CO_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
C2H4
Mole Fraction
2.0E-004
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
1080 1100 1120 1140 1160 1180 1200 1220 1240 1260
T / K

(b)



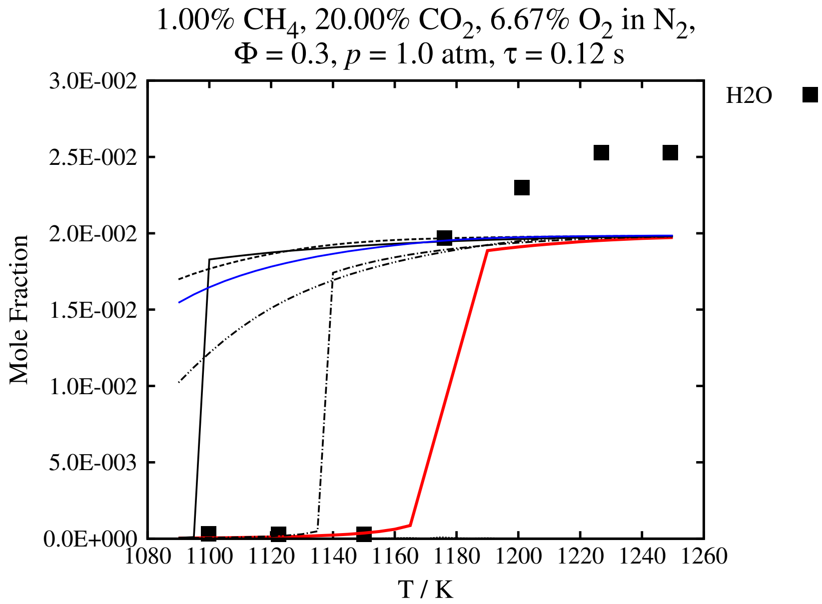
1.00% CH4, 20.00% CO2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH2O
Mole Fraction
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
1080 1100 1120 1140 1160 1180 1200 1220 1240 1260
T / K

(c)



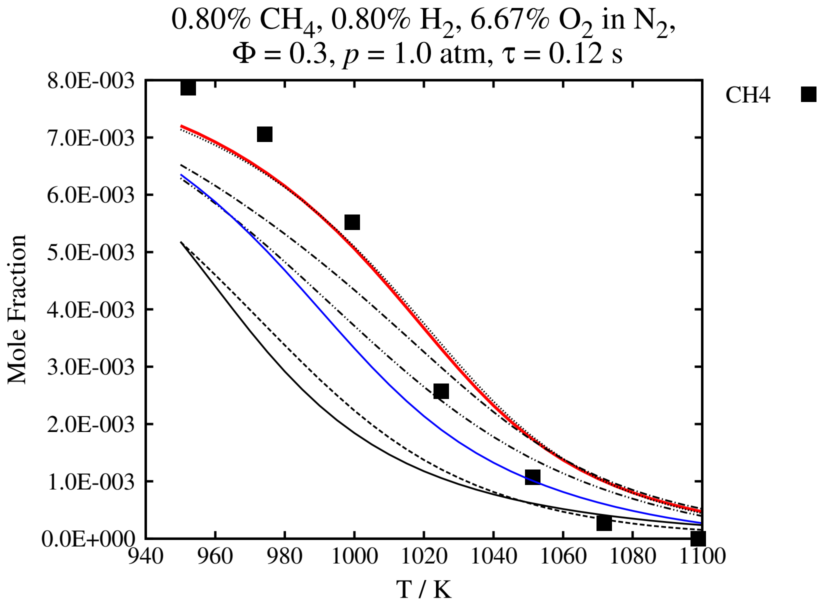
1.00% CH4, 20.00% CO2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CO
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
1080 1100 1120 1140 1160 1180 1200 1220 1240 1260
T / K

(d)

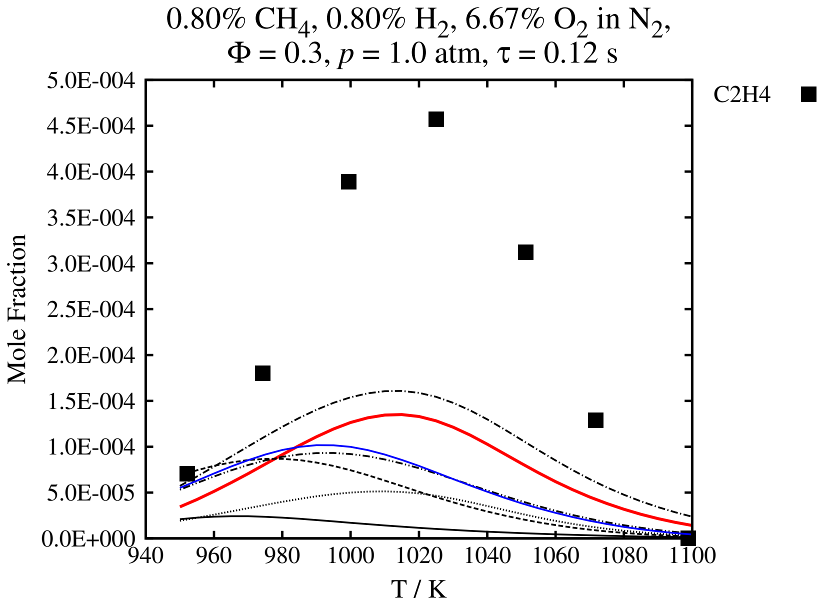


(e)

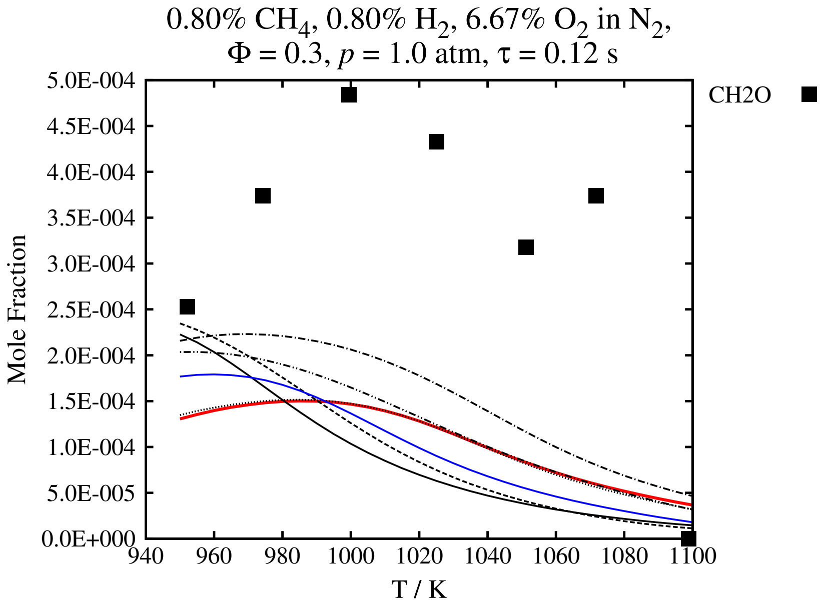
S12 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.80% CH_4, 0.80% H_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH4
Mole Fraction
T / K
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
940
960
980
1000
1020
1040
1060
1080
1100

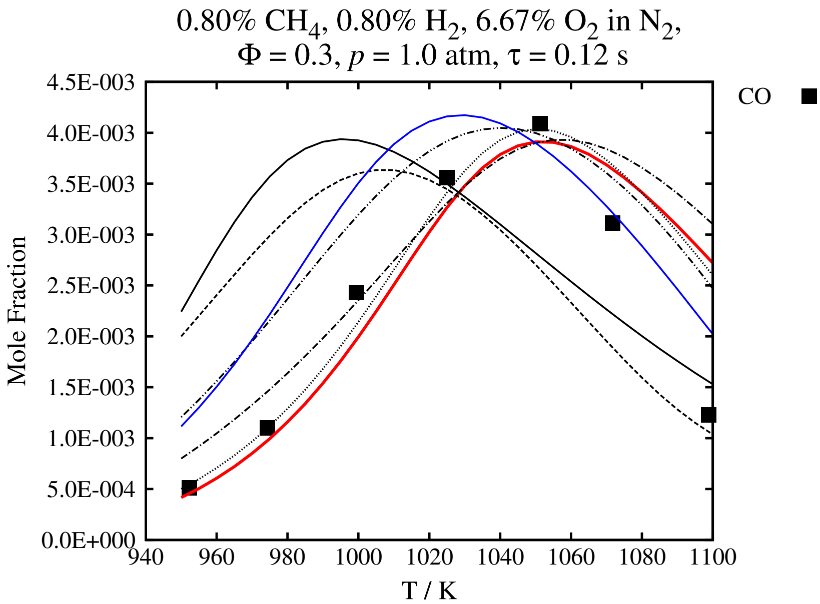
(a)


0.80% CH_4, 0.80% H_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
C2H4
Mole Fraction
T / K
5.0E-004
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
940
960
980
1000
1020
1040
1060
1080
1100

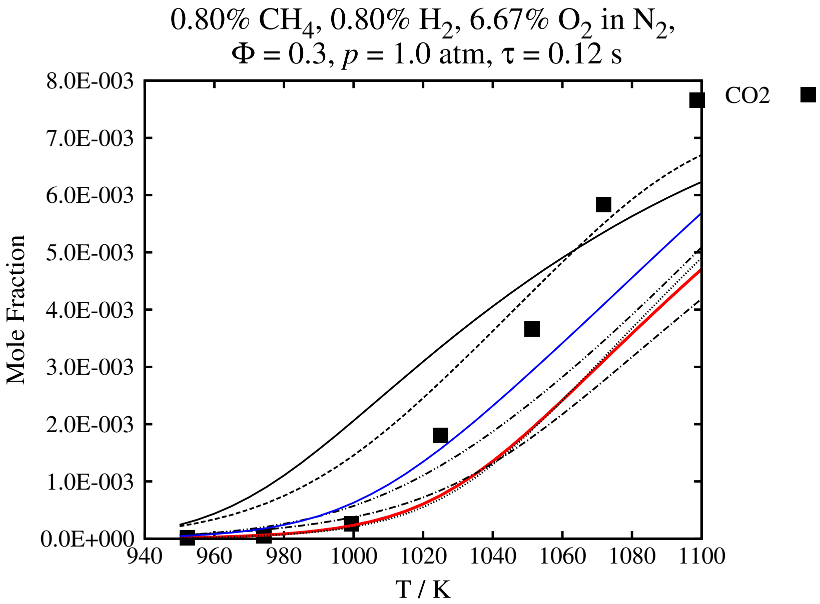
(b)


0.80% CH_4, 0.80% H_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
Mole Fraction
T / K
CH2O
5.0E-004
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
940
960
980
1000
1020
1040
1060
1080
1100

(c)

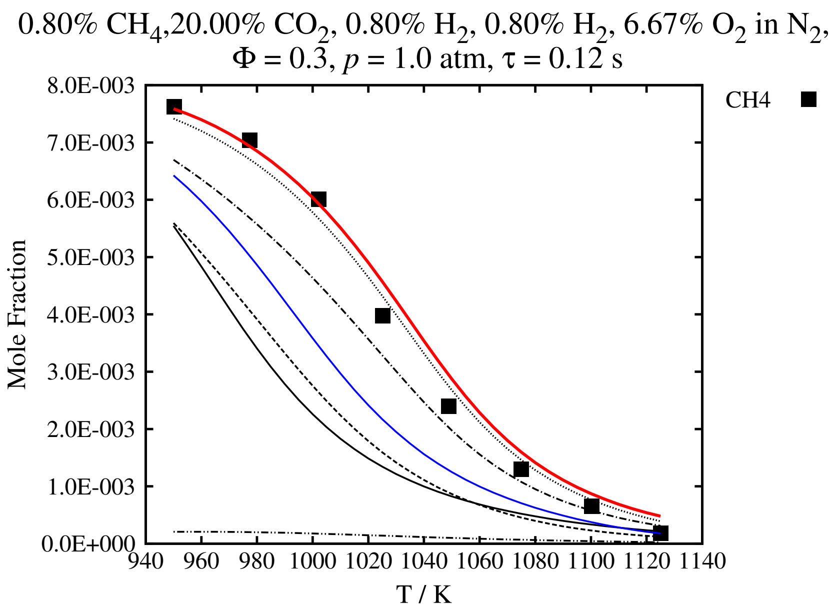

0.80% CH_4, 0.80% H_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
Mole Fraction
T / K
CO
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
940
960
980
1000
1020
1040
1060
1080
1100

(d)

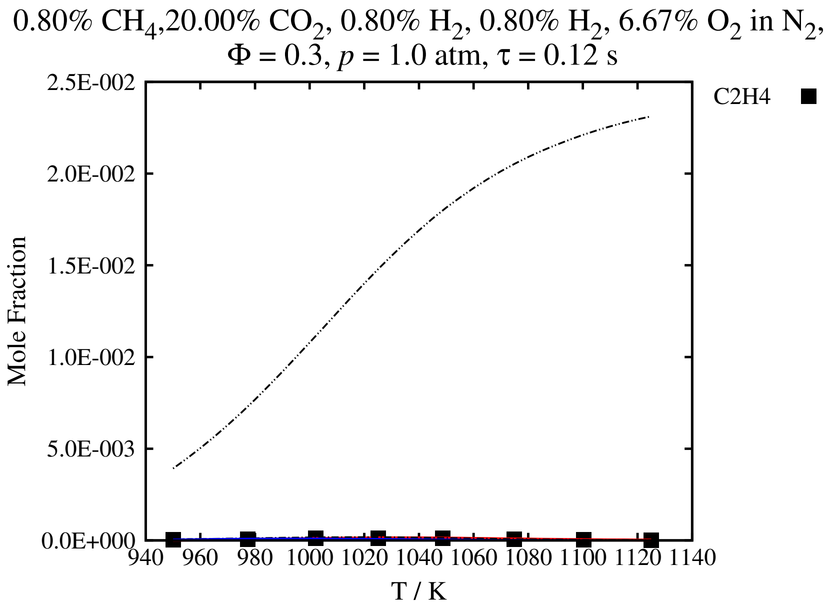


(e)

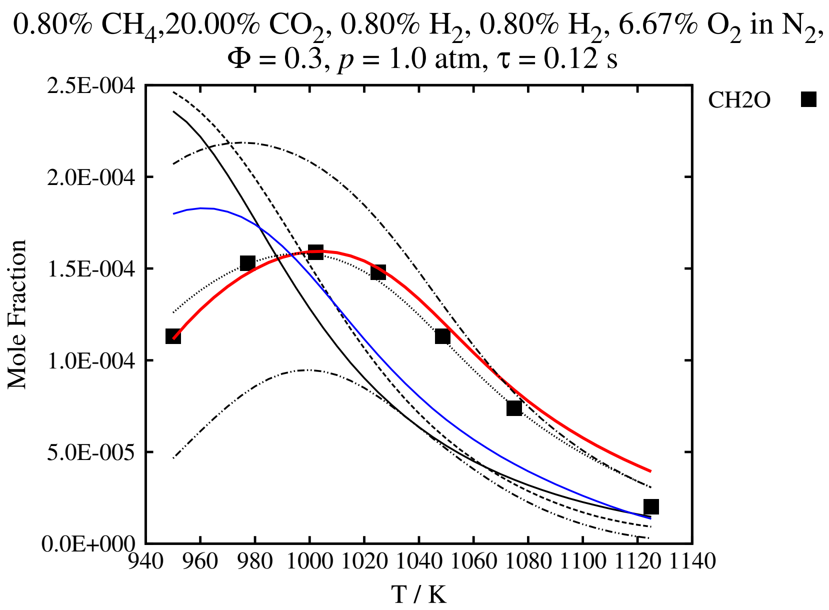
S13 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH4
Mole Fraction
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
940 960 980 1000 1020 1040 1060 1080 1100 1120 1140
T / K

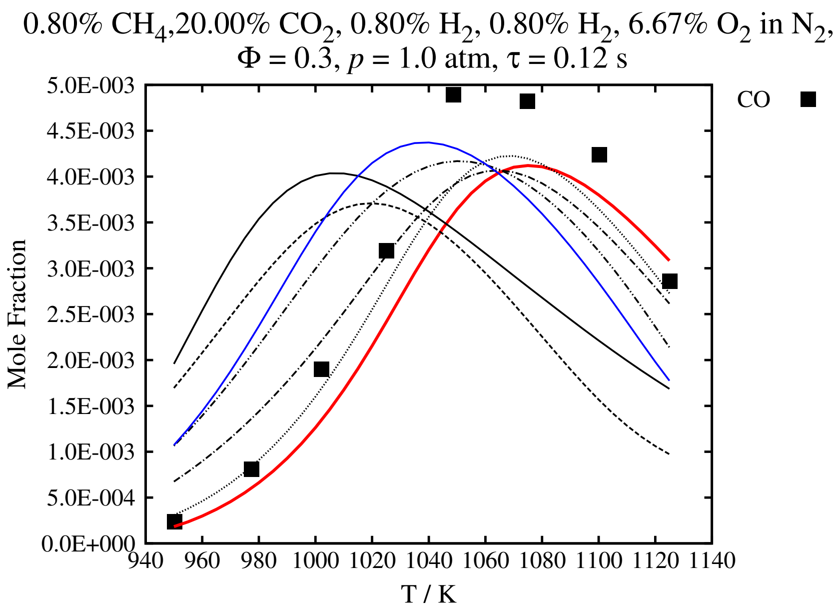
(a)


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
C2H4
Mole Fraction
2.5E-002
2.0E-002
1.5E-002
1.0E-002
5.0E-003
0.0E+000
940 960 980 1000 1020 1040 1060 1080 1100 1120 1140
T / K

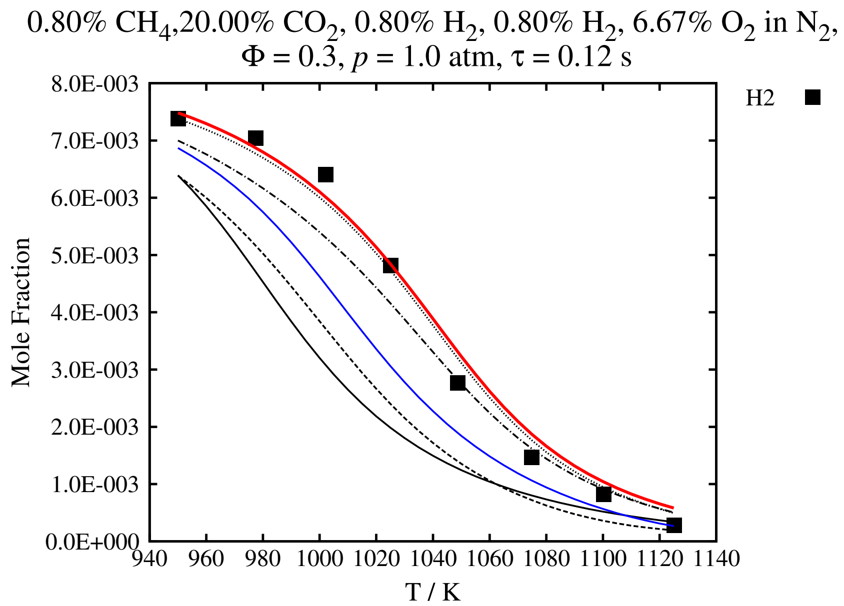
(b)


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH2O
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
940 960 980 1000 1020 1040 1060 1080 1100 1120 1140
T / K

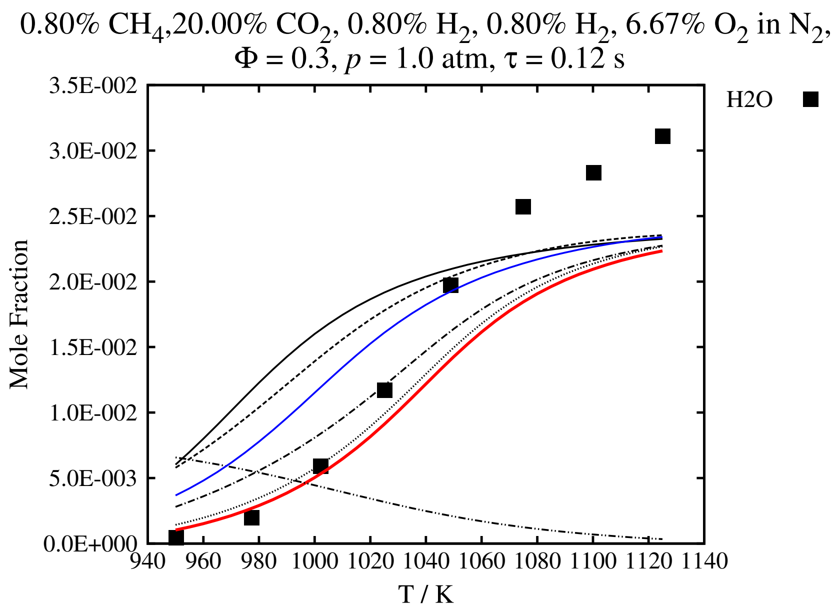
(c)


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CO
Mole Fraction
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
940 960 980 1000 1020 1040 1060 1080 1100 1120 1140
T / K

(d)



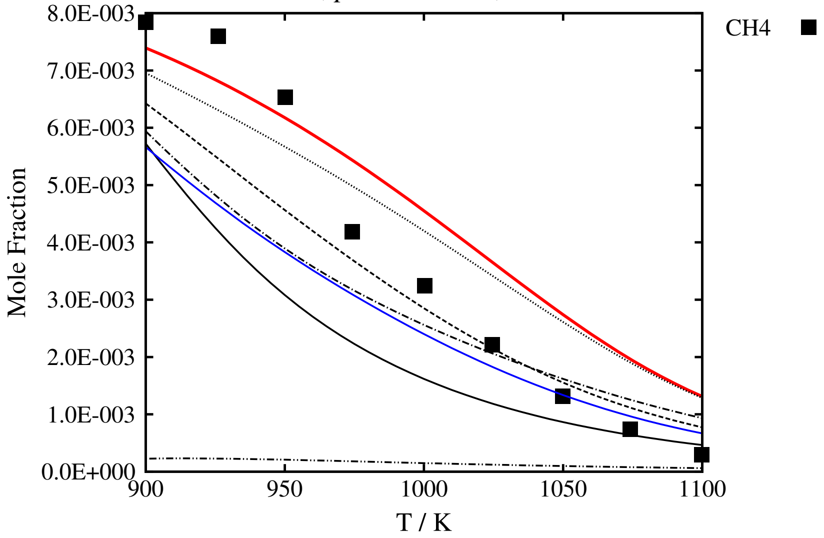
(e)



(f)

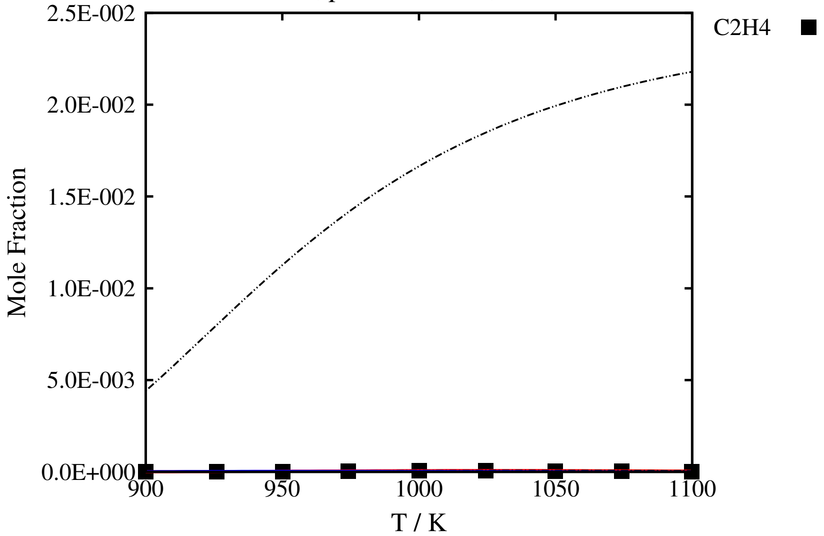
S14 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

0.80% CH_4, 0.80% H_2, 0.80% H_2, 6.67% O_2 in N_2,
$\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s

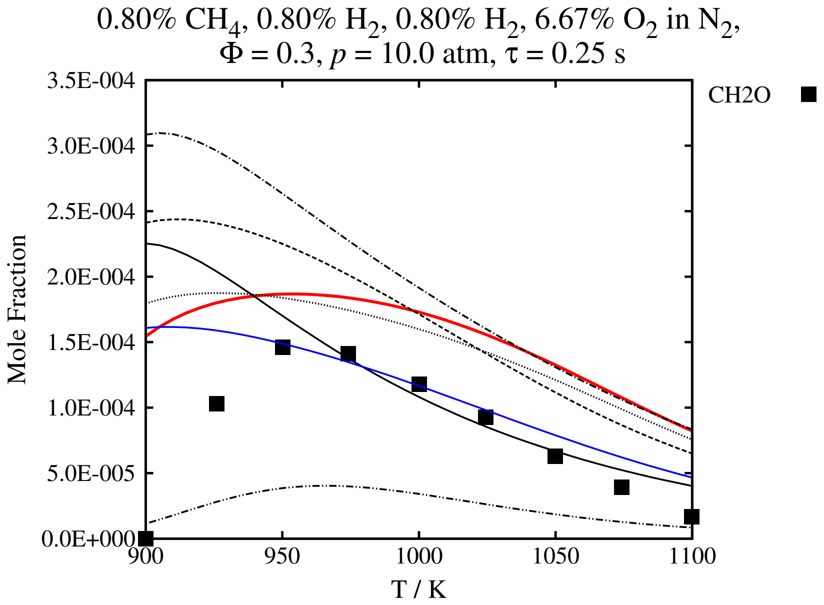


(a)

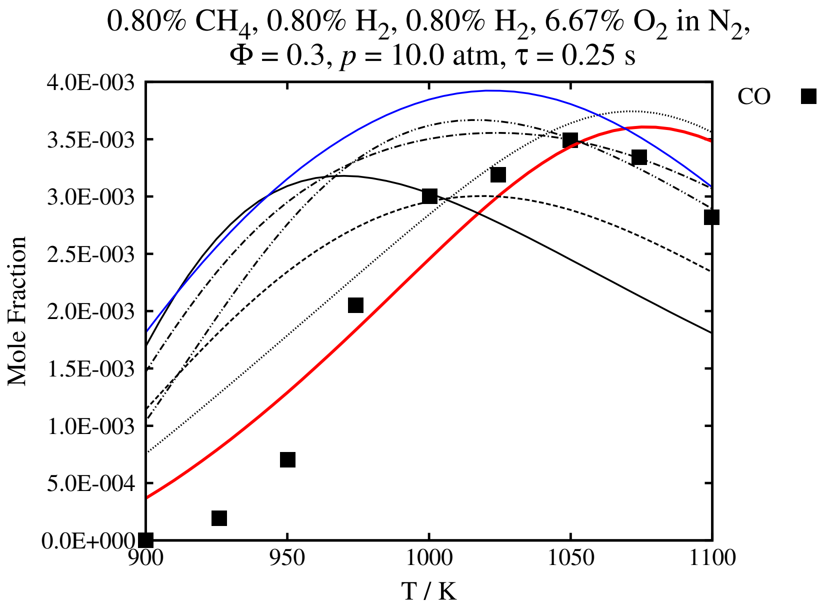
0.80% CH_4, 0.80% H_2, 0.80% H_2, 6.67% O_2 in N_2,
$\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s



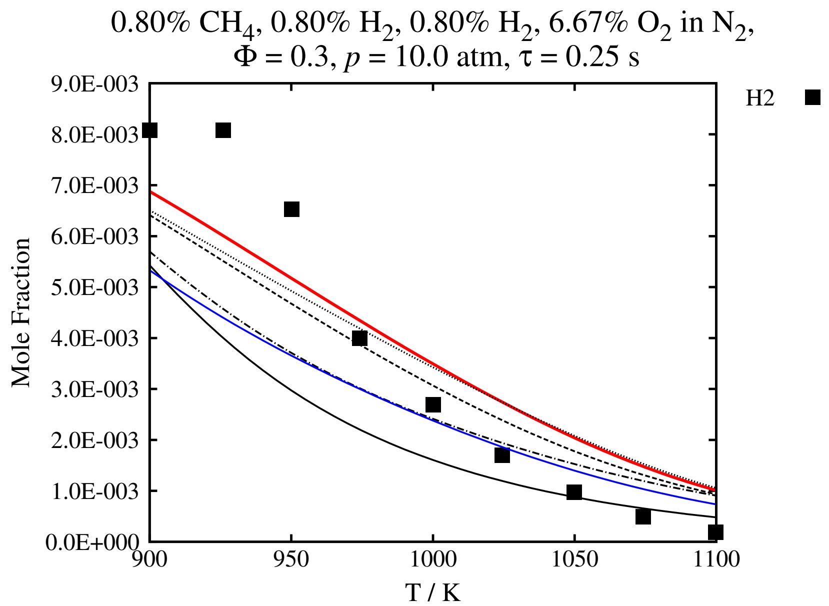
(b)


0.80% CH_4, 0.80% H_2, 0.80% H_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
T / K
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
900
950
1000
1050
1100

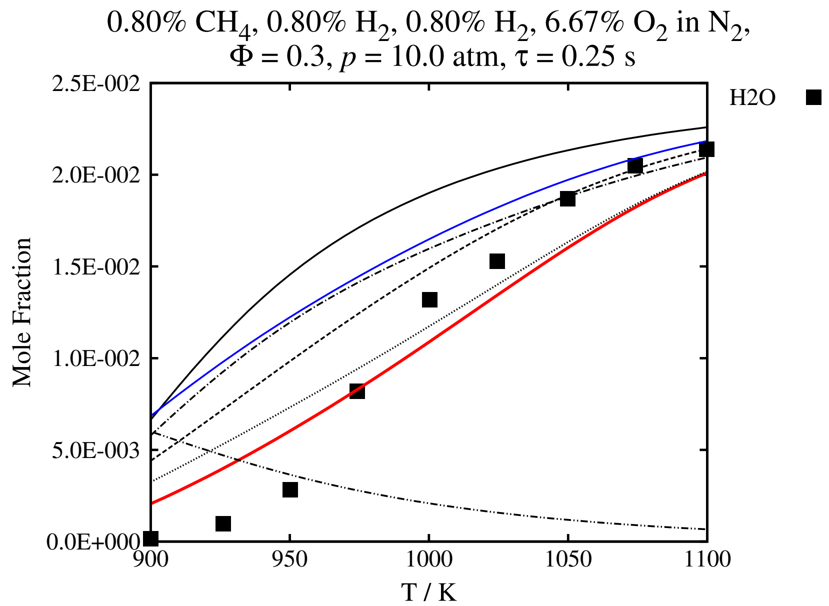
(c)


0.80% CH_4, 0.80% H_2, 0.80% H_2, 6.67% O_2 in N_2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
T / K
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
900
950
1000
1050
1100

(d)

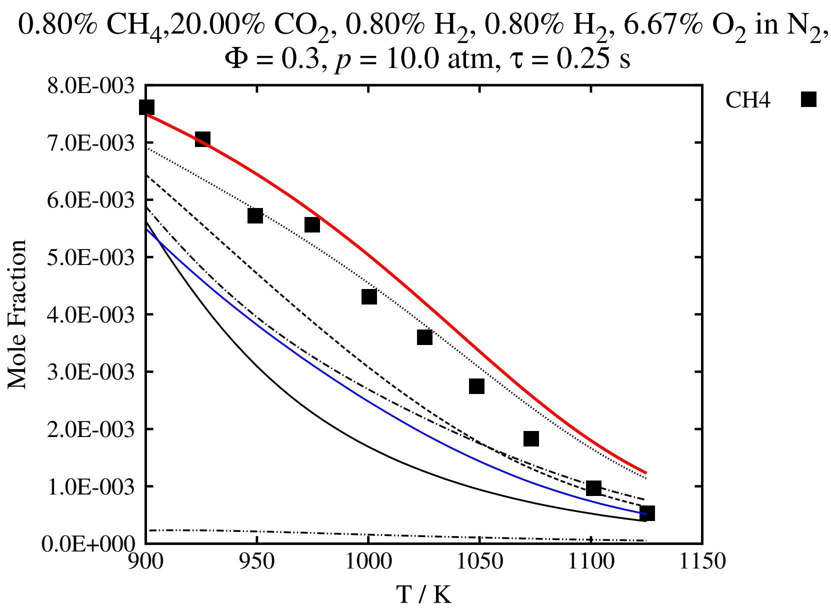


(e)

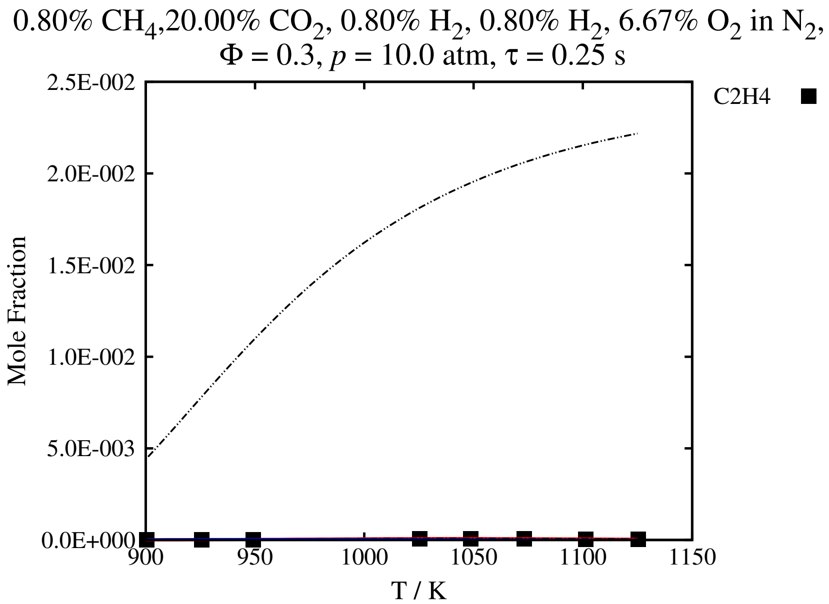


(f)

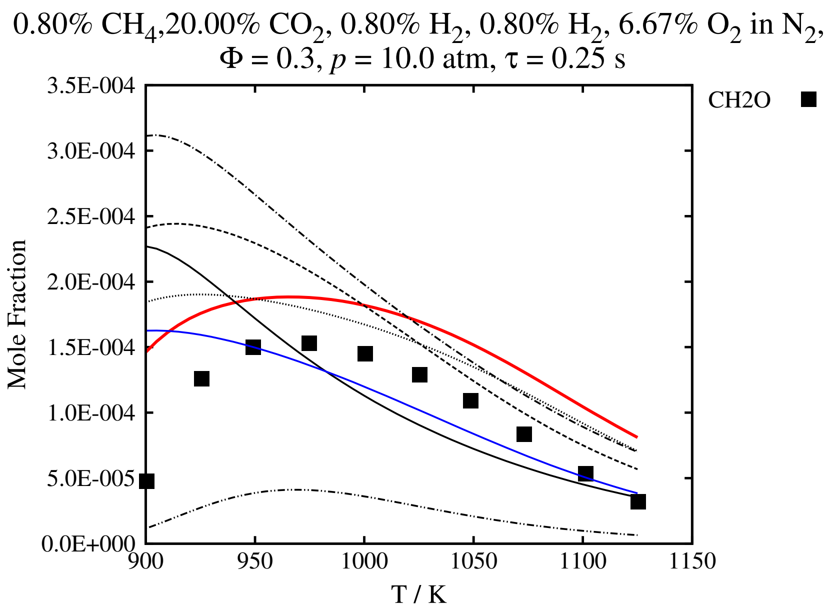
S15 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
900
950
1000
1050
1100
1150
T / K

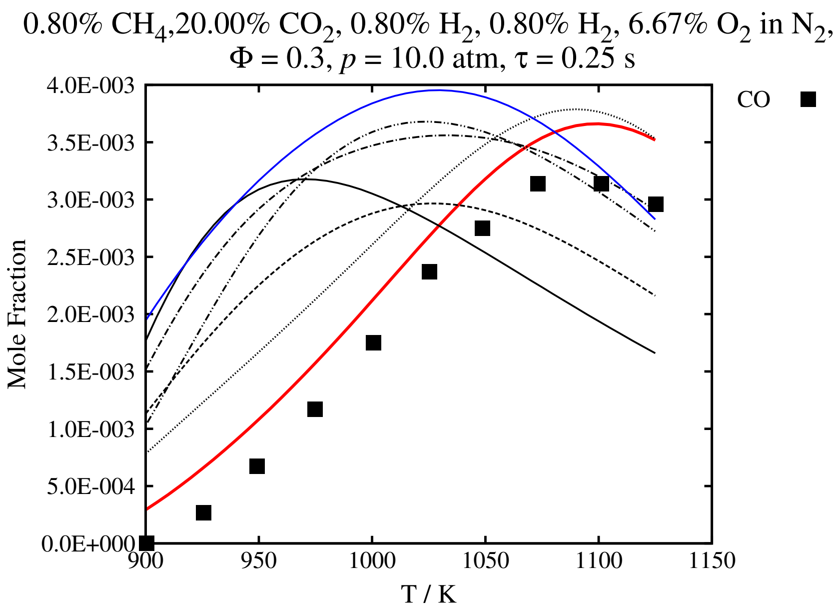
(a)


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
C2H4
Mole Fraction
2.5E-002
2.0E-002
1.5E-002
1.0E-002
5.0E-003
0.0E+000
900
950
1000
1050
1100
1150
T / K

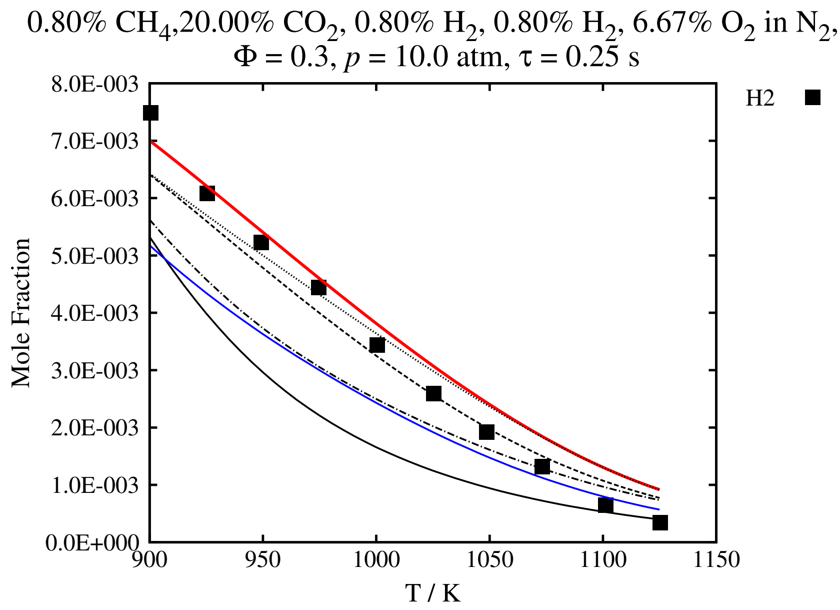
(b)


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
900
950
1000
1050
1100
1150
T / K

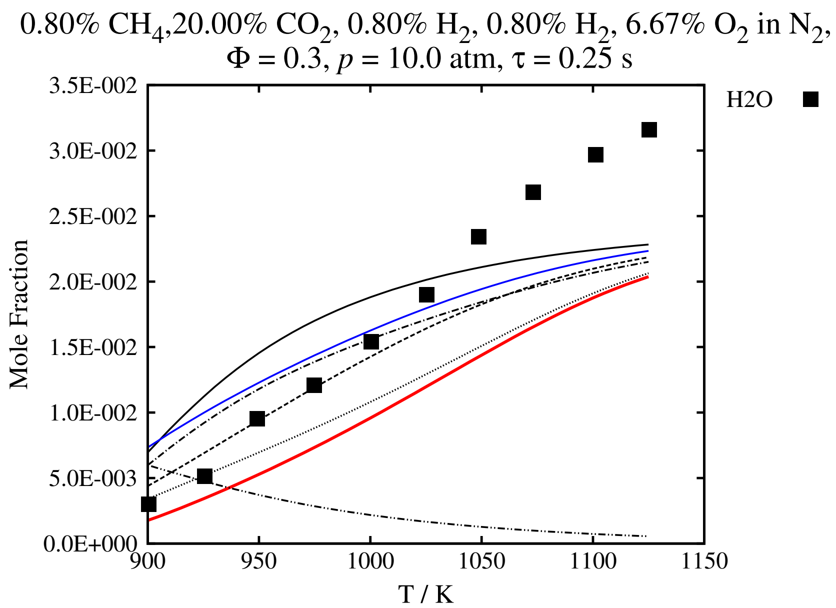
(c)


0.80% CH4,20.00% CO2, 0.80% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
900
950
1000
1050
1100
1150
T / K

(d)

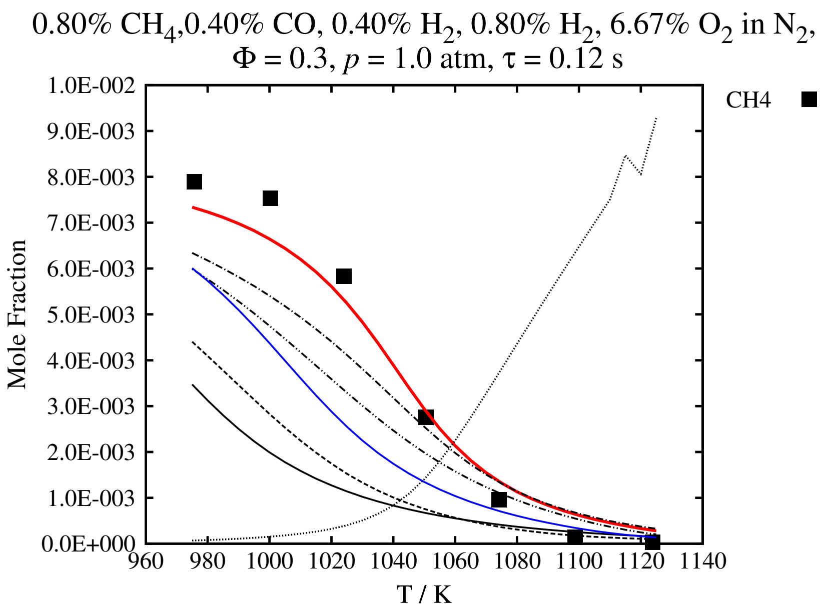


(e)

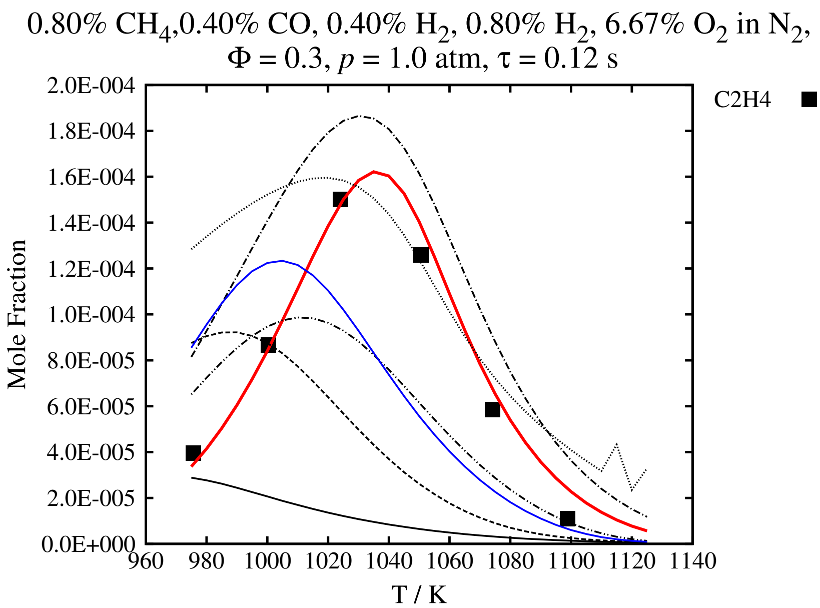


(f)

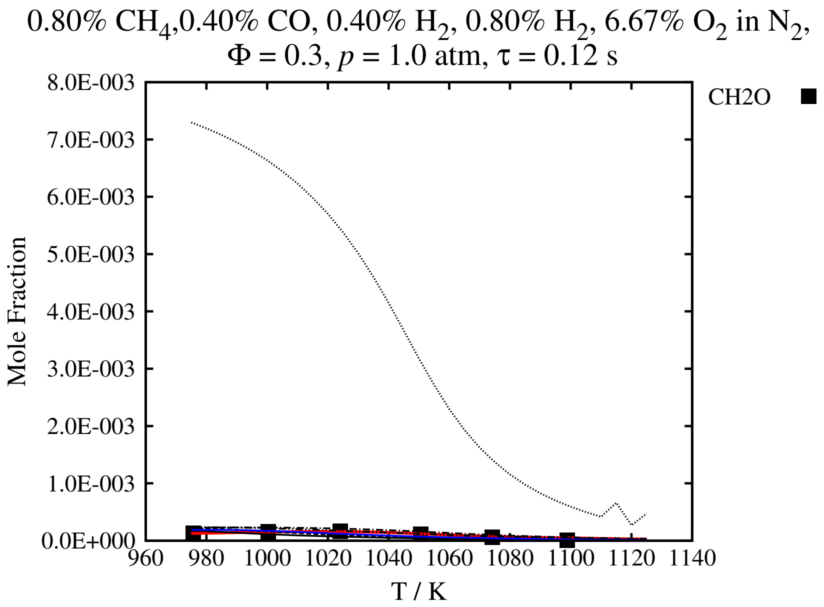
S16 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.80% CH4,0.40% CO, 0.40% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH4
Mole Fraction
T / K

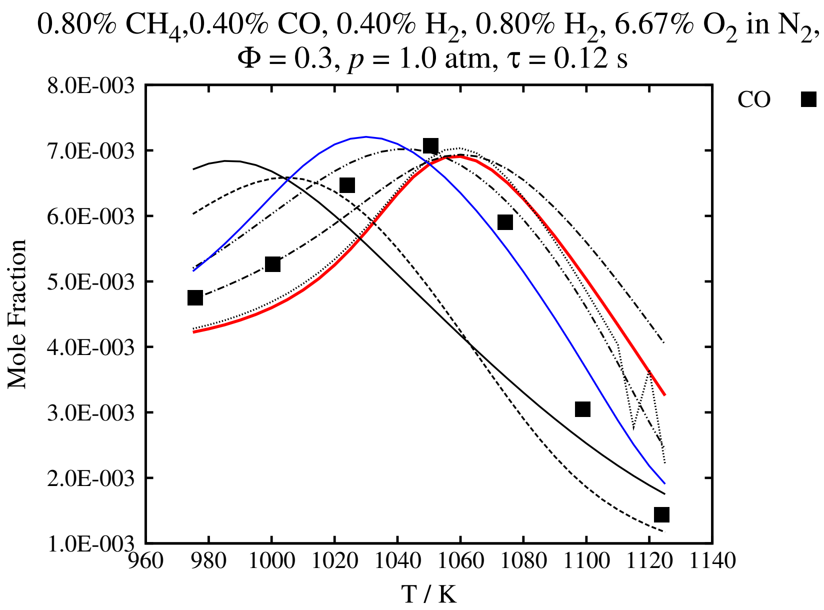
(a)


0.80% CH4,0.40% CO, 0.40% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
C2H4
Mole Fraction
T / K

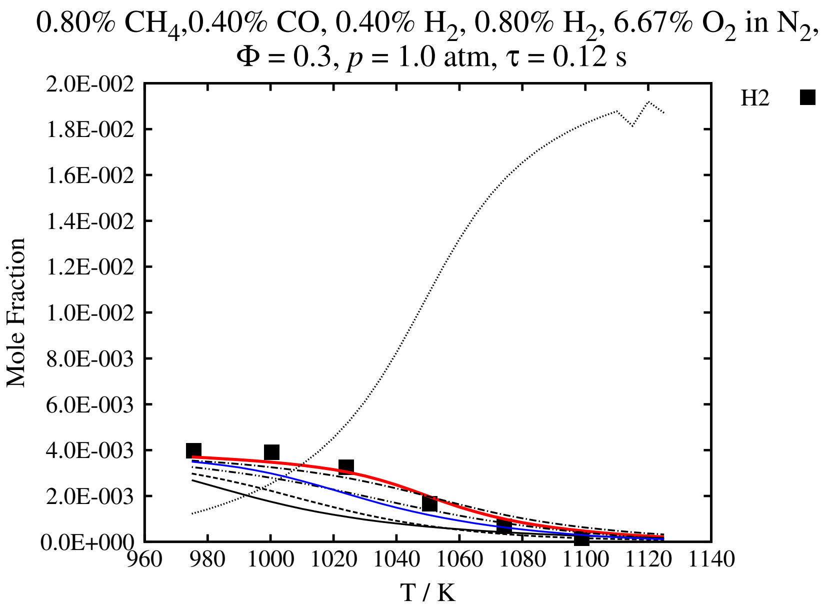
(b)


0.80% CH4,0.40% CO, 0.40% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CH2O
Mole Fraction
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
960 980 1000 1020 1040 1060 1080 1100 1120 1140
T / K

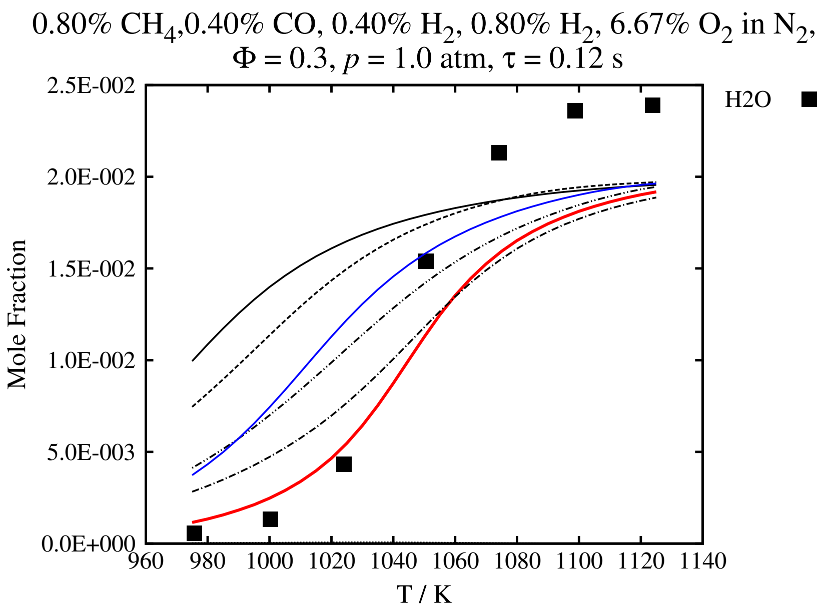
(c)


0.80% CH4,0.40% CO, 0.40% H2, 0.80% H2, 6.67% O2 in N2,
Φ = 0.3, p = 1.0 atm, τ = 0.12 s
CO
Mole Fraction
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
960 980 1000 1020 1040 1060 1080 1100 1120 1140
T / K

(d)

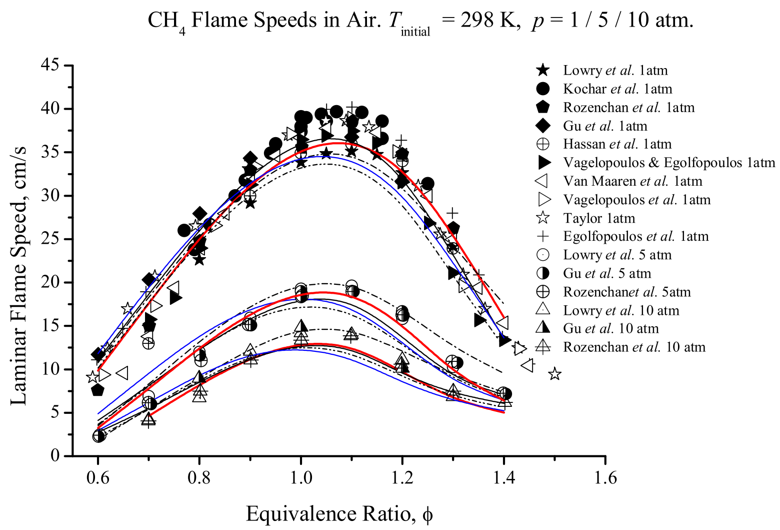


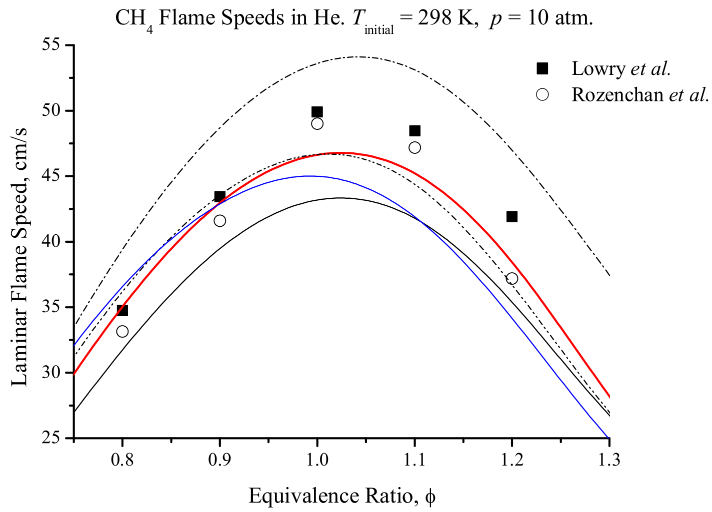
(e)



(f)

S17 Jet-stirred reactor species profiles of methane/air mixtures. Symbols are experimental data [14] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

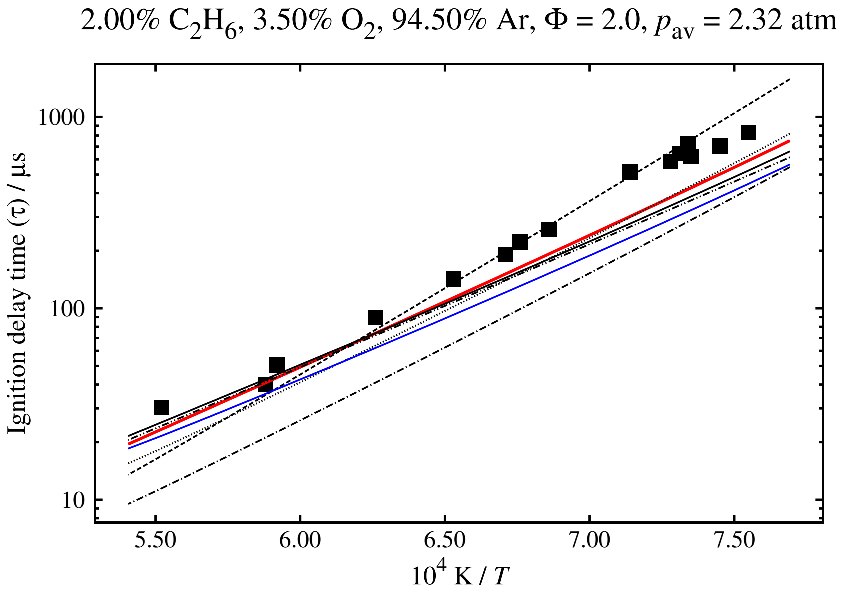




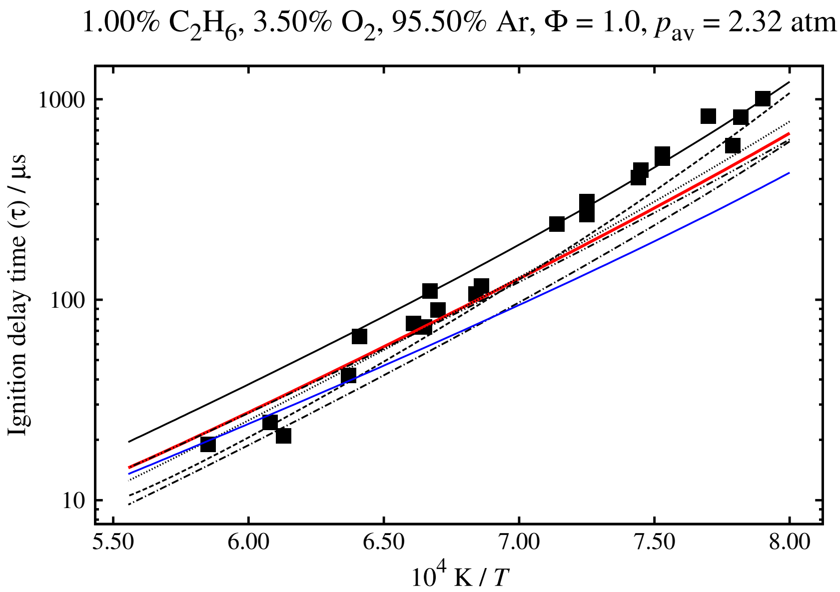
S18 Laminar flame speed measurements methane/air or methane/helium mixtures. Symbols are experimental data [15]–[24] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

2.2. *Ethane*

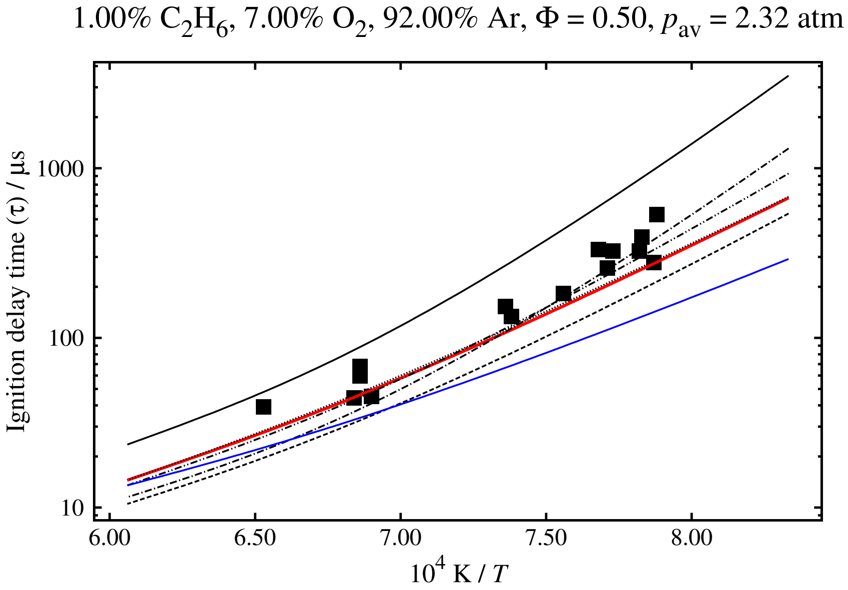
2.2.1. *Shock Tube*



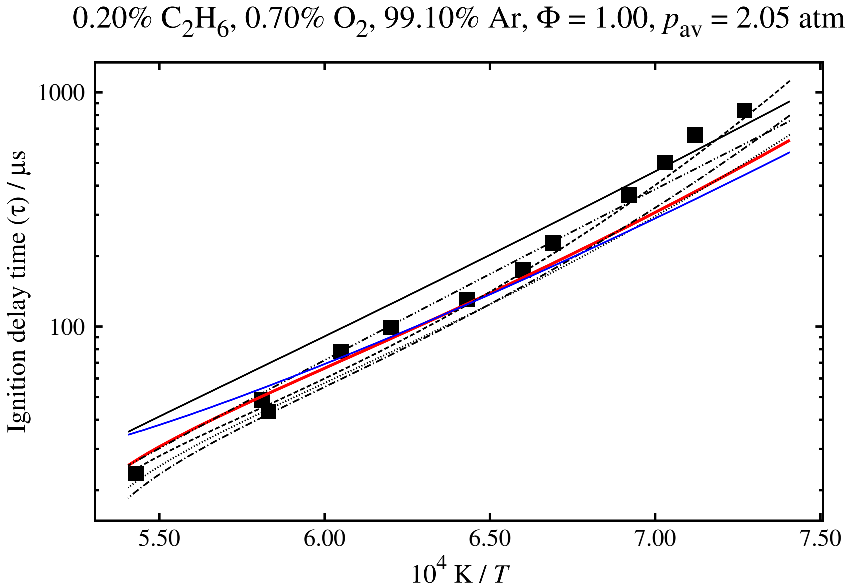
(a)



(b)

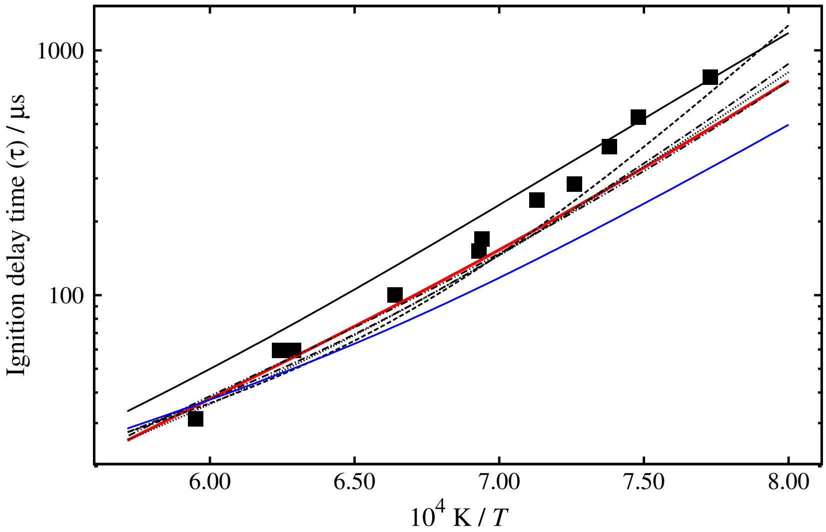

1.00% C_2H_6, 7.00% O_2, 92.00% Ar, Φ = 0.50, p_{av} = 2.32 atm
Ignition delay time (τ) / µs
1000
100
10
6.00
6.50
7.00
7.50
8.00
10^4 K / T

(c)


0.20% C_2H_6, 0.70% O_2, 99.10% Ar, Φ = 1.00, p_{av} = 2.05 atm
Ignition delay time (τ) / µs
1000
100
5.50
6.00
6.50
7.00
7.50
10^4 K / T

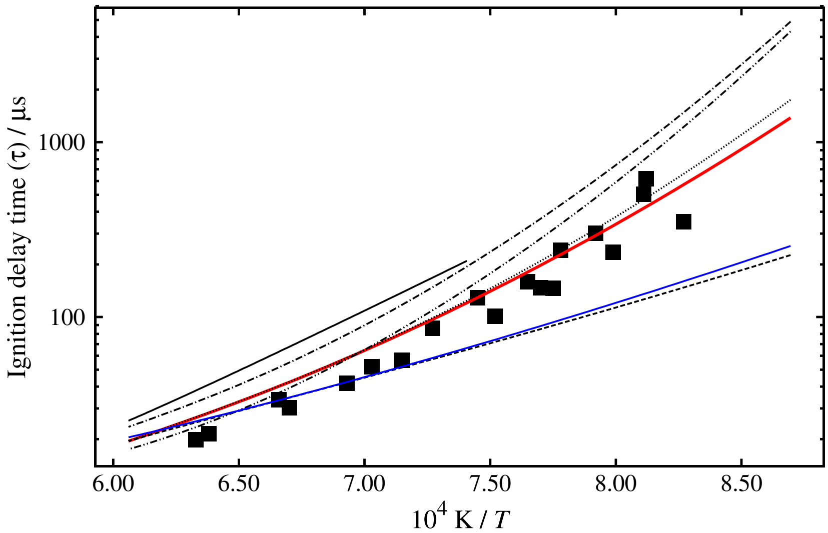
(d)

0.20% C_2H_6, 1.40% O_2, 98.40% Ar, $\Phi = 0.50$, $p_{av} = 2.05$ atm



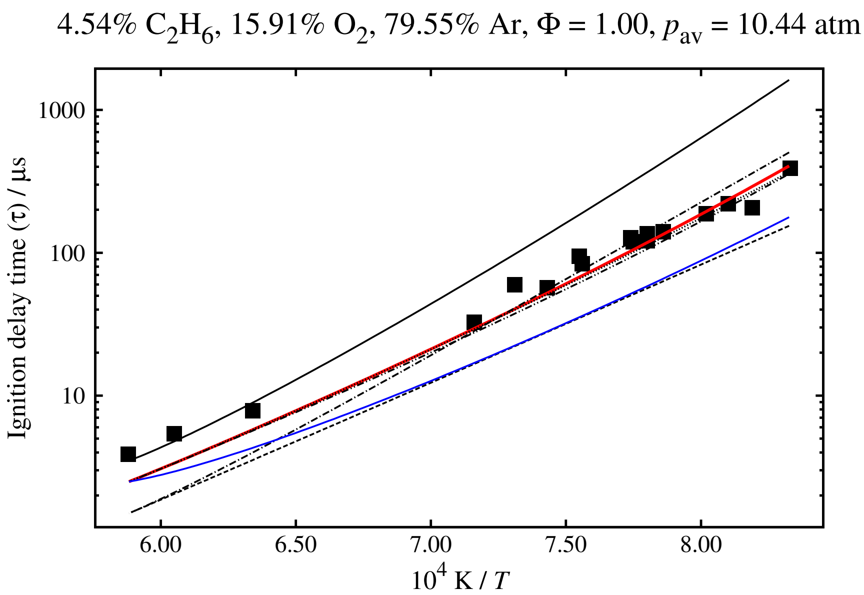
(e)

0.20% C_2H_6, 7.00% O_2, 92.80% Ar, $\Phi = 0.10$, $p_{av} = 2.05$ atm

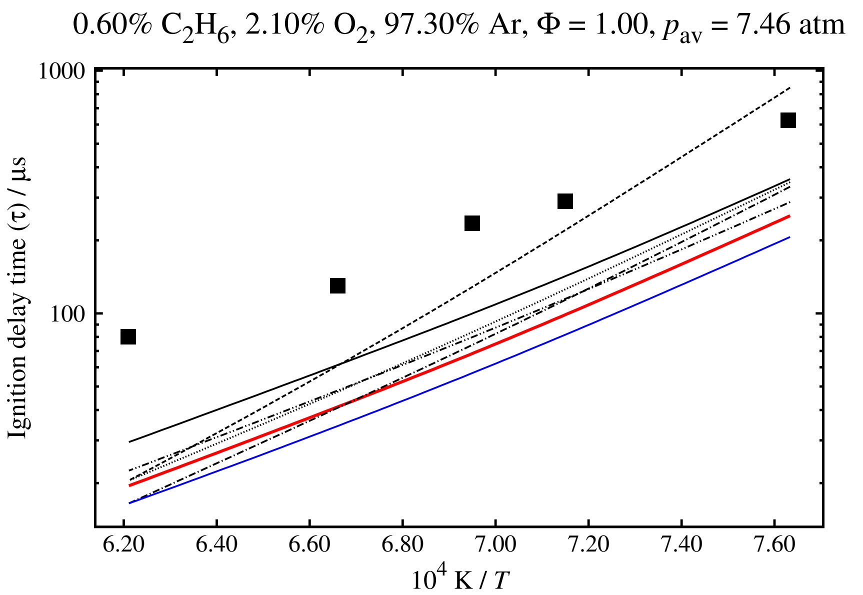


(f)

S19 Shock tube ignition delay times of ethane/oxygen/argon mixtures. Symbols are experimental data [25] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

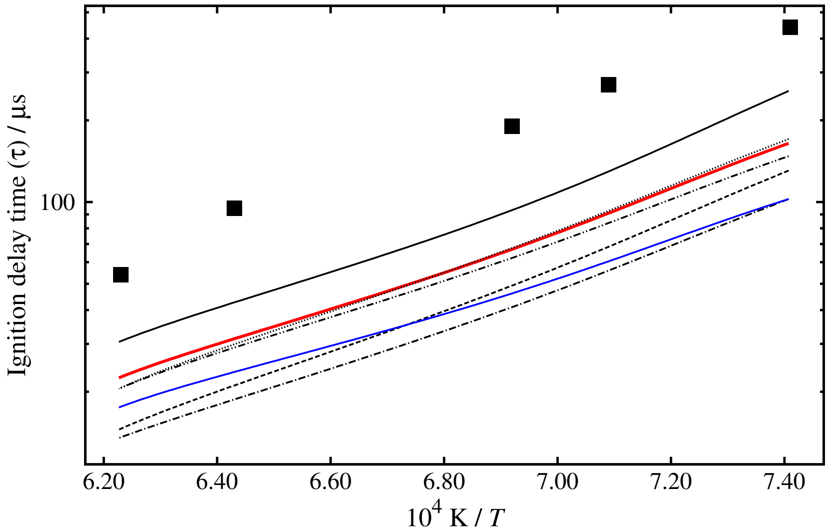

4.54% C_2H_6, 15.91% O_2, 79.55% Ar, Φ = 1.00, p_{av} = 10.44 atm
Ignition delay time (τ) / μs
1000
100
10
6.00
6.50
7.00
7.50
8.00
10^4 K / T

(a)


0.60% C_2H_6, 2.10% O_2, 97.30% Ar, Φ = 1.00, p_{av} = 7.46 atm
Ignition delay time (τ) / μs
1000
100
6.20
6.40
6.60
6.80
7.00
7.20
7.40
7.60
10^4 K / T

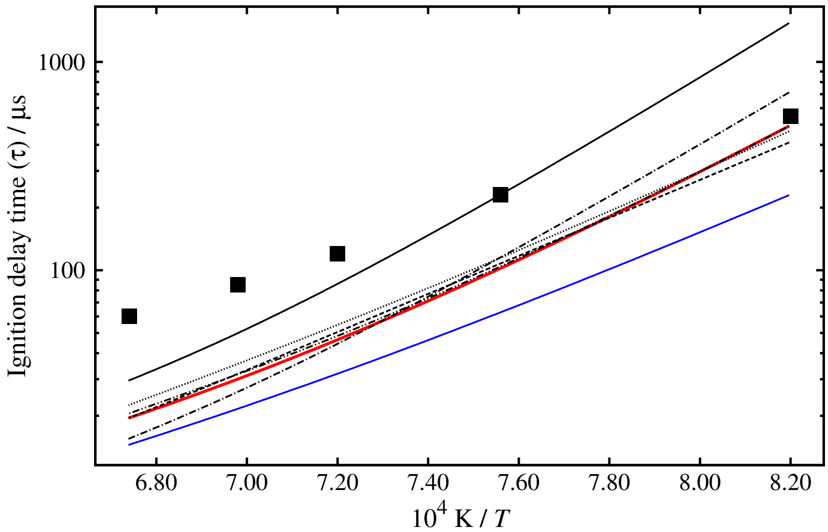
(b)

2.00% C_2H_6, 7.00% O_2, 97.30% Ar, Φ = 1.00, p_{av} = 2.29 atm



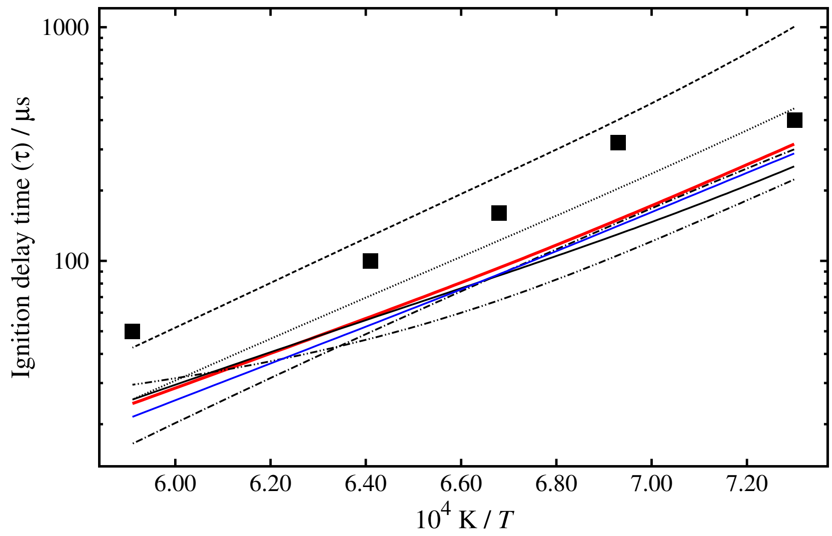
(c)

2.00% C_2H_6, 7.00% O_2, 97.30% Ar, Φ = 1.00, p_{av} = 7.72 atm



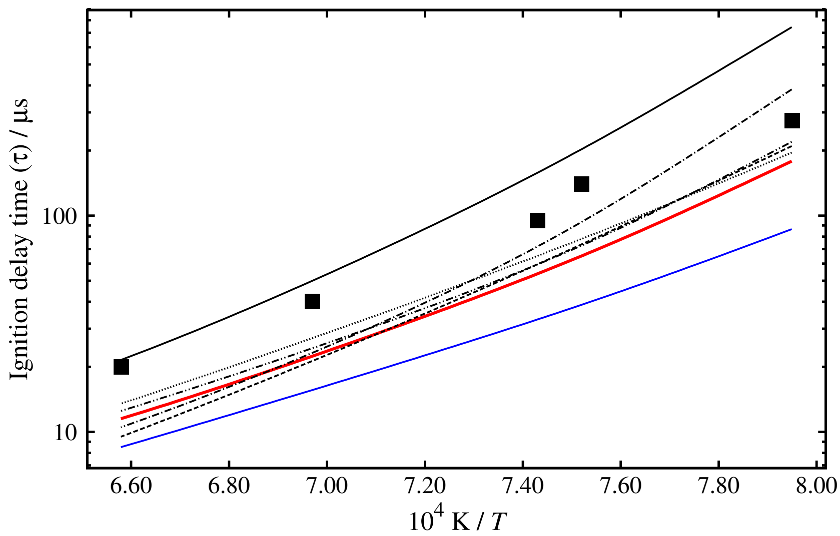
(d)

1.06% C_2H_6, 1.85% O_2, 97.09% Ar, Φ = 2.00, p_{av} = 7.63 atm

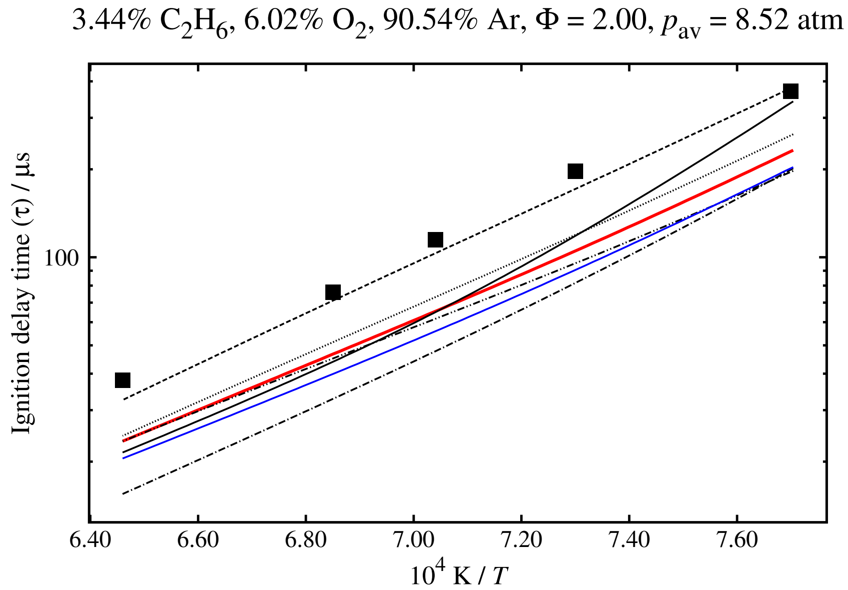


(e)

1.00% C_2H_6, 7.00% O_2, 92.00% Ar, Φ = 0.50, p_{av} = 7.10 atm

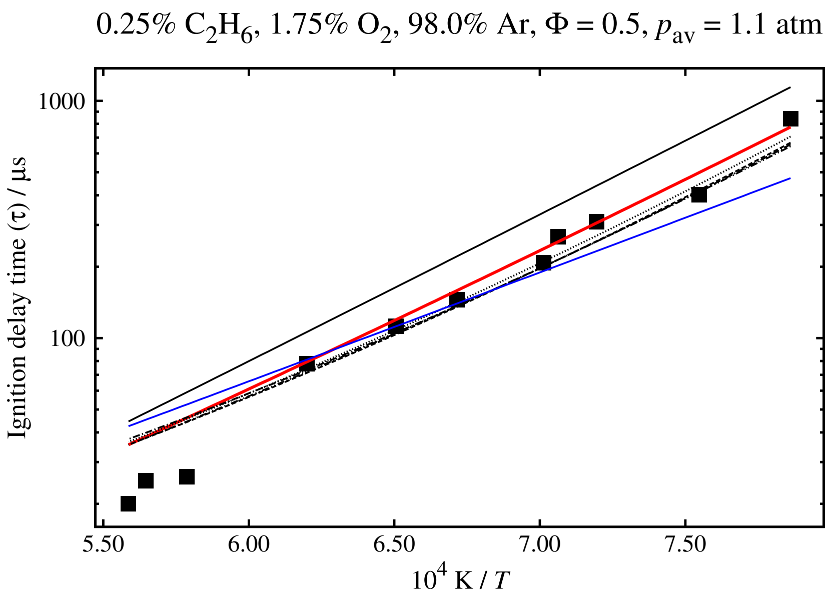


(f)

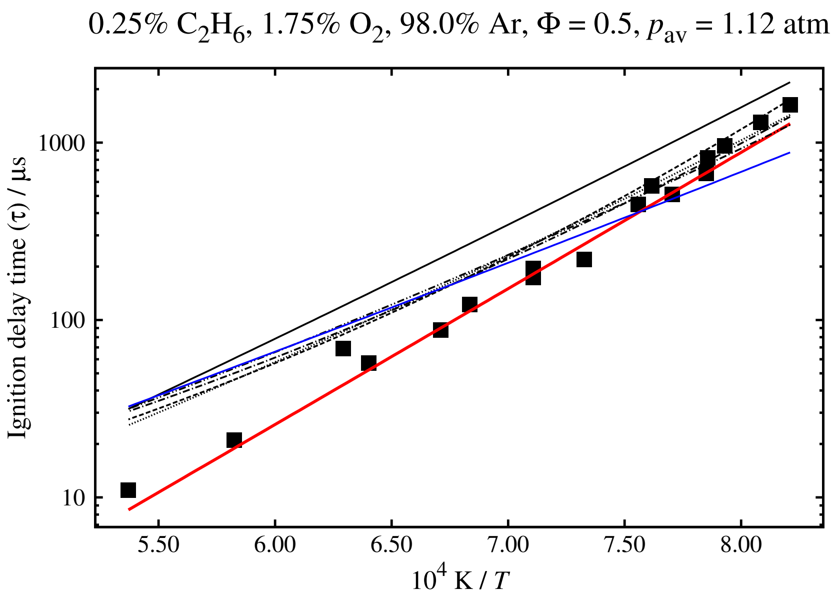


(g)

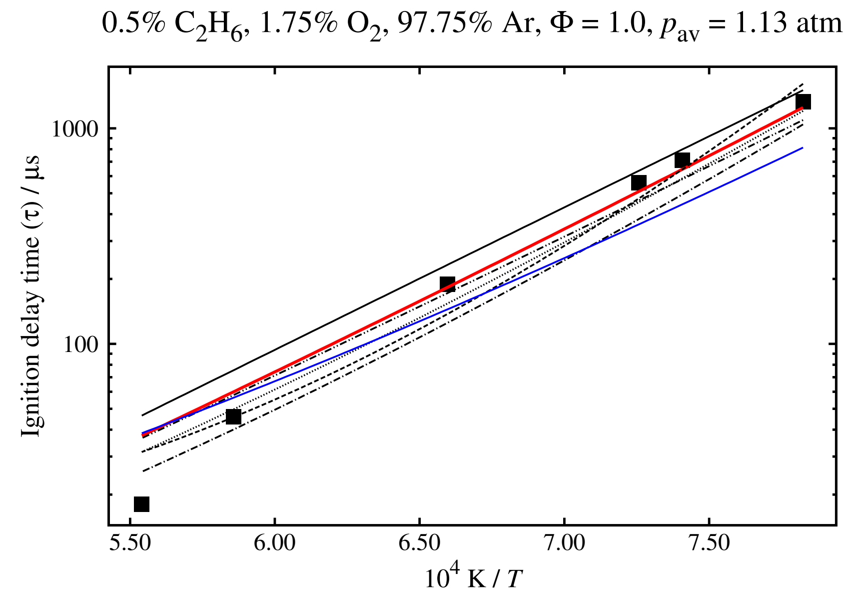
S20 Shock tube ignition delay times of ethane/oxygen/argon mixtures. Symbols are experimental data [26] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.25% C_2H_6, 1.75% O_2, 98.0% Ar, Φ = 0.5, p_{av} = 1.1 atm
Ignition delay time (τ) / μs
1000
100
5.50
6.00
6.50
7.00
7.50
10^4 K / T

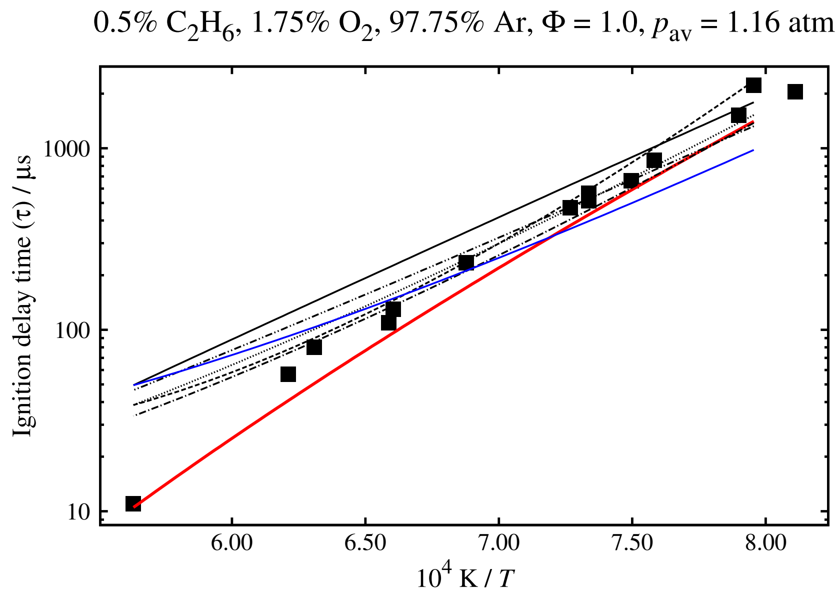
(a)


0.25% C_2H_6, 1.75% O_2, 98.0% Ar, Φ = 0.5, p_{av} = 1.12 atm
Ignition delay time (τ) / μs
1000
100
10
5.50
6.00
6.50
7.00
7.50
8.00
10^4 K / T

(b)

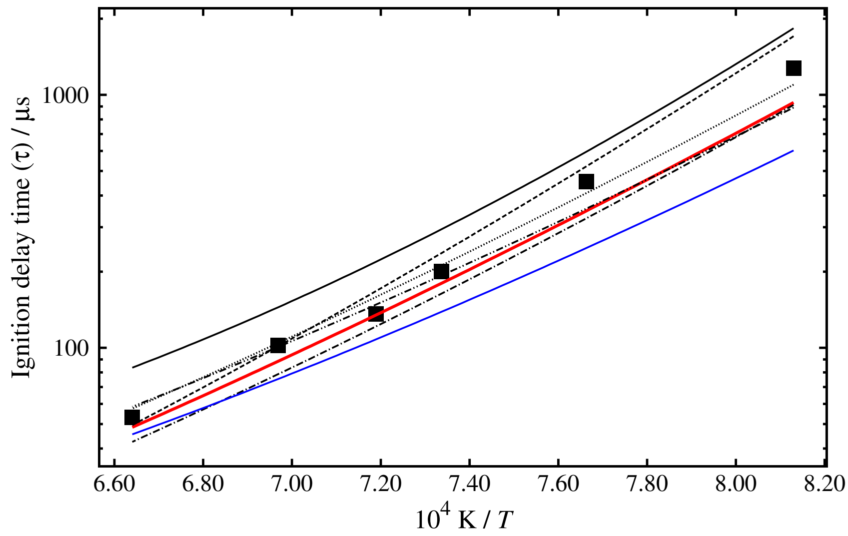

0.5% C2H6, 1.75% O2, 97.75% Ar, Φ = 1.0, pav = 1.13 atm
Ignition delay time (τ) / µs
1000
100
5.50
6.00
6.50
7.00
7.50
10^4 K / T

(c)


0.5% C2H6, 1.75% O2, 97.75% Ar, Φ = 1.0, pav = 1.16 atm
Ignition delay time (τ) / µs
1000
100
10
6.00
6.50
7.00
7.50
8.00
10^4 K / T

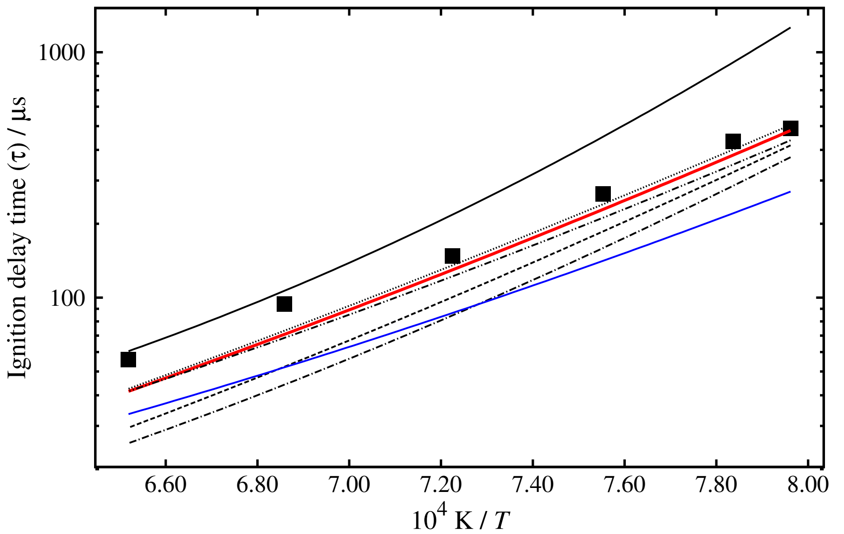
(d)

0.93% C_2H_6, 3.24% O_2, 95.83% Ar, Φ = 1.0, p_{av} = 2.67 atm

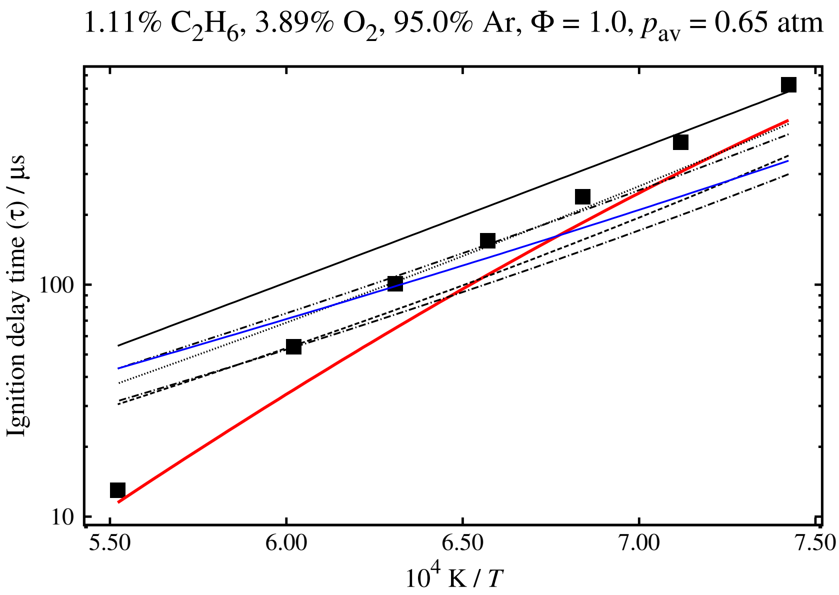


(e)

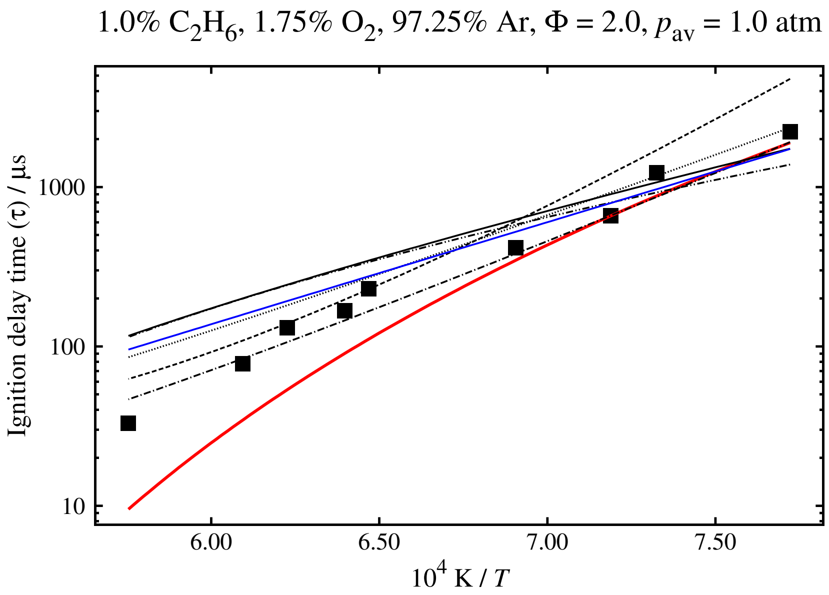
2.0% C_2H_6, 7.0% O_2, 91.0% Ar, Φ = 1.0, p_{av} = 1.89 atm



(f)

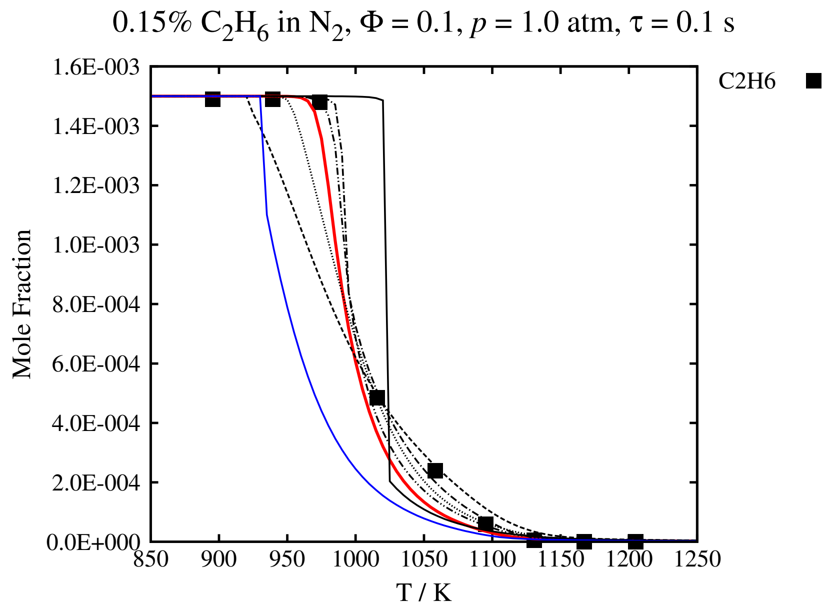


(g)

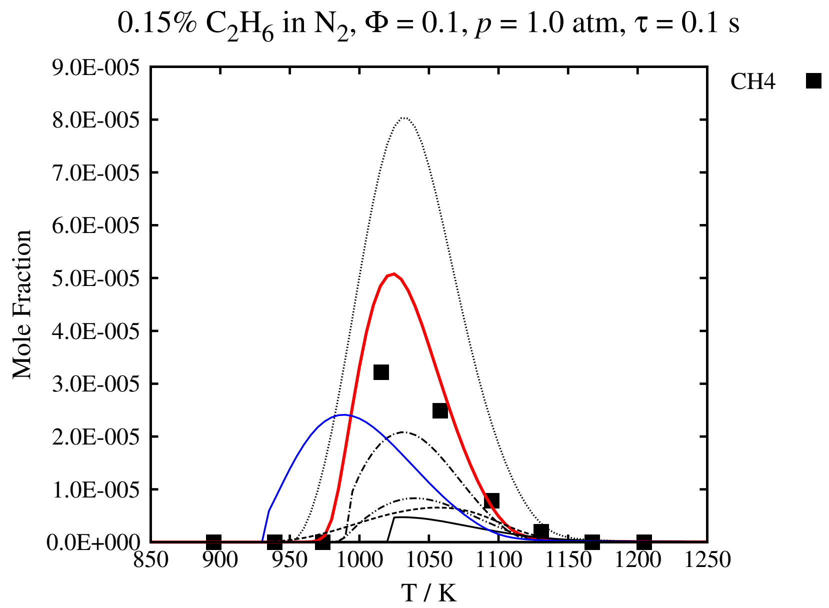


(h)

S21 Shock tube ignition delay times of ethane/oxygen/argon mixtures. Symbols are experimental data [27] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, — USC II.

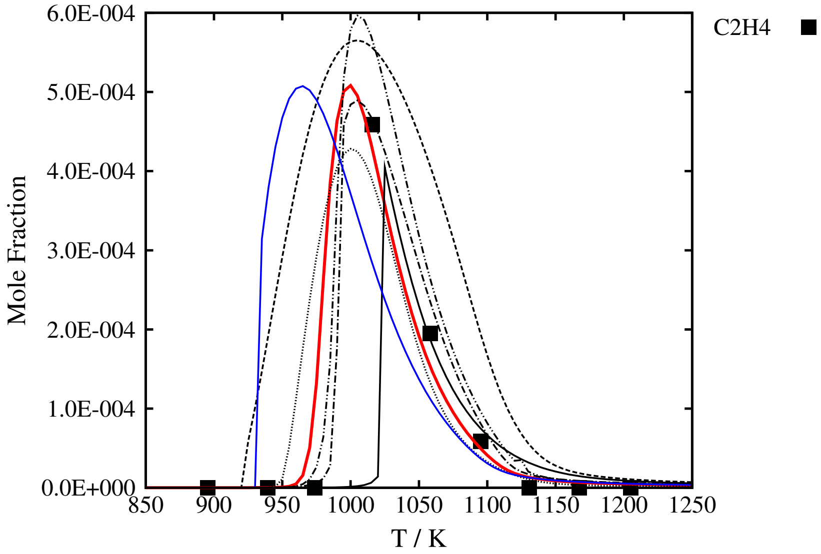

0.15% C_2H_6 in N_2, Φ = 0.1, p = 1.0 atm, τ = 0.1 s
C2H6
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

(a)


0.15% C_2H_6 in N_2, Φ = 0.1, p = 1.0 atm, τ = 0.1 s
CH4
Mole Fraction
9.0E-005
8.0E-005
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

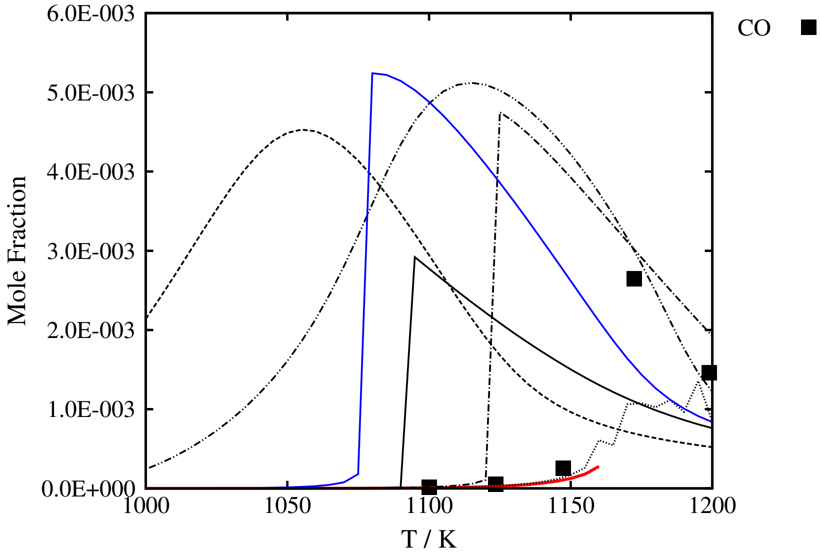
(b)

0.15% C_2H_6 in N_2, $\Phi = 0.1$, $p = 1.0$ atm, $\tau = 0.1$ s

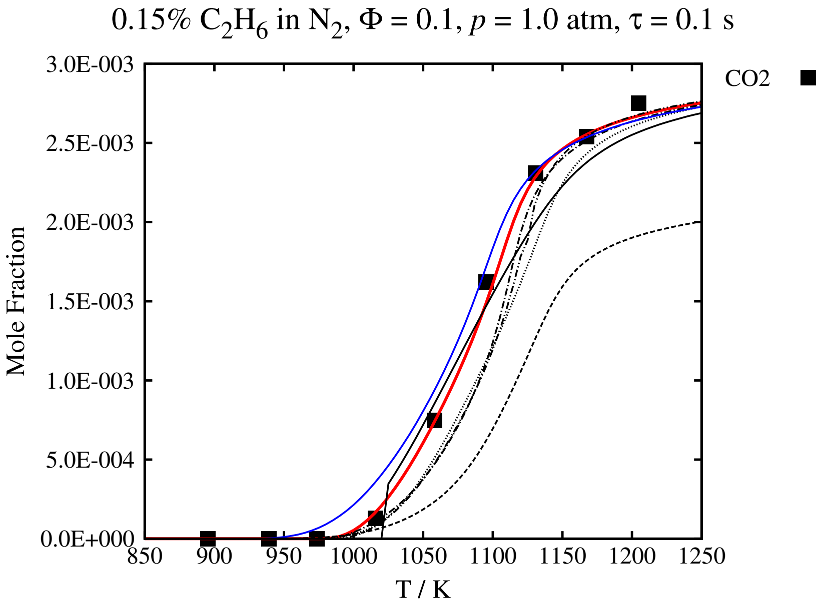


(c)

1.0% CH_4, 6.67% O_2 in N_2, $\Phi = 0.3$, $p = 1.0$ atm, $\tau = 0.12$ s

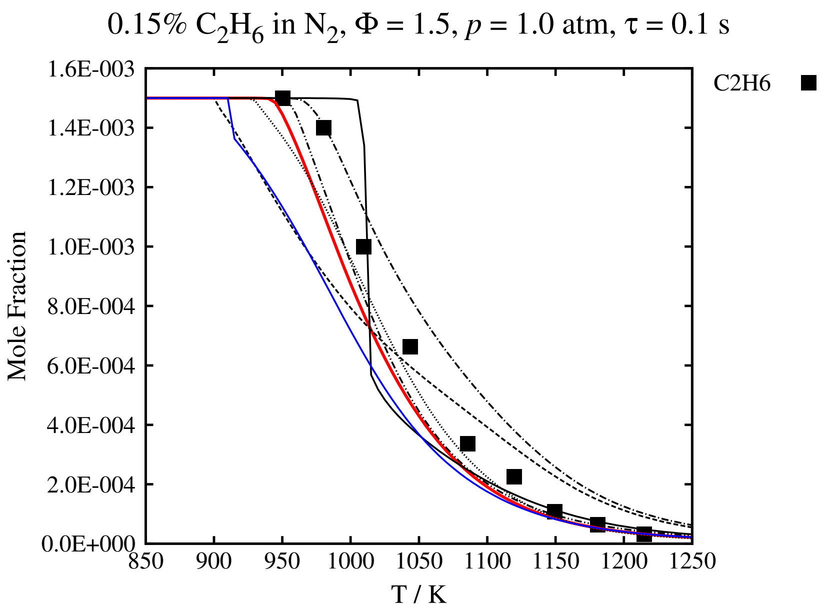


(d)

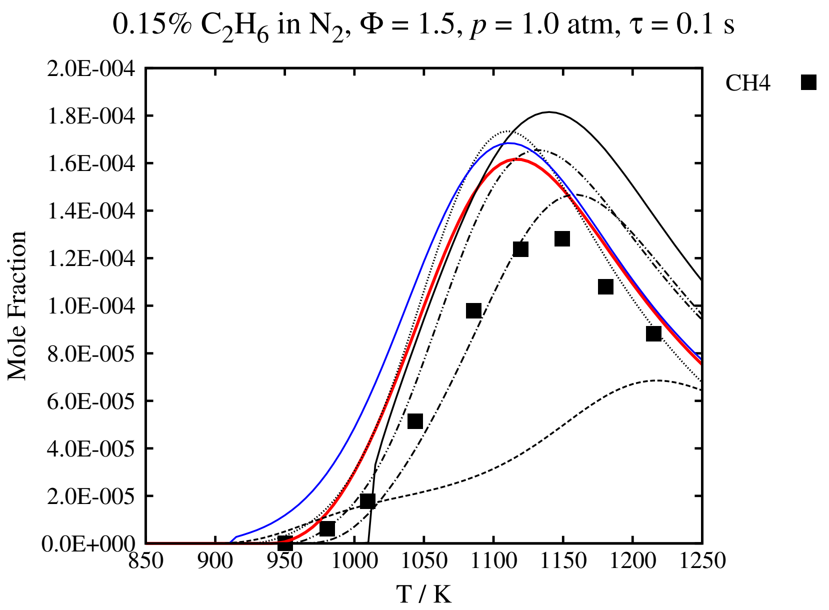


(e)

S22 Jet-stirred reactor species profiles of methane/oxygen/nitrogen mixtures. Symbols are experimental data [28] lines are model predictions. —— AramcoMech 1.3, —— GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, —— USC II.

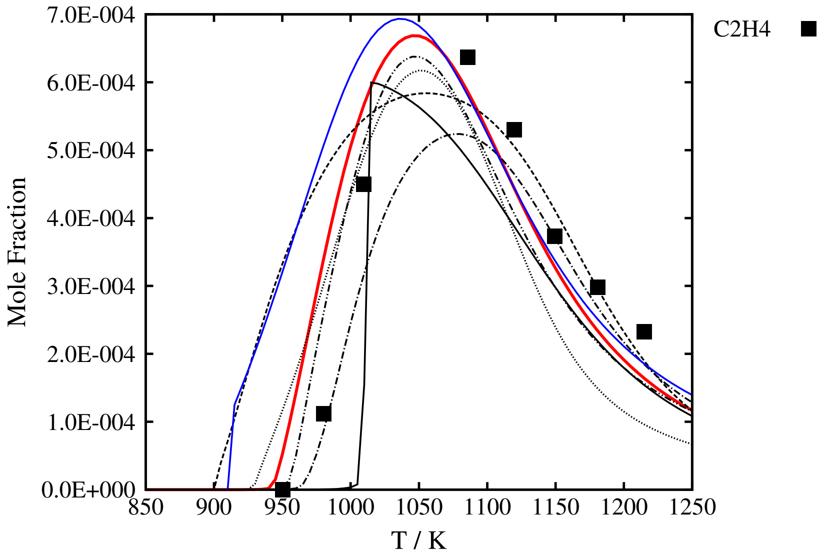

0.15% C2H6 in N2, Φ = 1.5, p = 1.0 atm, τ = 0.1 s
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K
C2H6

(a)


0.15% C2H6 in N2, Φ = 1.5, p = 1.0 atm, τ = 0.1 s
Mole Fraction
2.0E-004
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K
CH4

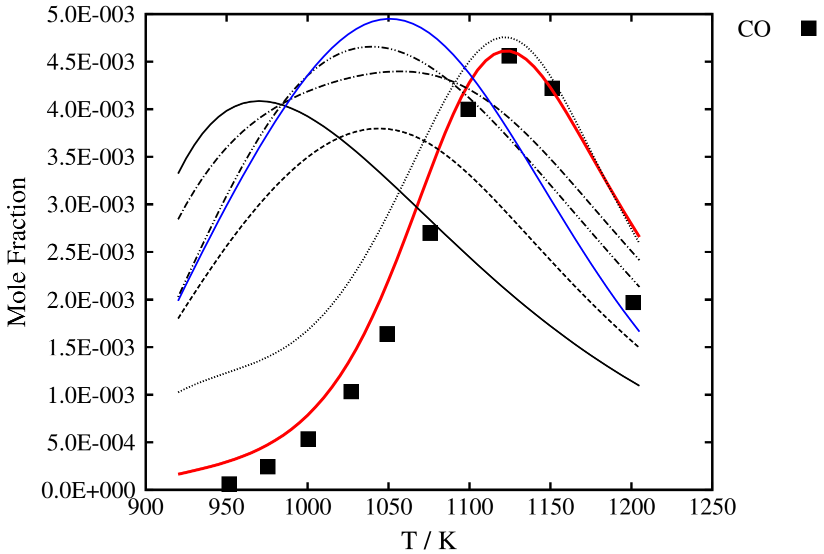
(b)

0.15% C_2H_6 in N_2, Φ = 1.5, p = 1.0 atm, τ = 0.1 s

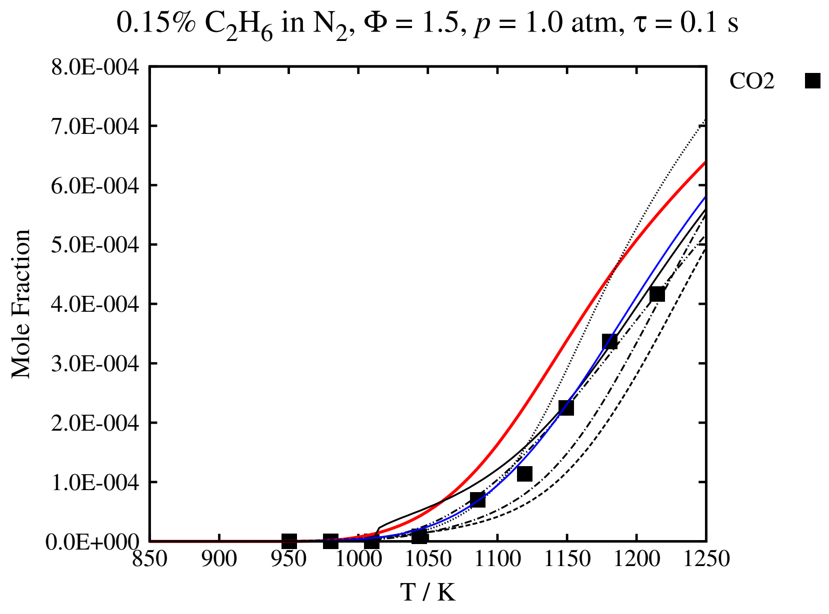


(c)

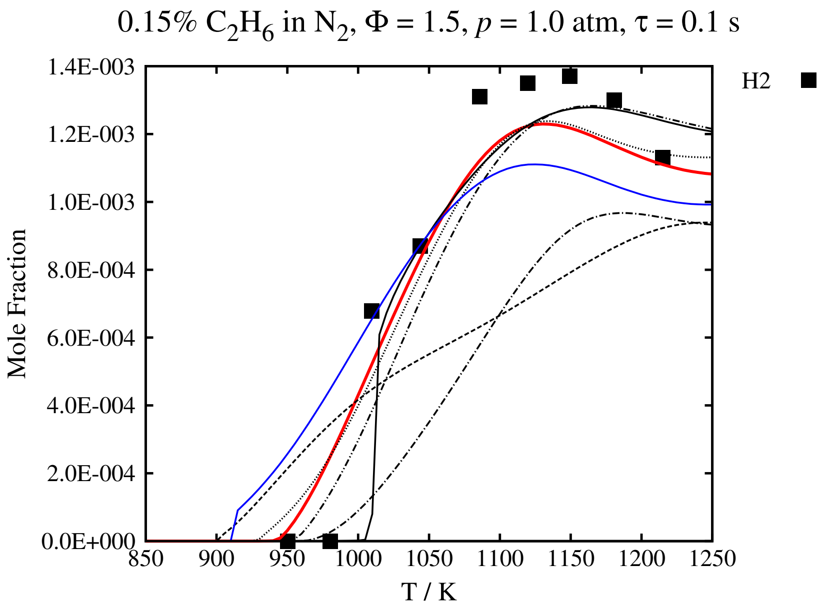
1.0% CH_4, 6.67% O_2 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s



(d)

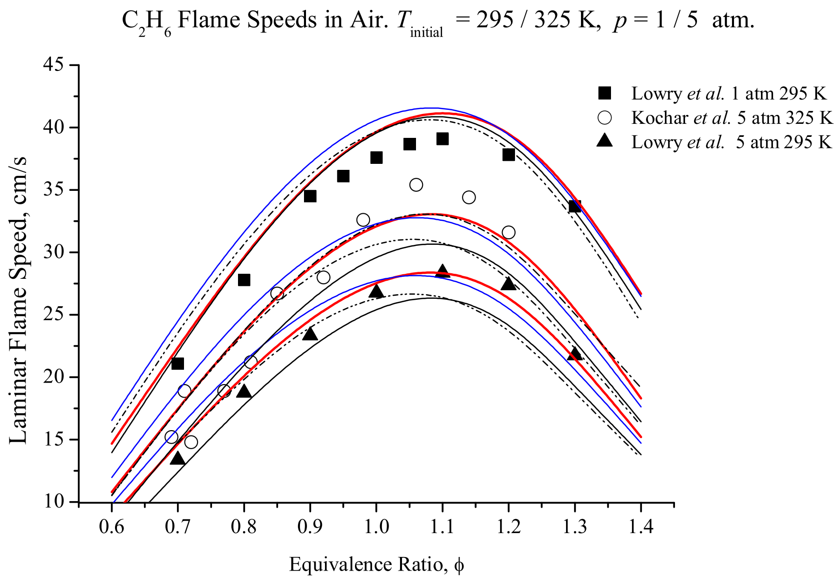


(e)



(f)

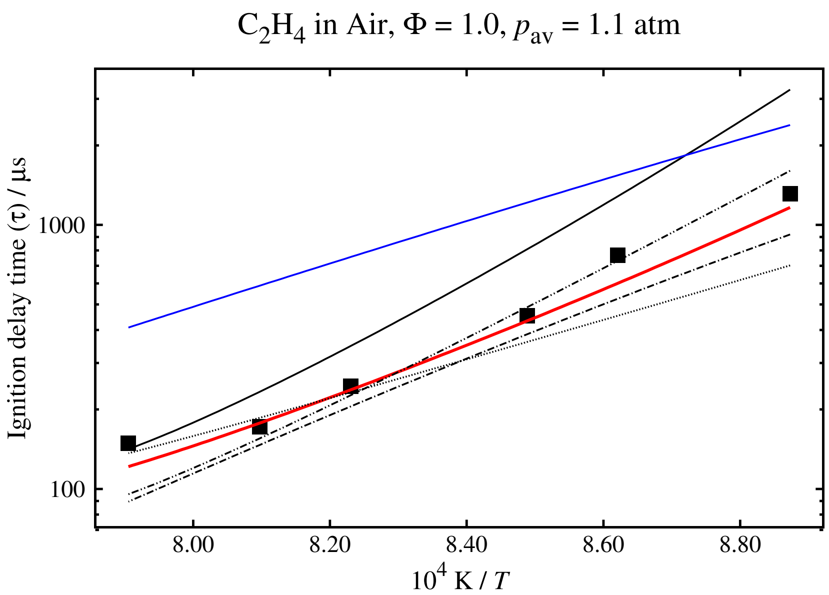
S23 Jet-stirred reactor species profiles of methane/oxygen/nitrogen mixtures. Symbols are experimental data [28] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



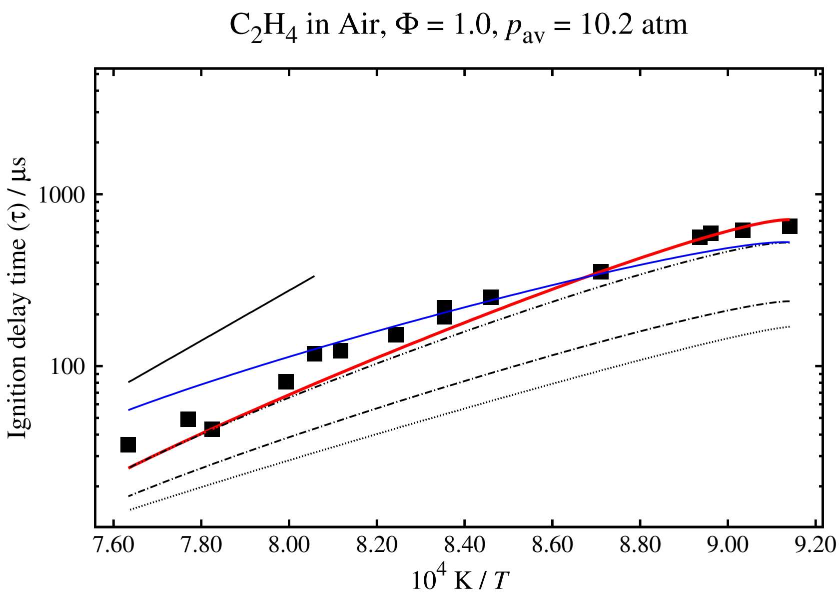
S24 Laminar flame speed measurements ethane/air mixtures. Symbols are experimental data [15, 16] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

2.3. Ethylene

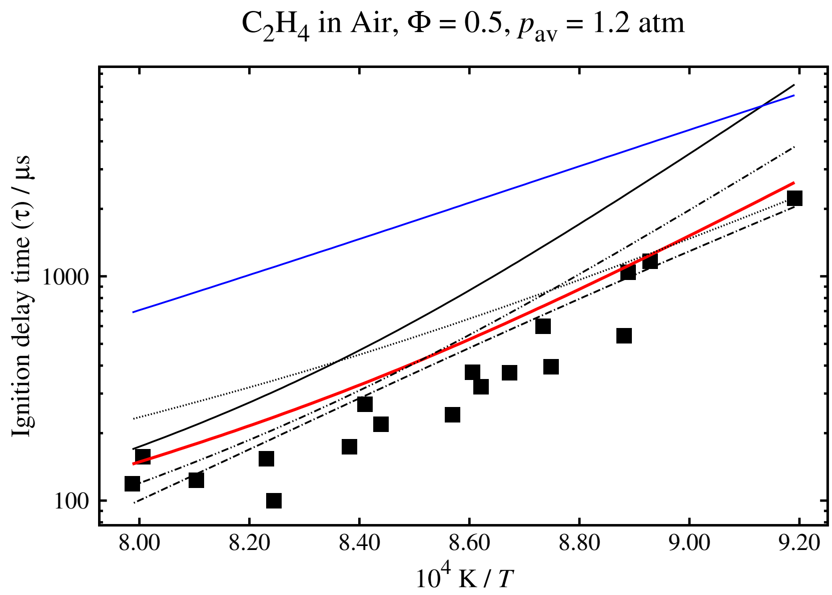
2.3.1. Shock Tube



(a)

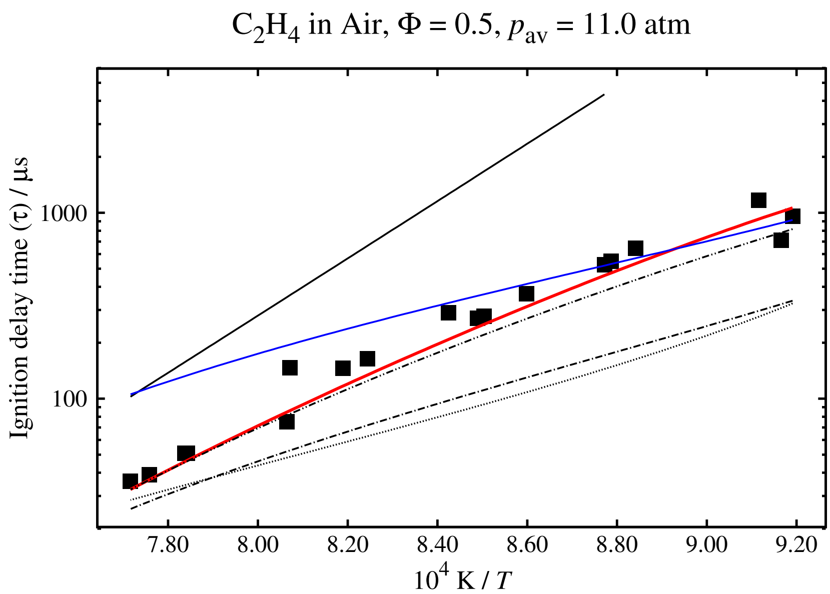


(b)



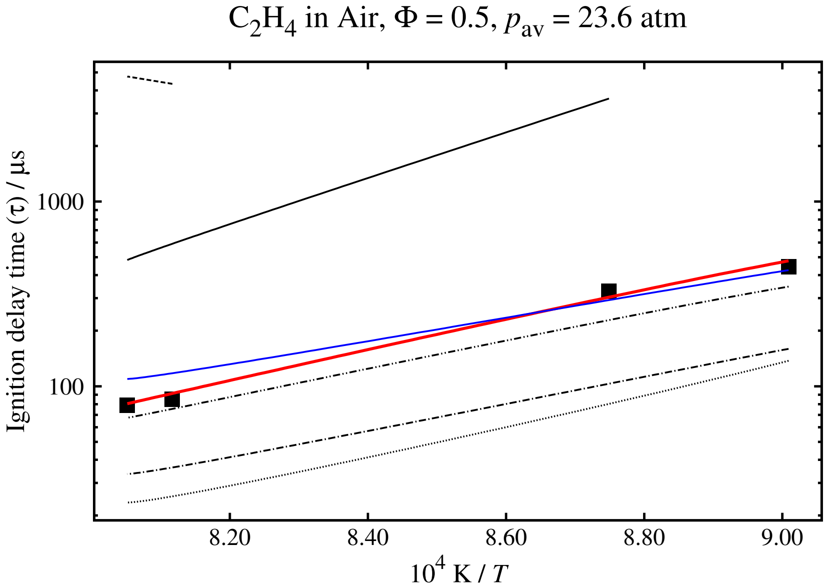
C_2H_4 in Air, $\Phi = 0.5$, $p_{av} = 1.2$ atm
Ignition delay time (τ) / μs
1000
100
8.00
8.20
8.40
8.60
8.80
9.00
9.20
10^4 K / T

(c)

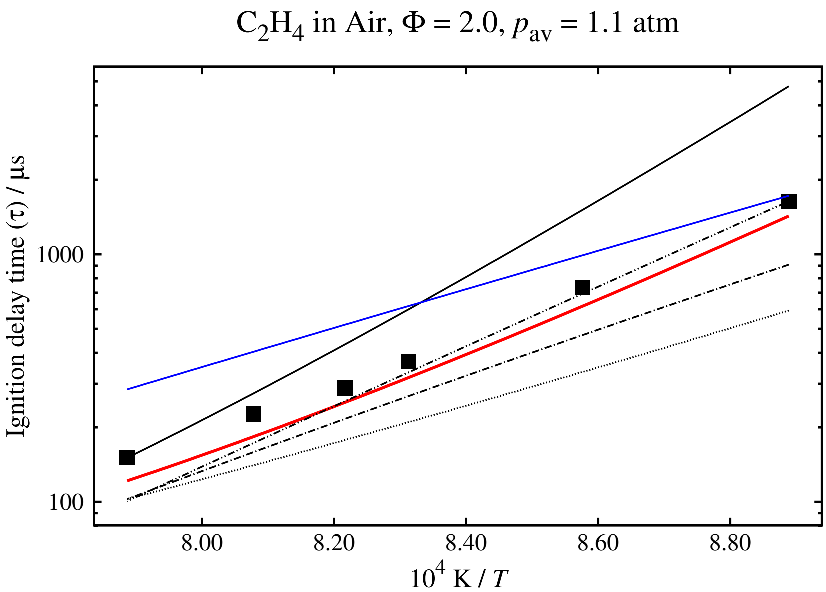


C_2H_4 in Air, $\Phi = 0.5$, $p_{av} = 11.0$ atm
Ignition delay time (τ) / μs
1000
100
7.80
8.00
8.20
8.40
8.60
8.80
9.00
9.20
10^4 K / T

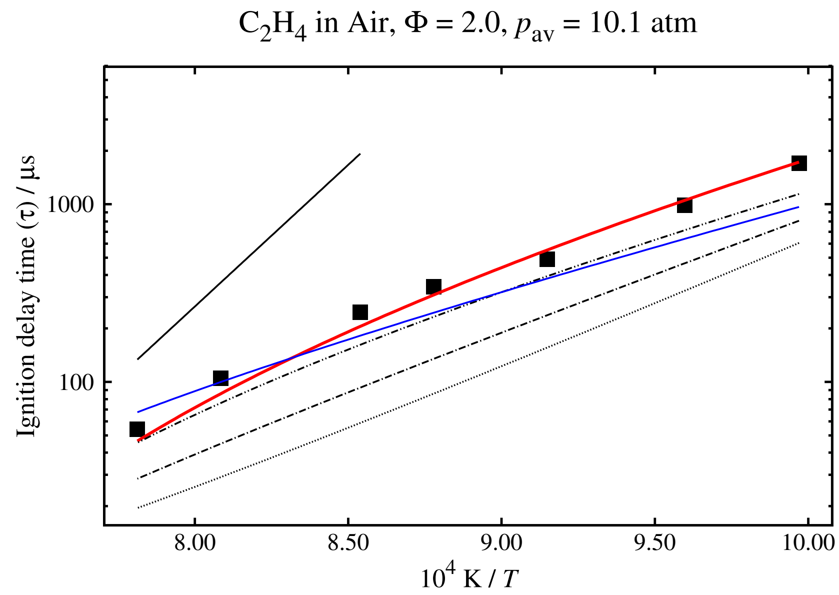
(d)


C2H4 in Air, Φ = 0.5, pav = 23.6 atm
Ignition delay time (τ) / µs
1000
100
8.20
8.40
8.60
8.80
9.00
10^4 K / T

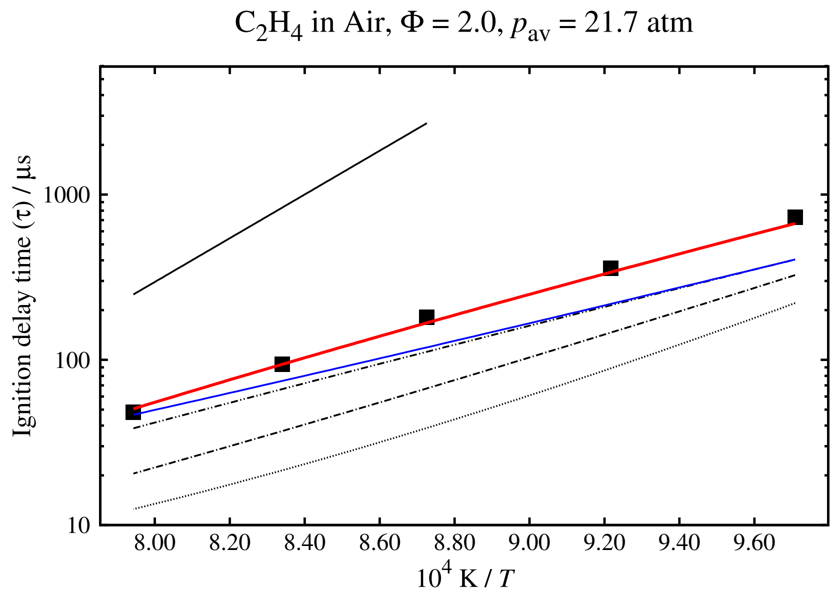
(e)


C2H4 in Air, Φ = 2.0, pav = 1.1 atm
Ignition delay time (τ) / µs
1000
100
8.00
8.20
8.40
8.60
8.80
10^4 K / T

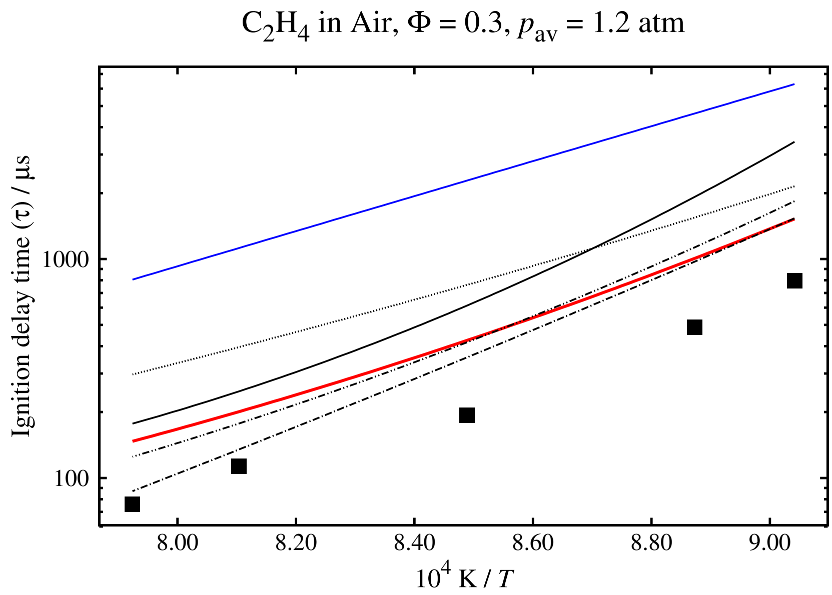
(f)


C2H4 in Air, Φ = 2.0, pav = 10.1 atm
Ignition delay time (τ) / μs
1000
100
8.00
8.50
9.00
9.50
10.00
10^4 K / T

(g)

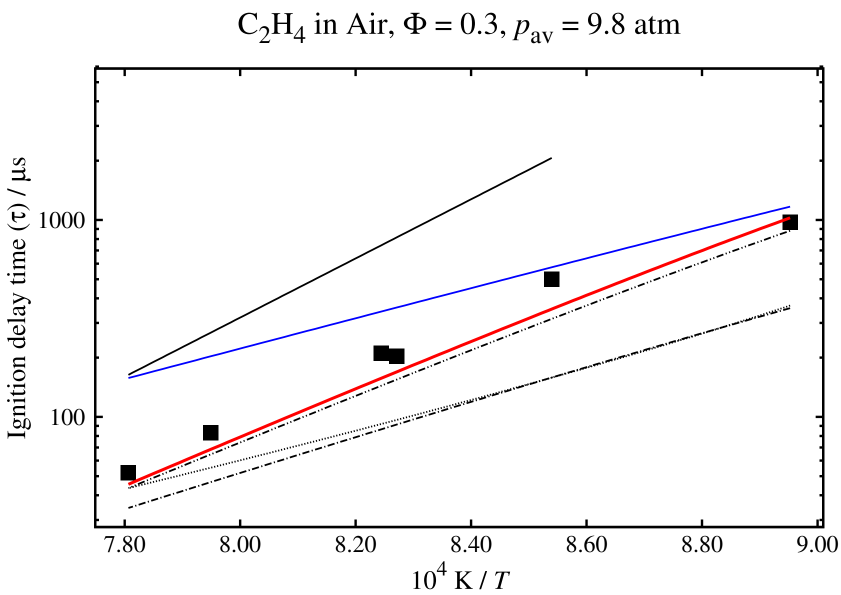

C2H4 in Air, Φ = 2.0, pav = 21.7 atm
Ignition delay time (τ) / μs
1000
100
10
8.00
8.20
8.40
8.60
8.80
9.00
9.20
9.40
9.60
10^4 K / T

(h)



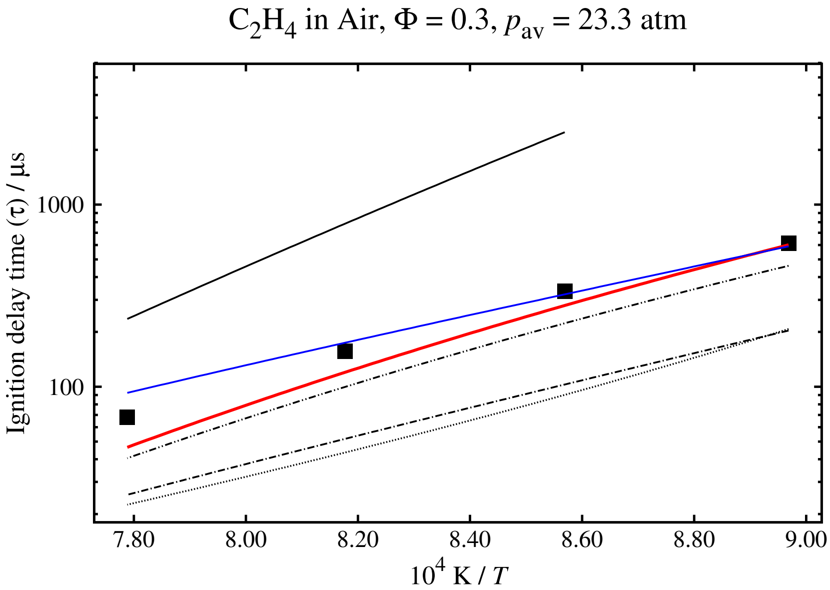
C_2H_4 in Air, $\Phi = 0.3$, $p_{av} = 1.2$ atm
Ignition delay time (τ) / µs
1000
100
8.00
8.20
8.40
8.60
8.80
9.00
10^4 K / T

(i)



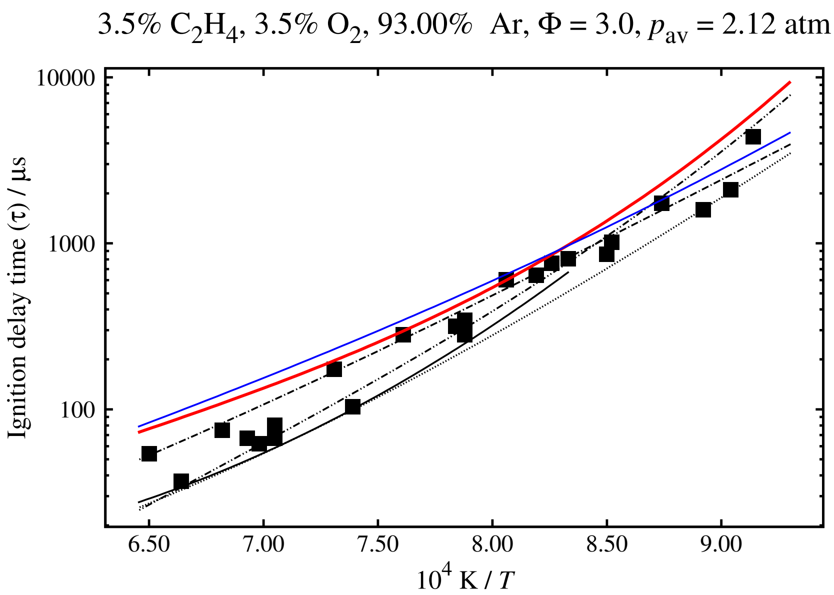
C_2H_4 in Air, $\Phi = 0.3$, $p_{av} = 9.8$ atm
Ignition delay time (τ) / µs
1000
100
7.80
8.00
8.20
8.40
8.60
8.80
9.00
10^4 K / T

(j)

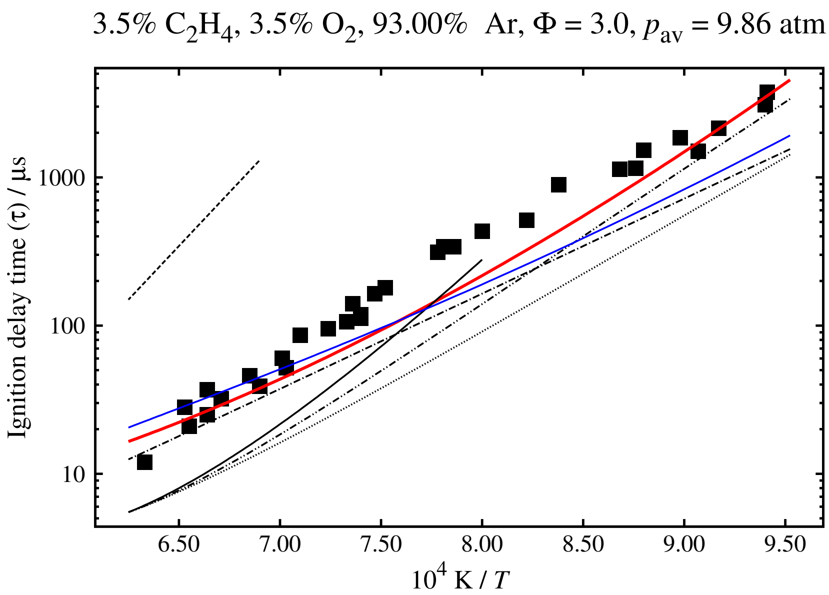


(k)

S25 Shock tube ignition delay times of ethylene/air mixtures. Symbols are experimental data [29] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

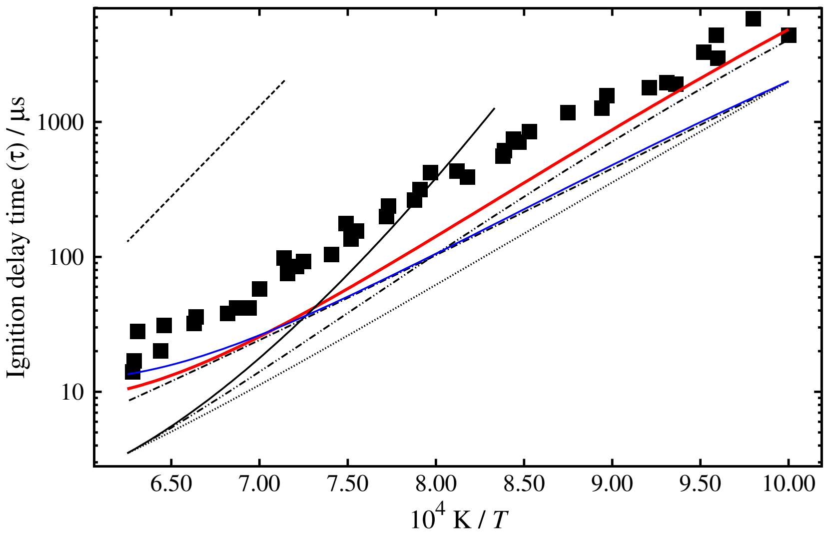

3.5% C2H4, 3.5% O2, 93.00% Ar, Φ = 3.0, pav = 2.12 atm
Ignition delay time (τ) / µs
10000
1000
100
6.50
7.00
7.50
8.00
8.50
9.00
10^4 K / T

(a)


3.5% C2H4, 3.5% O2, 93.00% Ar, Φ = 3.0, pav = 9.86 atm
Ignition delay time (τ) / µs
1000
100
10
6.50
7.00
7.50
8.00
8.50
9.00
9.50
10^4 K / T

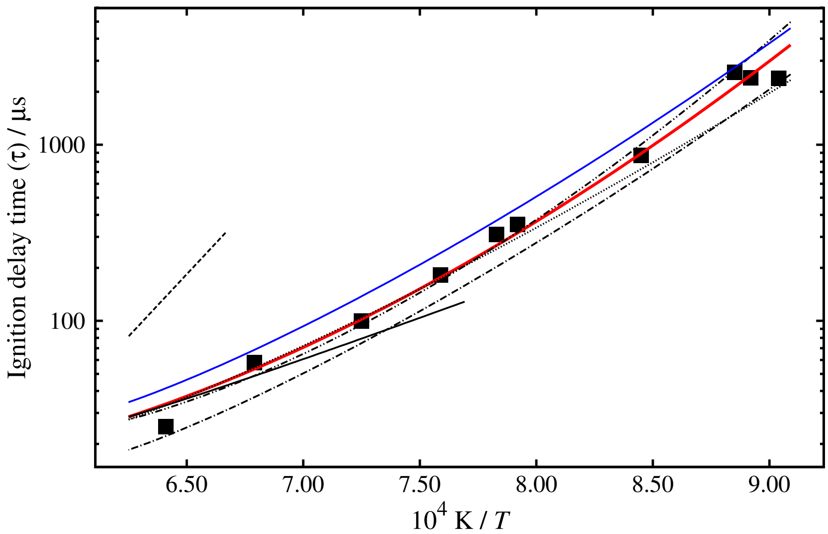
(b)

3.5% C_2H_4, 3.5% O_2, 93.00% Ar, Φ = 3.0, p_{av} = 18.03 atm



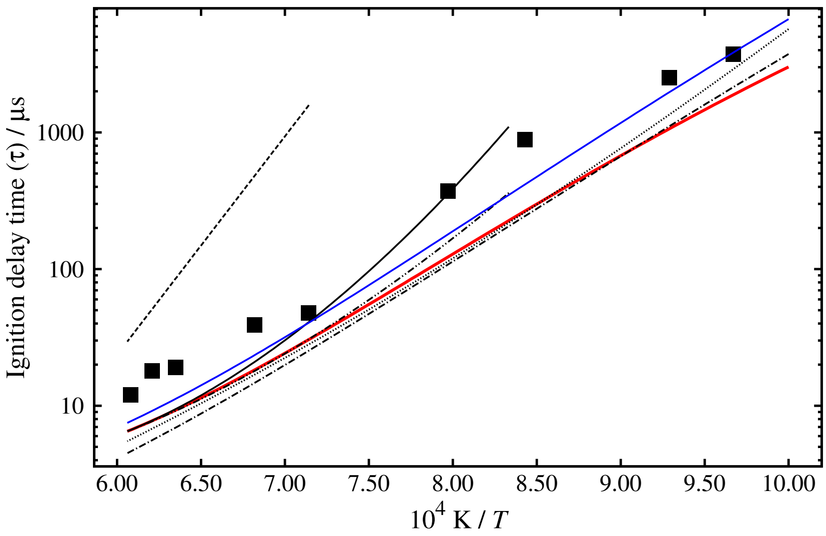
(c)

1.75% C_2H_4, 5.25% O_2, 93.00% Ar, Φ = 1.0, p_{av} = 2.13 atm



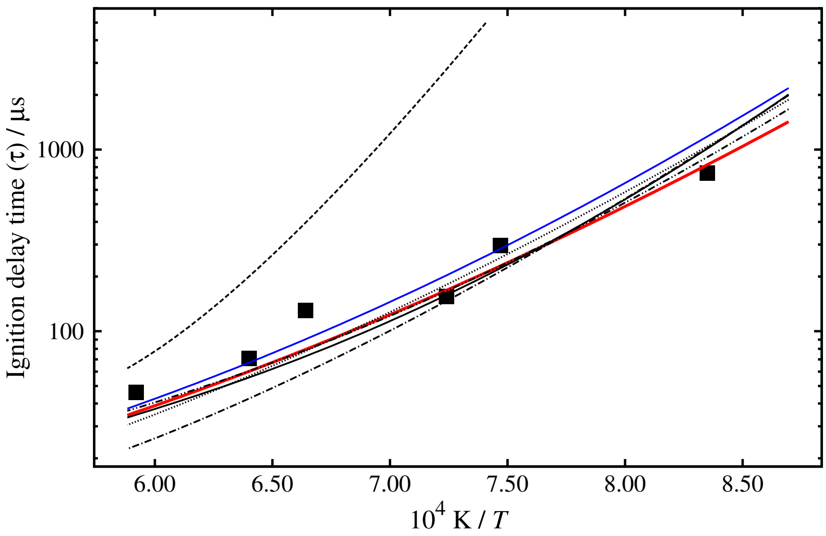
(d)

1.75% C_2H_4, 5.25% O_2, 93.00% Ar, Φ = 1.0, p_{av} = 9.32 atm



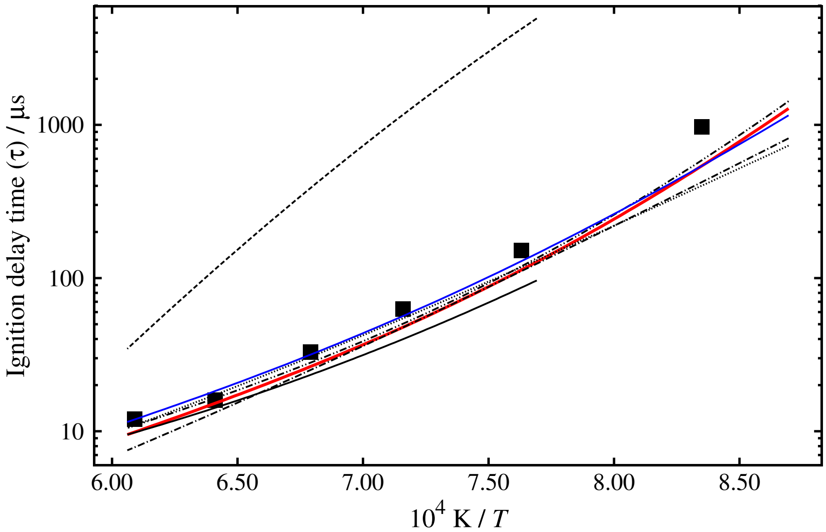
(e)

1.00% C_2H_4, 3.00% O_2, 96.00% Ar, Φ = 1.0, p_{av} = 2.03 atm



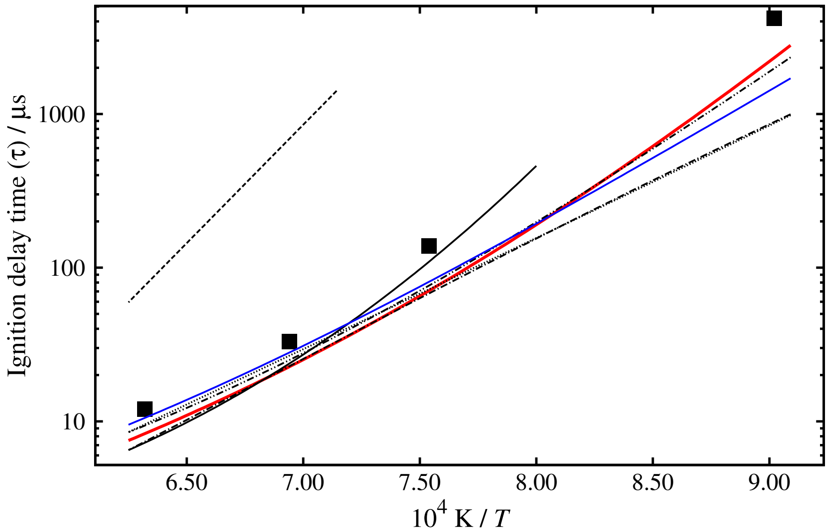
(f)

1.00% C_2H_4, 3.00% O_2, 96.00% Ar, Φ = 1.0, p_{av} = 9.85 atm



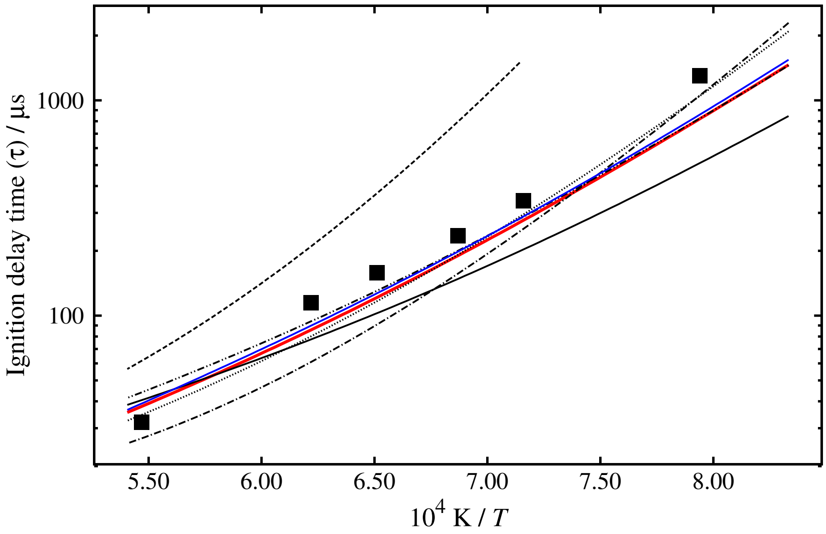
(g)

1.00% C_2H_4, 3.00% O_2, 96.00% Ar, Φ = 1.0, p_{av} = 17.9 atm



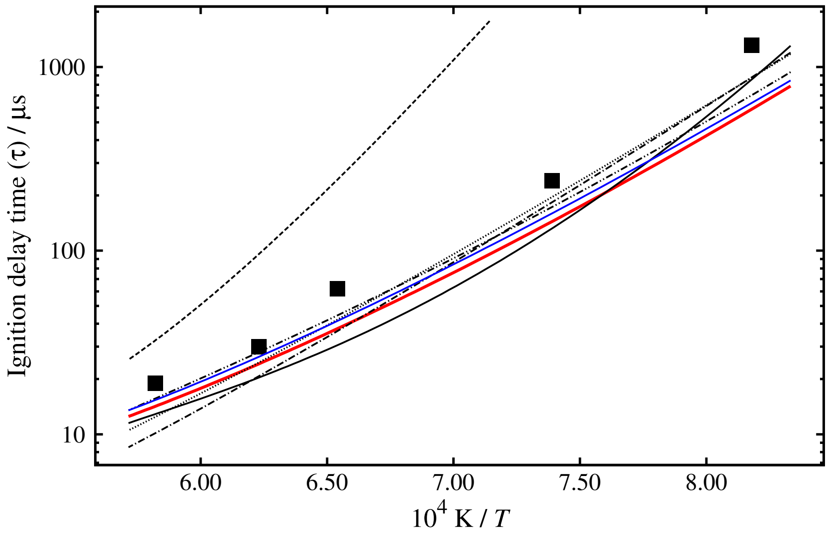
(h)

0.50% C_2H_4, 1.50% O_2, 98.00% Ar, Φ = 1.0, p_{av} = 2.12 atm

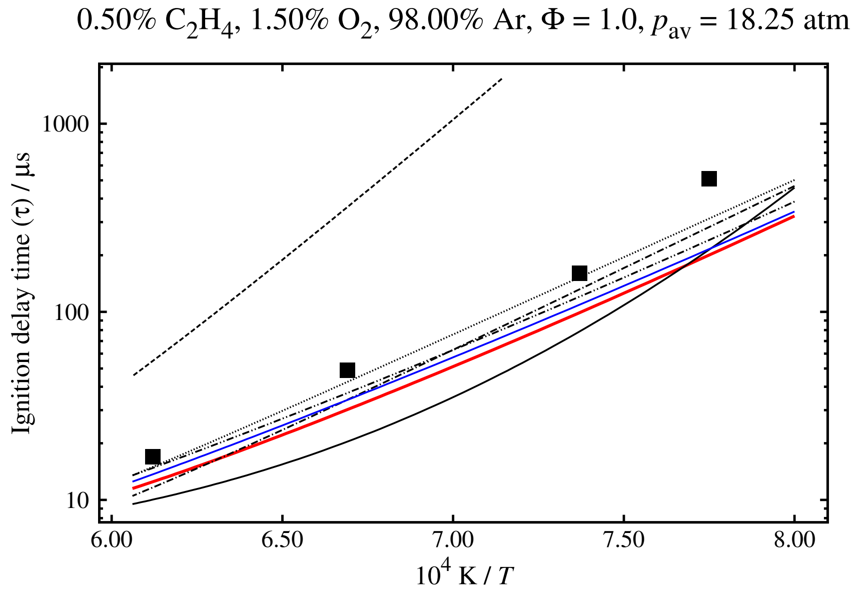


(i)

0.50% C_2H_4, 1.50% O_2, 98.00% Ar, Φ = 1.0, p_{av} = 9.80 atm

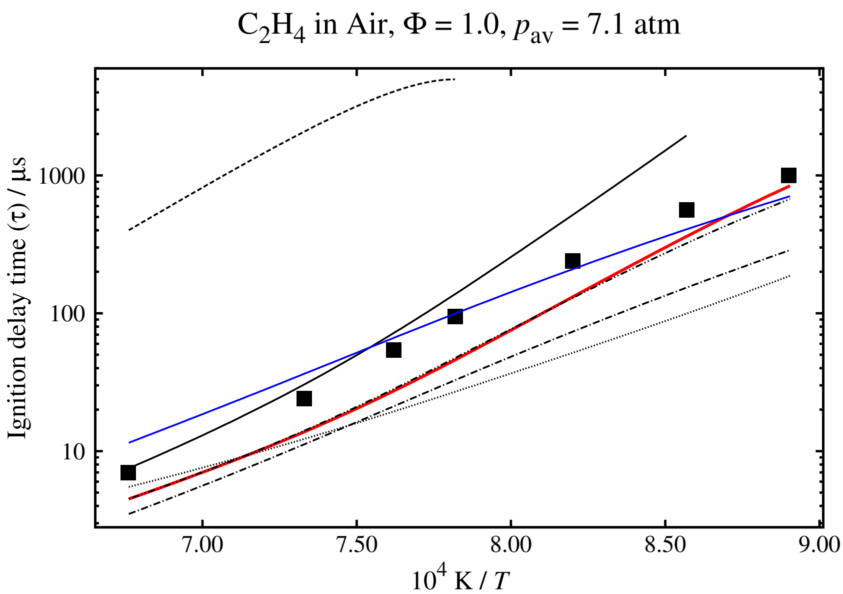


(j)



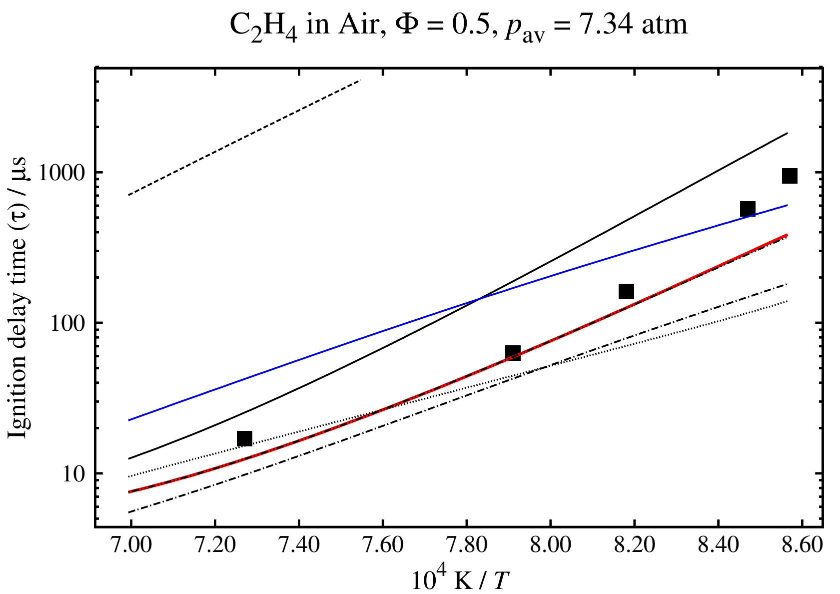
(k)

S26 Shock tube ignition delay times of thylene/oxygen/argon mixtures. Symbols are experimental data [31] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



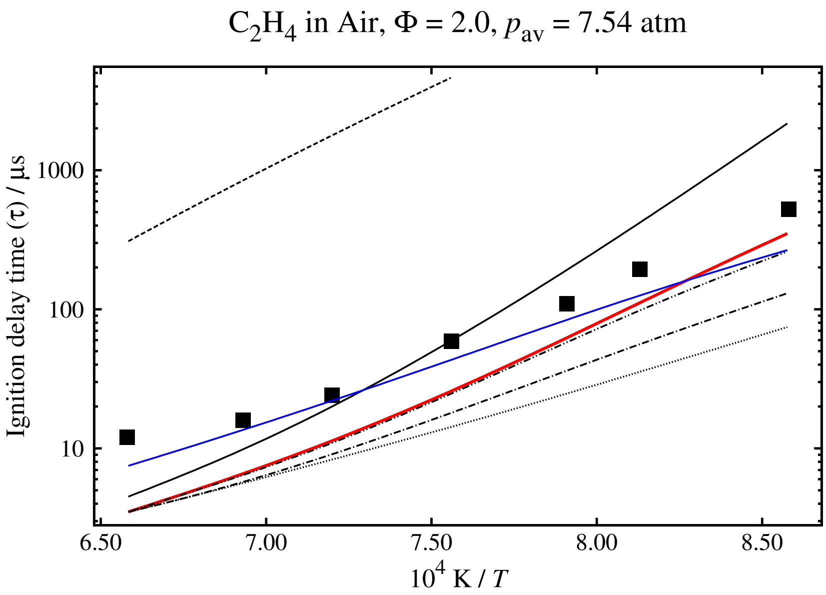
C$_2$H$_4$ in Air, Φ = 1.0, p_{av} = 7.1 atm
1000
100
10
Ignition delay time (τ) / μs
7.00
7.50
8.00
8.50
9.00
10^4 K / T

(a)

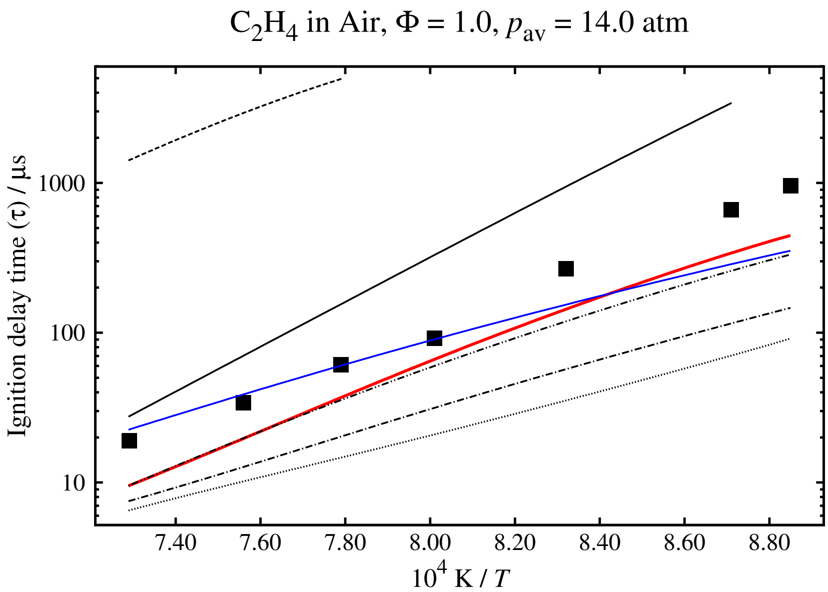


C$_2$H$_4$ in Air, Φ = 0.5, p_{av} = 7.34 atm
1000
100
10
Ignition delay time (τ) / μs
7.00
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
10^4 K / T

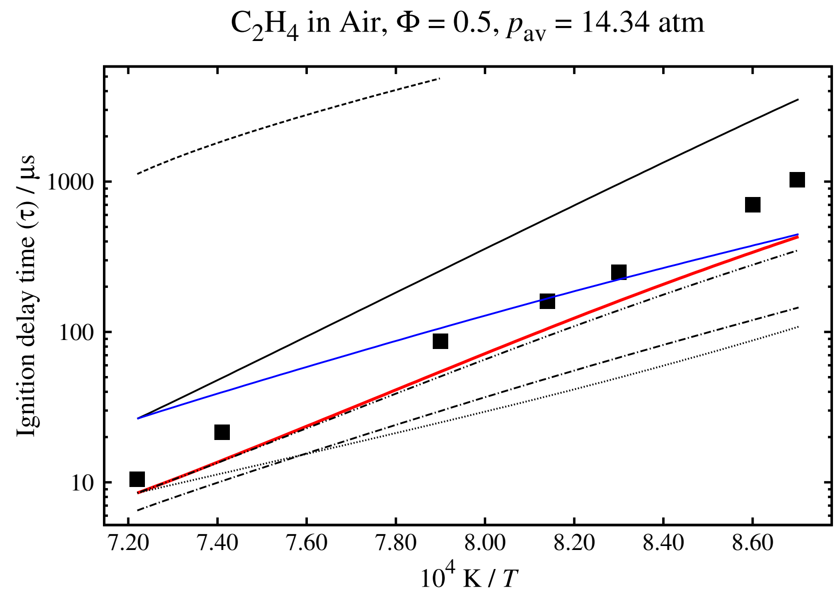
(b)


C2H4 in Air, Φ = 2.0, pav = 7.54 atm
Ignition delay time (τ) / µs
1000
100
10
6.50
7.00
7.50
8.00
8.50
10^4 K / T

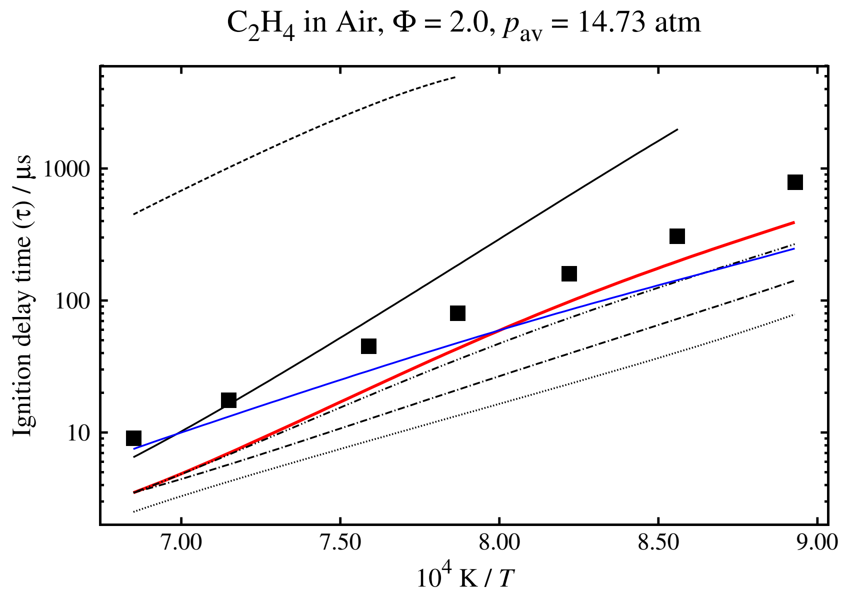
(c)


C2H4 in Air, Φ = 1.0, pav = 14.0 atm
Ignition delay time (τ) / µs
1000
100
10
7.40
7.60
7.80
8.00
8.20
8.40
8.60
8.80
10^4 K / T

(d)

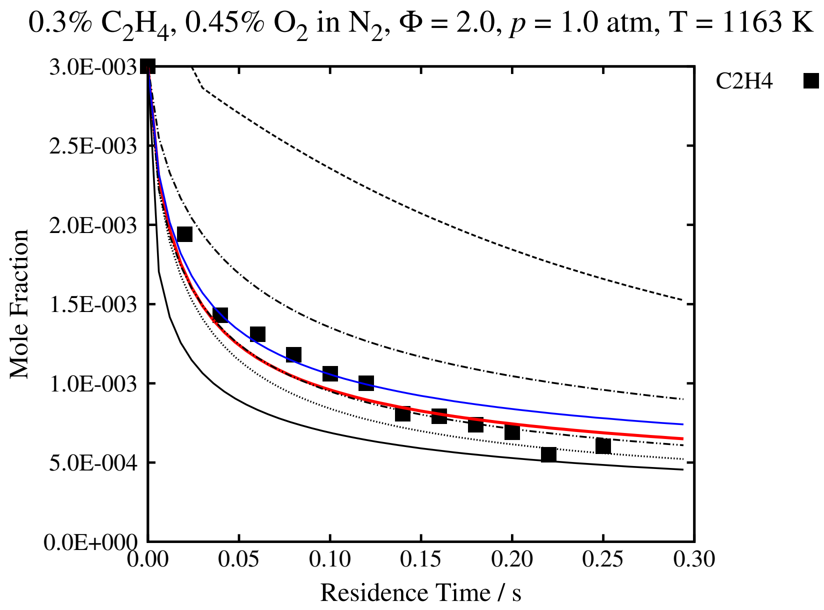


(e)

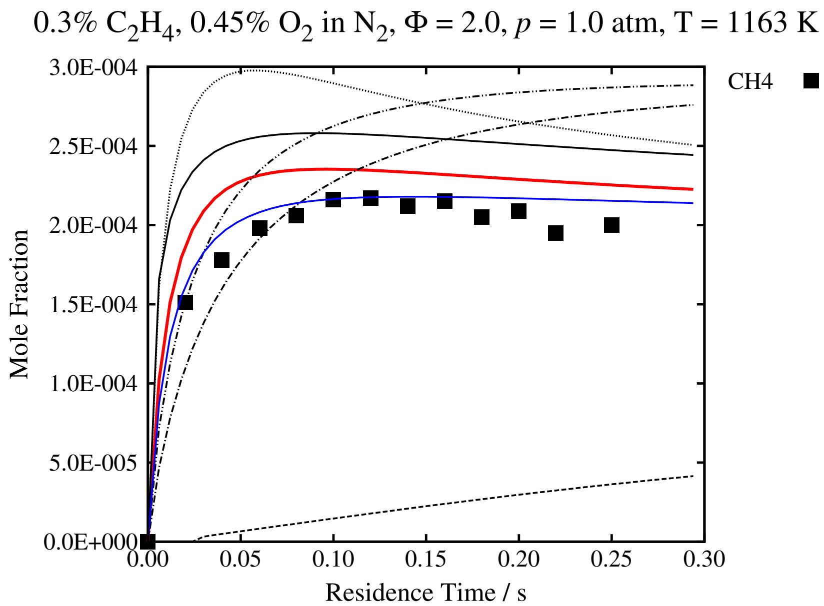


(f)

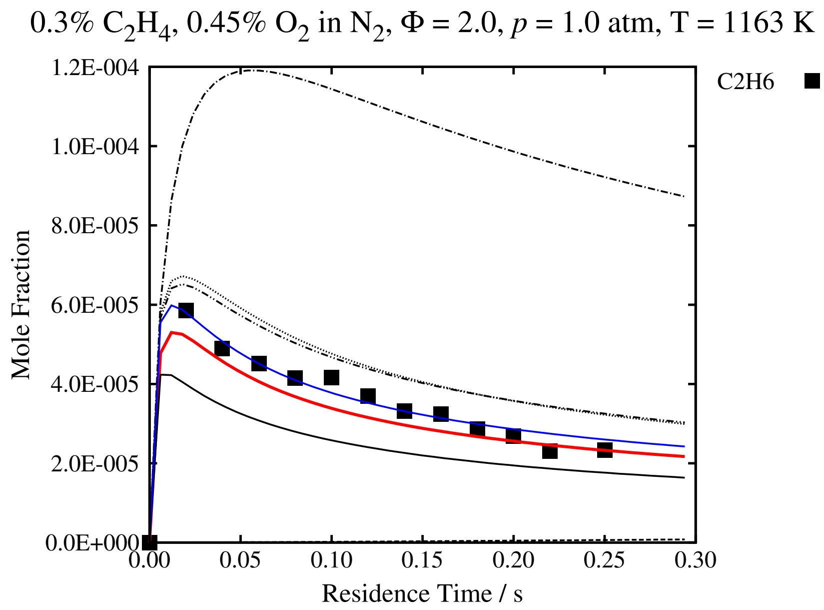
S27 Shock tube ignition delay times of ethylene/air mixtures. Symbols are experimental data [30] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.3% C2H4, 0.45% O2 in N2, Φ = 2.0, p = 1.0 atm, T = 1163 K
C2H4
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Residence Time / s

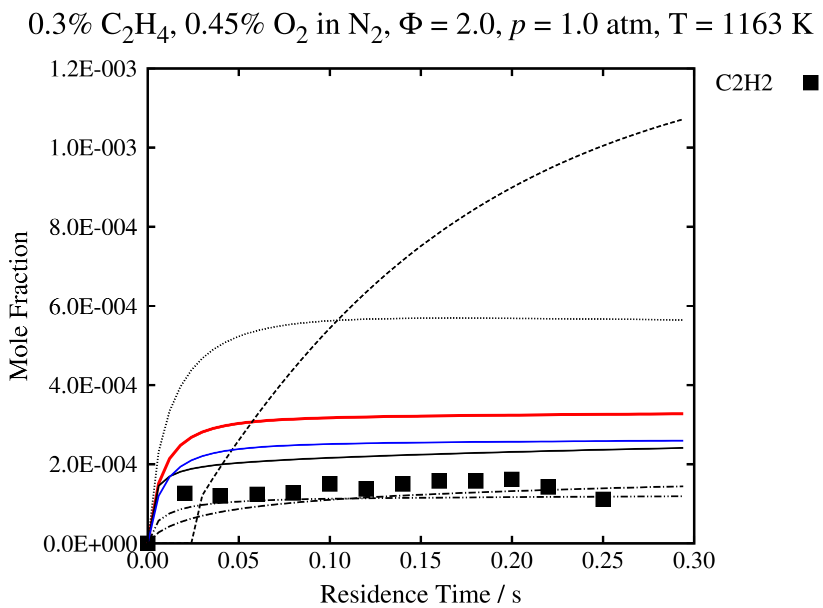
(a)


0.3% C2H4, 0.45% O2 in N2, Φ = 2.0, p = 1.0 atm, T = 1163 K
CH4
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Residence Time / s

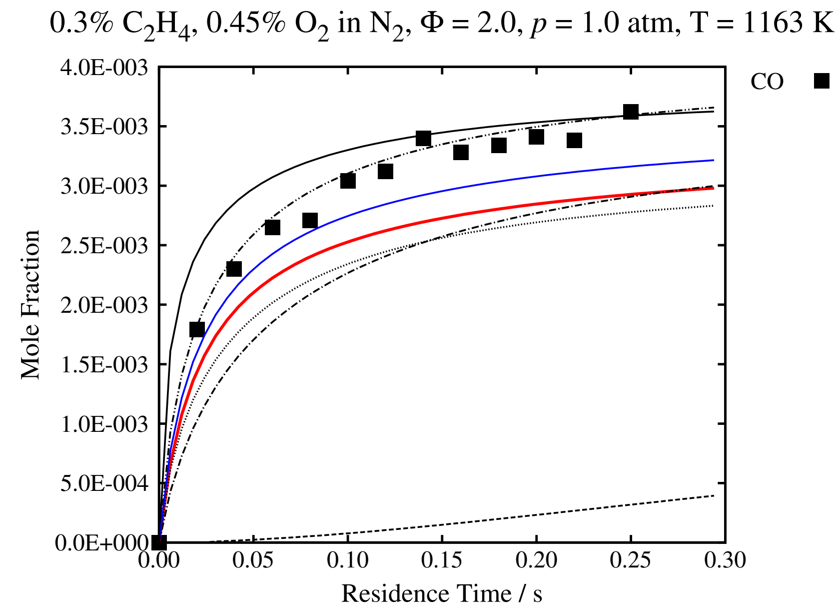
(b)


0.3% C2H4, 0.45% O2 in N2, Φ = 2.0, p = 1.0 atm, T = 1163 K
C2H6
Mole Fraction
Residence Time / s
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30

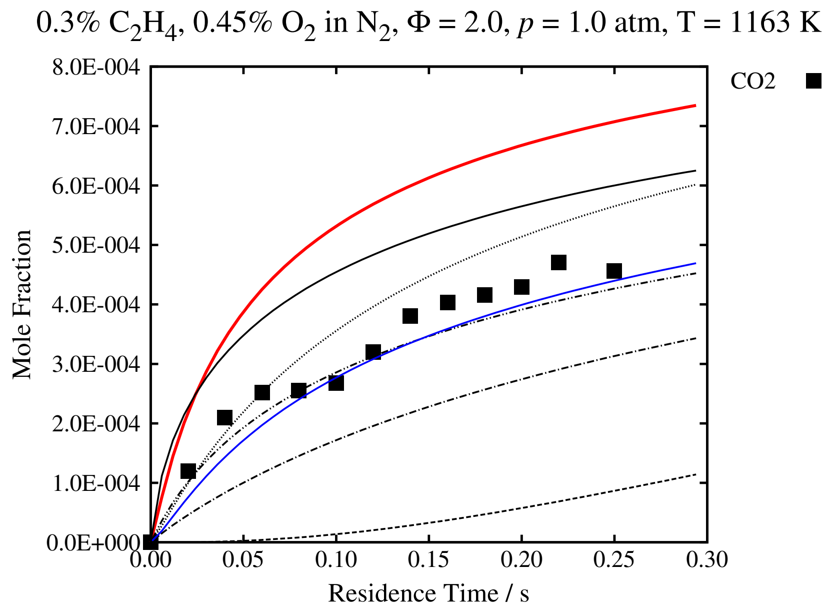
(c)


0.3% C2H4, 0.45% O2 in N2, Φ = 2.0, p = 1.0 atm, T = 1163 K
C2H2
Mole Fraction
Residence Time / s
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30

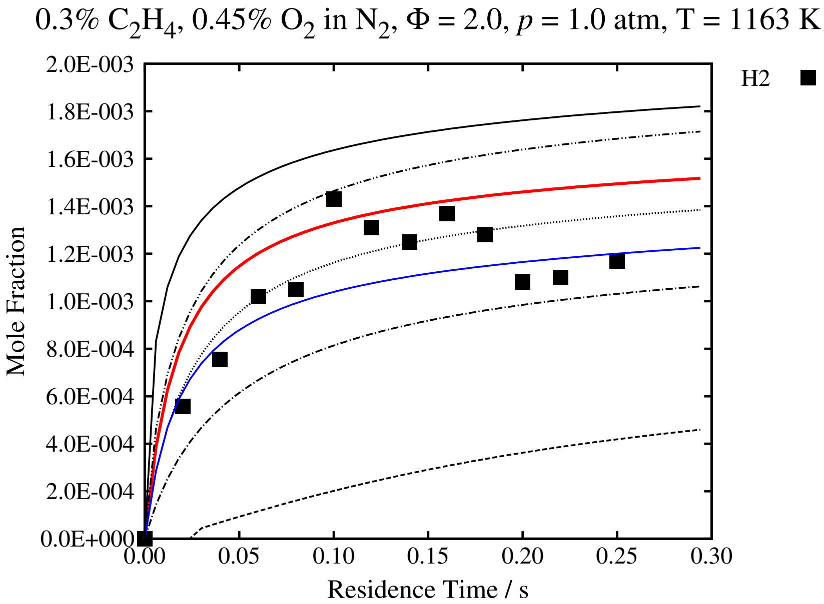
(d)


0.3% C2H4, 0.45% O2 in N2, Φ = 2.0, p = 1.0 atm, T = 1163 K
CO
Mole Fraction
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Residence Time / s

(e)

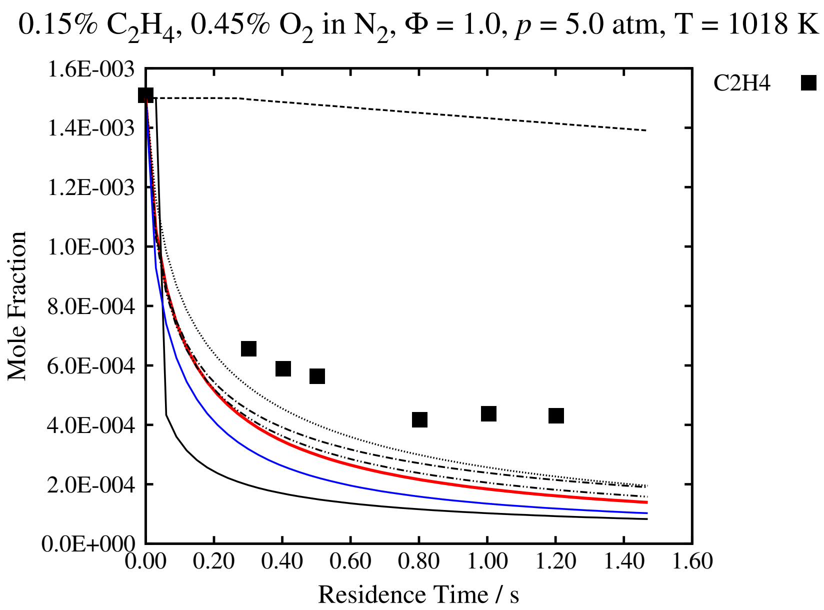

0.3% C2H4, 0.45% O2 in N2, Φ = 2.0, p = 1.0 atm, T = 1163 K
CO2
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Residence Time / s

(f)



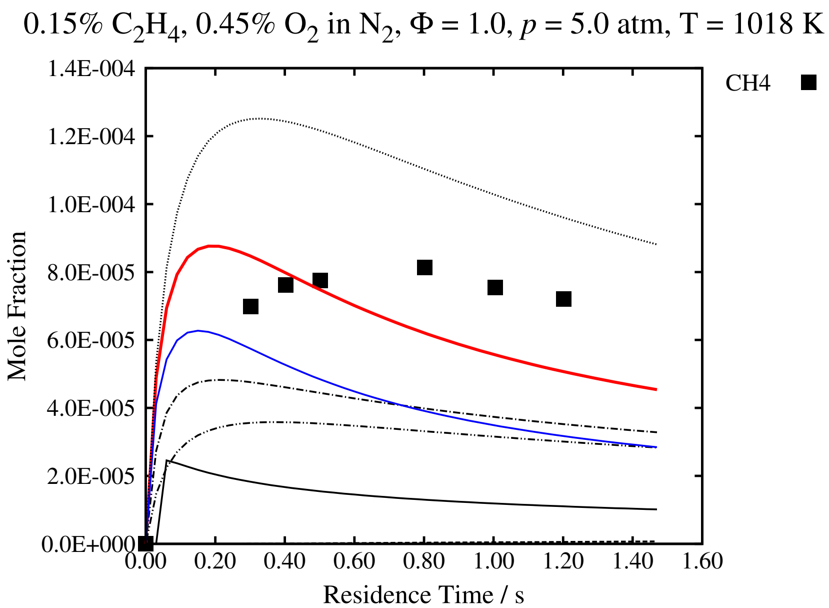
(g)

S28 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [32] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



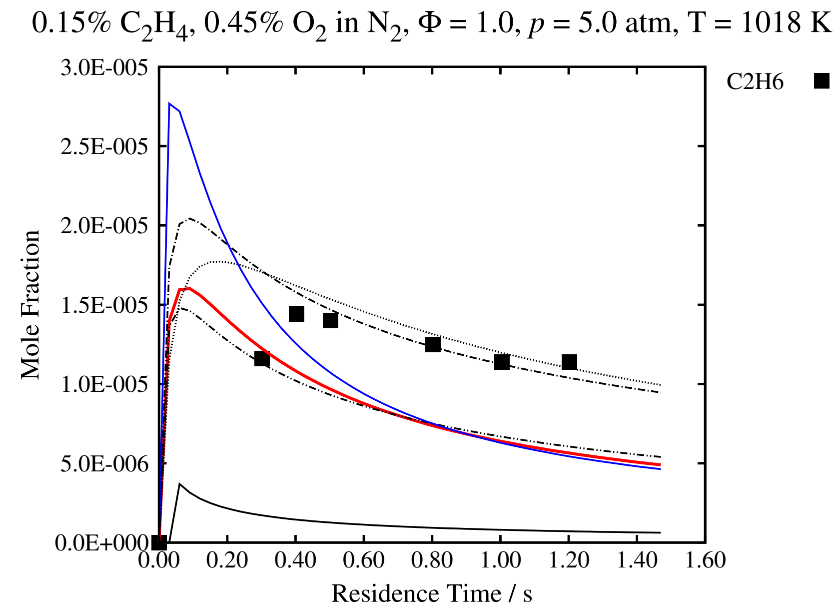
0.15% C2H4, 0.45% O2 in N2, Φ = 1.0, p = 5.0 atm, T = 1018 K
C2H4
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60
Residence Time / s

(a)

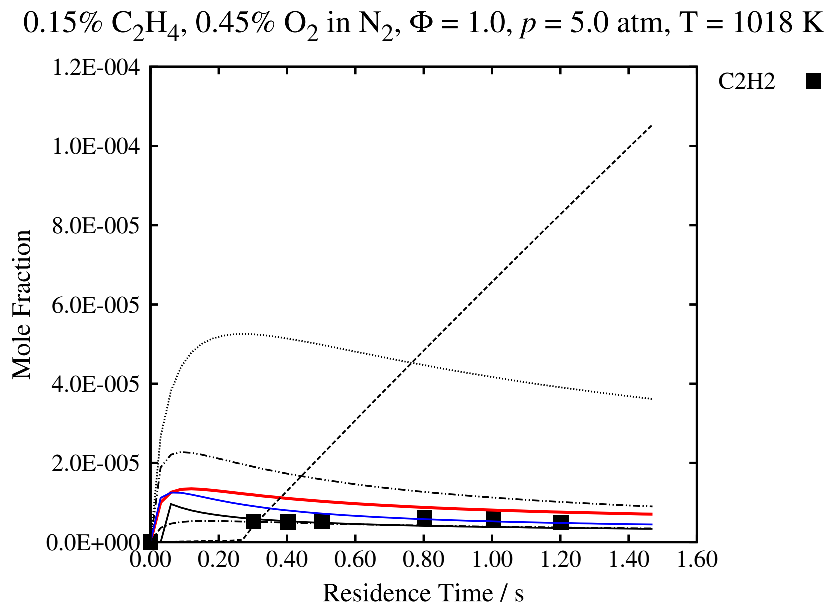


0.15% C2H4, 0.45% O2 in N2, Φ = 1.0, p = 5.0 atm, T = 1018 K
CH4
Mole Fraction
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60
Residence Time / s

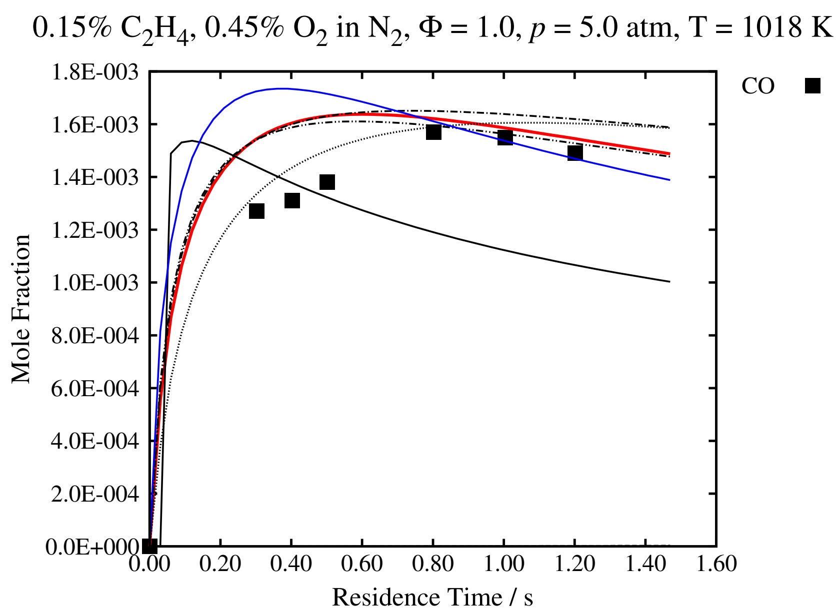
(b)


0.15% C_2H_4, 0.45% O_2 in N_2, Φ = 1.0, *p* = 5.0 atm, T = 1018 K
C2H6
Mole Fraction
Residence Time / s
3.0E-005
2.5E-005
2.0E-005
1.5E-005
1.0E-005
5.0E-006
0.0E+000
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

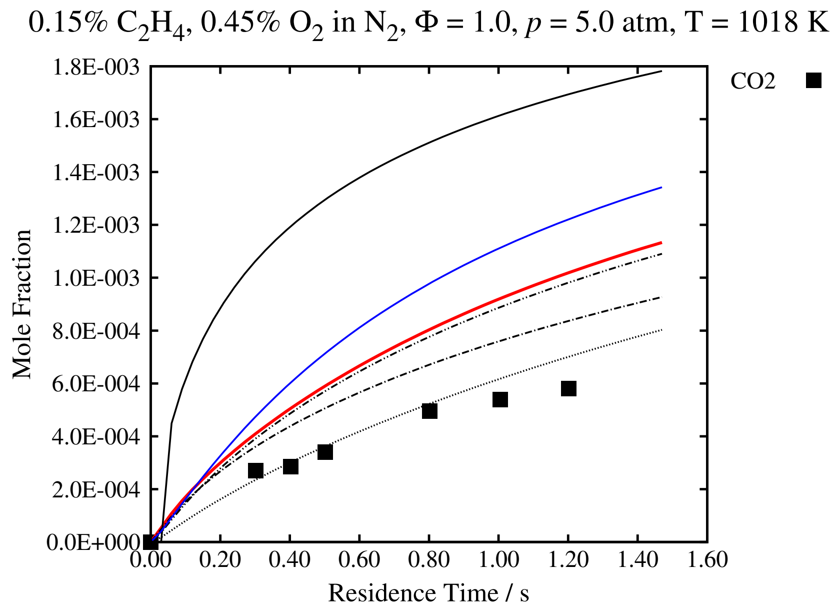
(c)


0.15% C_2H_4, 0.45% O_2 in N_2, Φ = 1.0, *p* = 5.0 atm, T = 1018 K
C2H2
Mole Fraction
Residence Time / s
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

(d)

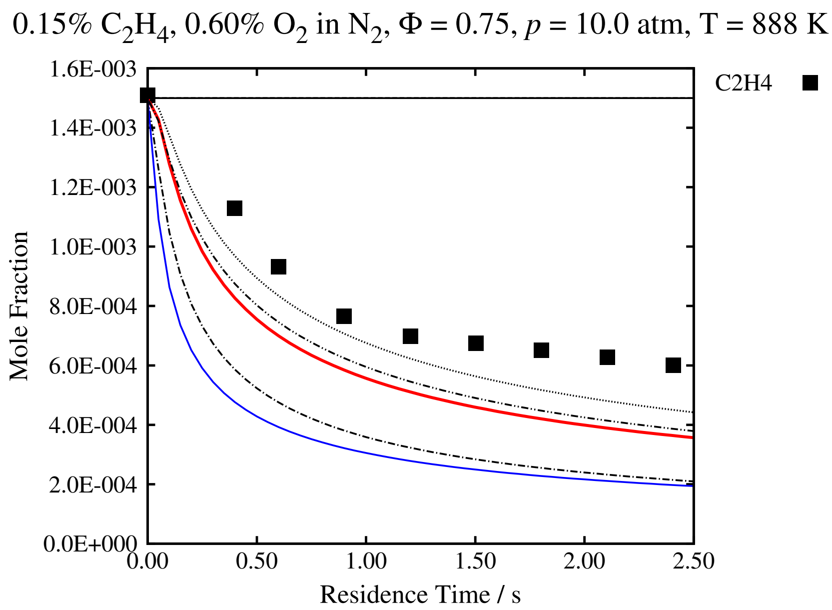


(e)

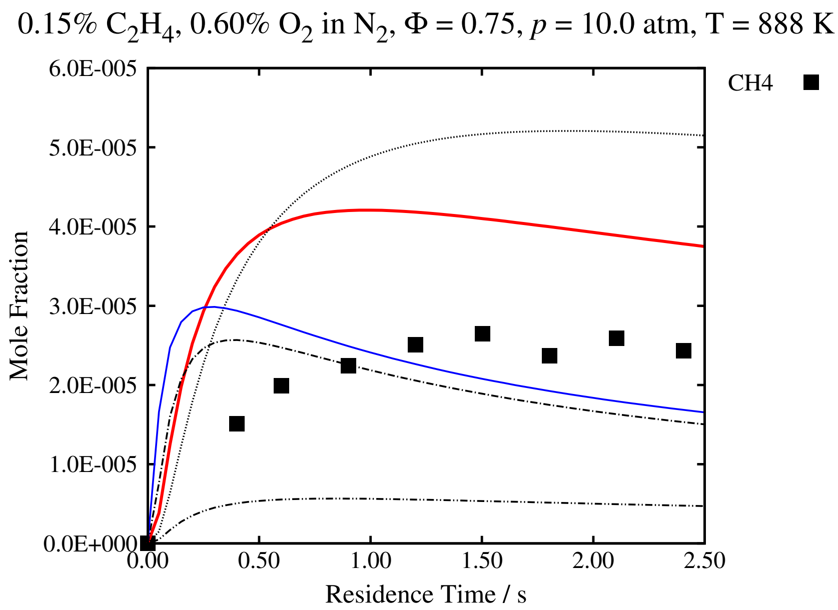


(f)

S29 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [32] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

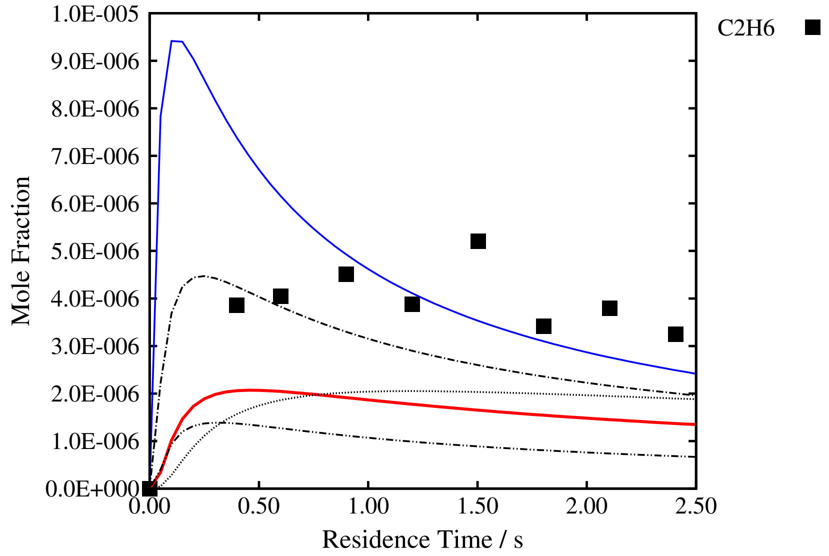

0.15% C_2H_4, 0.60% O_2 in N_2, Φ = 0.75, p = 10.0 atm, T = 888 K
C2H4
Mole Fraction
Residence Time / s
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.00
0.50
1.00
1.50
2.00
2.50

(a)


0.15% C_2H_4, 0.60% O_2 in N_2, Φ = 0.75, p = 10.0 atm, T = 888 K
CH4
Mole Fraction
Residence Time / s
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
0.00
0.50
1.00
1.50
2.00
2.50

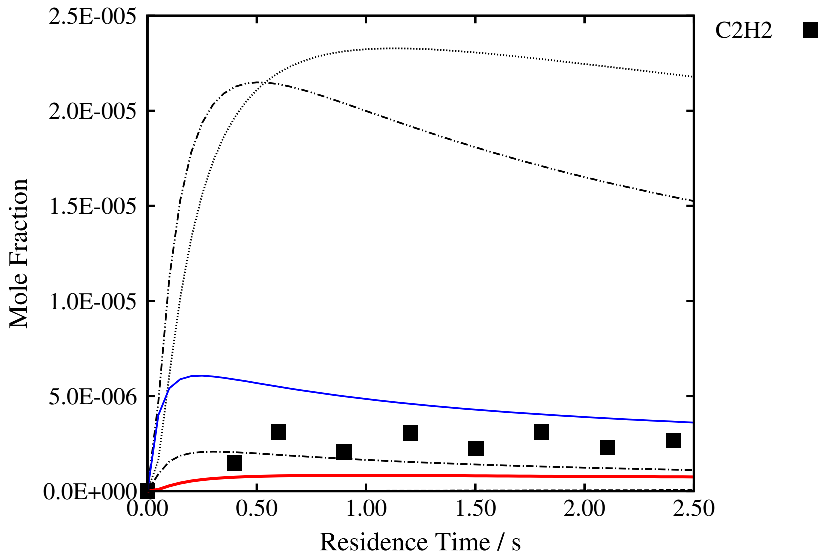
(b)

0.15% C_2H_4, 0.60% O_2 in N_2, Φ = 0.75, p = 10.0 atm, T = 888 K

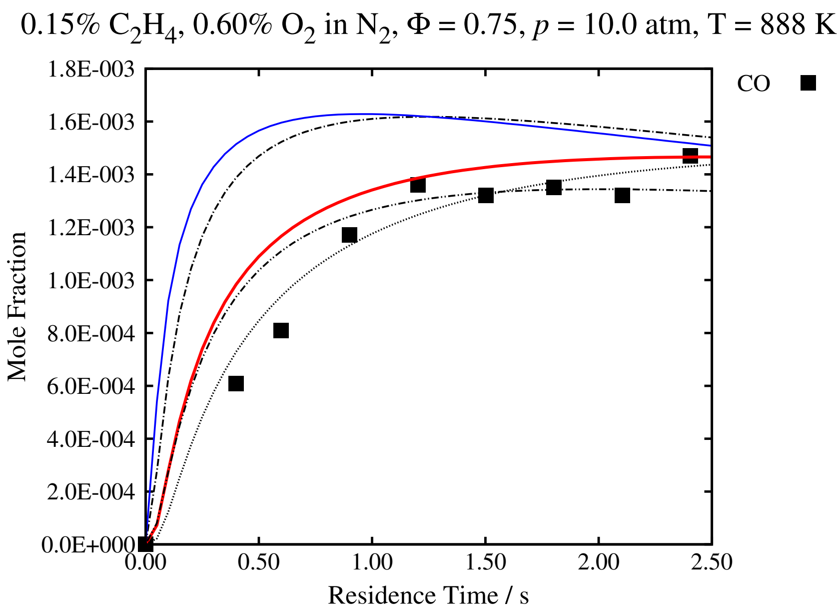


(c)

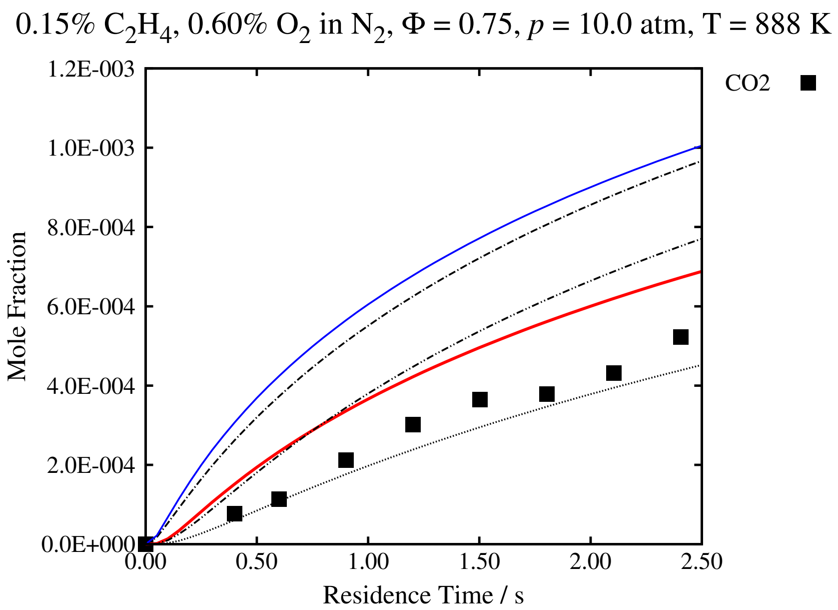
0.15% C_2H_4, 0.60% O_2 in N_2, Φ = 0.75, p = 10.0 atm, T = 888 K



(d)

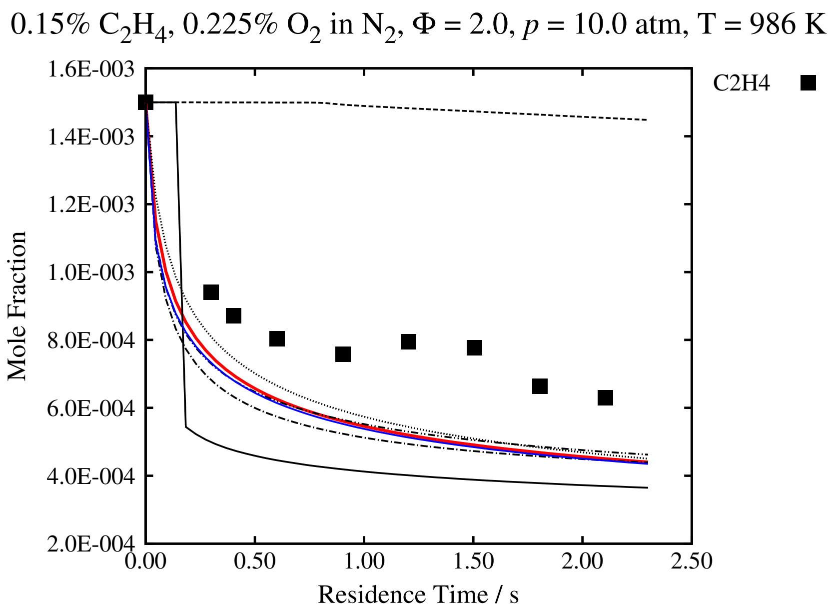


(e)

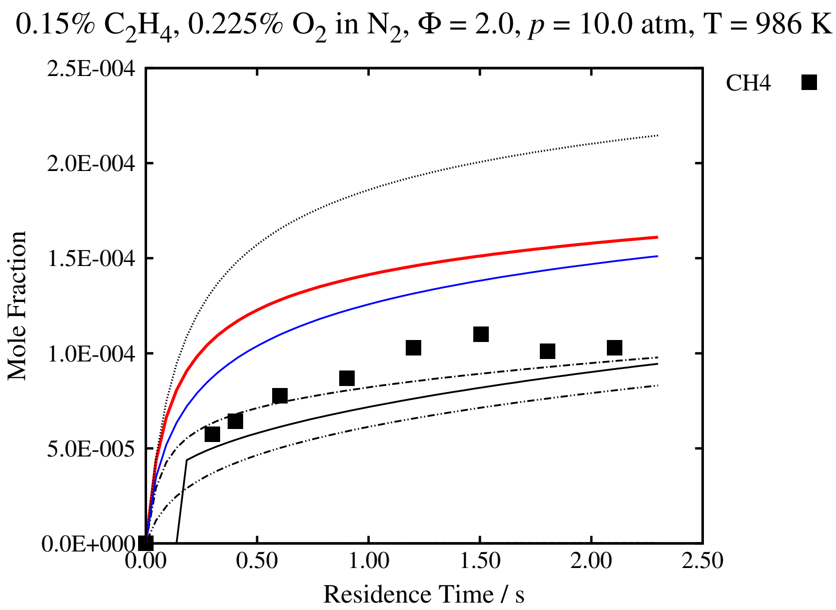


(f)

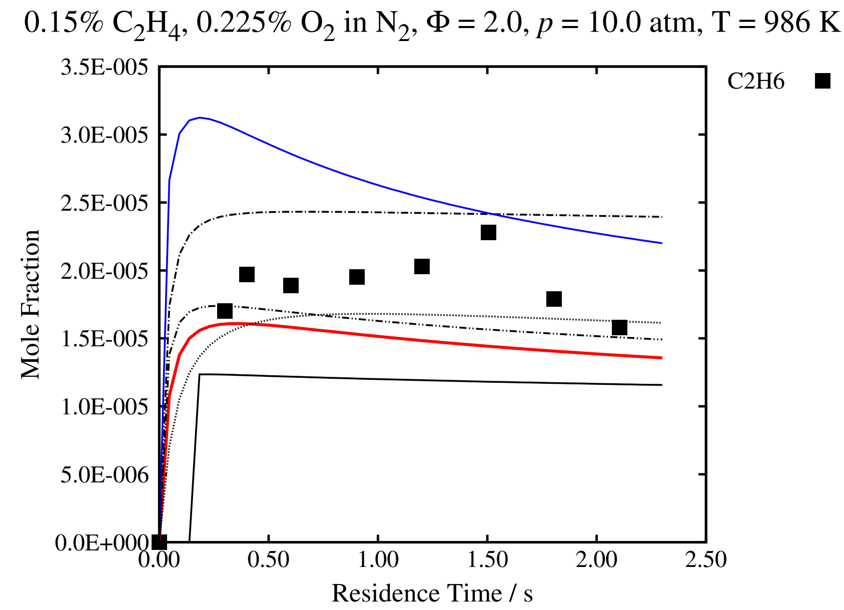
S30 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [32] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.15% C2H4, 0.225% O2 in N2, Φ = 2.0, p = 10.0 atm, T = 986 K
C2H4
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.00
0.50
1.00
1.50
2.00
2.50
Residence Time / s

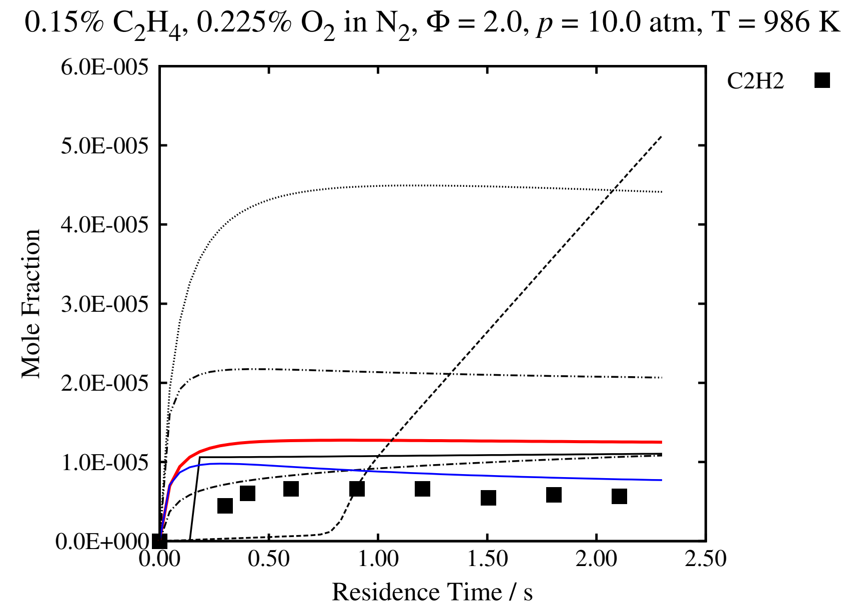
(a)


0.15% C2H4, 0.225% O2 in N2, Φ = 2.0, p = 10.0 atm, T = 986 K
CH4
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.00
0.50
1.00
1.50
2.00
2.50
Residence Time / s

(b)

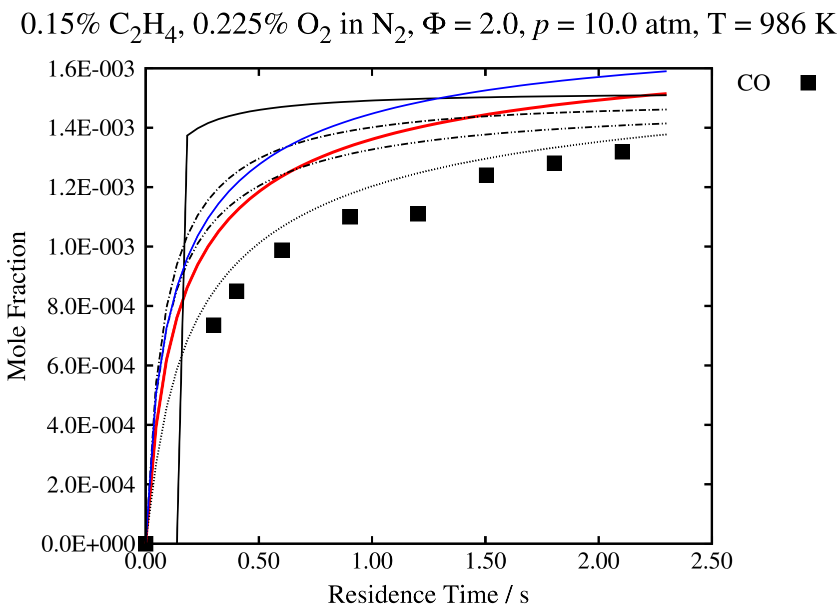


(c)

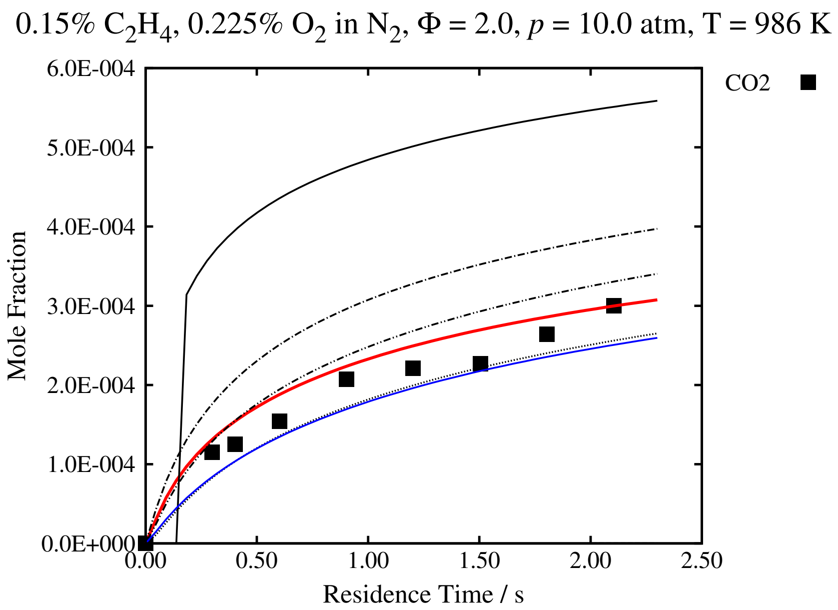


(d)

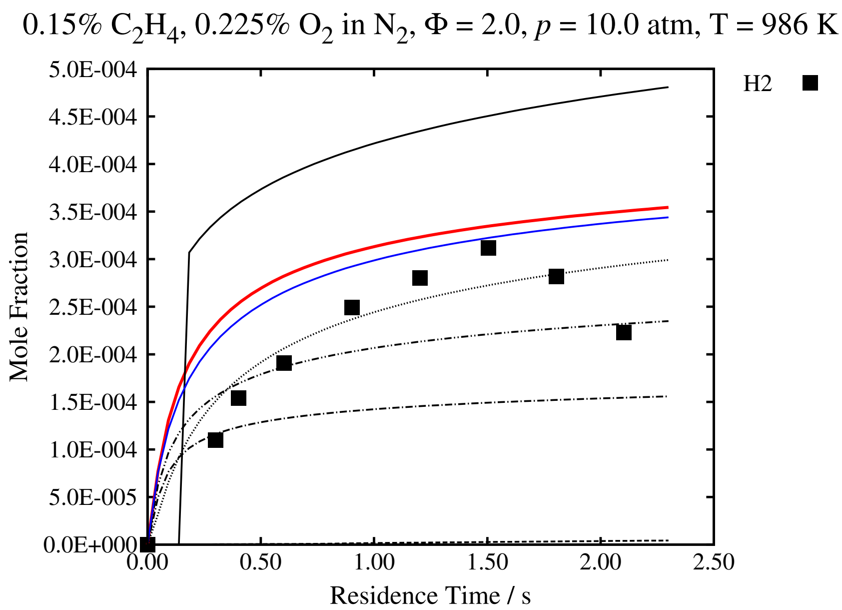
S31 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [32] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.15% C_2H_4, 0.225% O_2 in N_2, Φ = 2.0, *p* = 10.0 atm, T = 986 K
CO
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.00
0.50
1.00
1.50
2.00
2.50
Residence Time / s

(a)


0.15% C_2H_4, 0.225% O_2 in N_2, Φ = 2.0, *p* = 10.0 atm, T = 986 K
CO2
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.00
0.50
1.00
1.50
2.00
2.50
Residence Time / s

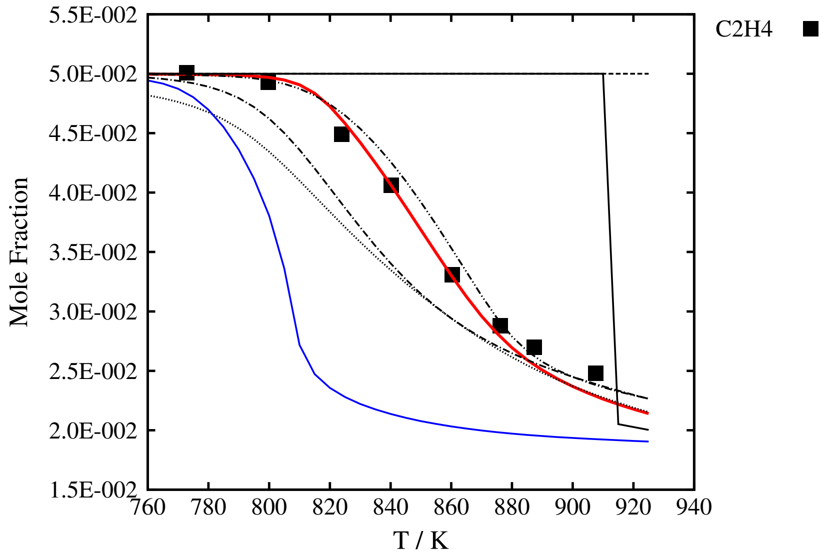
(b)



(c)

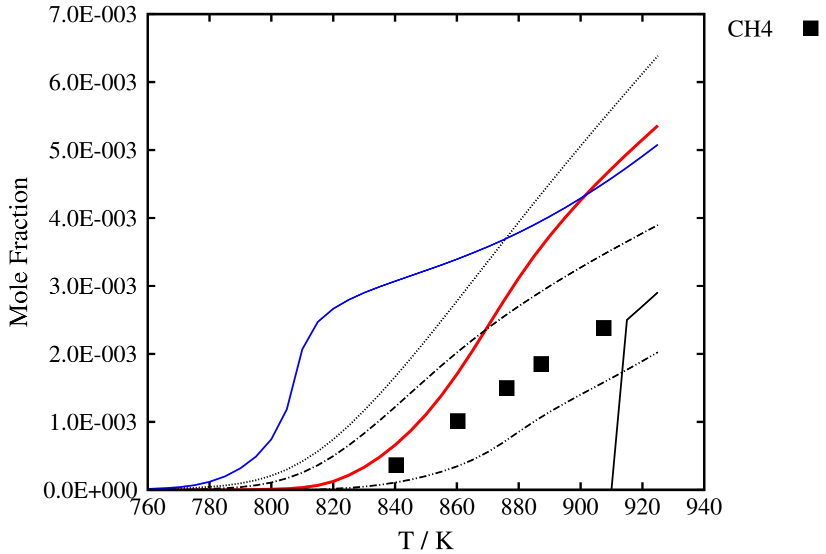
S32 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [32] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

5.0% C_2H_4 in N_2, Φ = 3.0, p = 1.0 atm, τ = 1.3 s

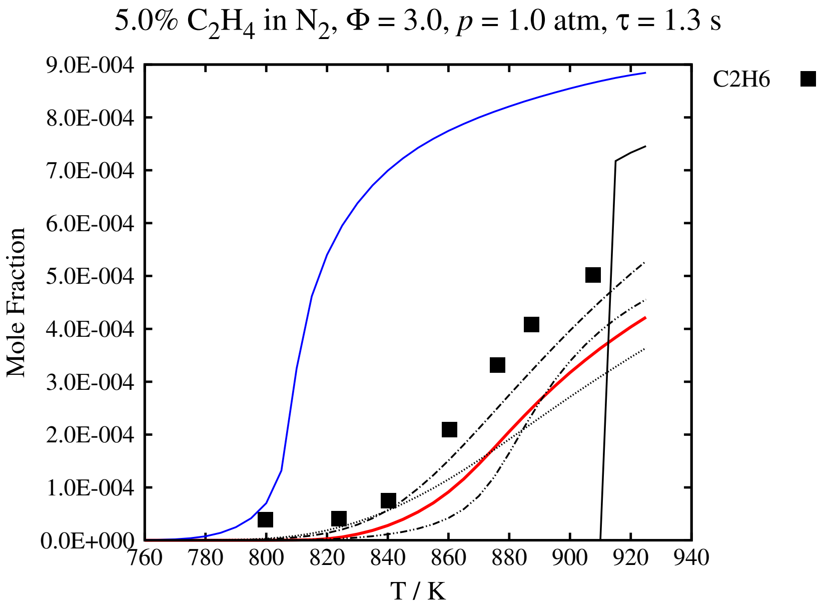


(a)

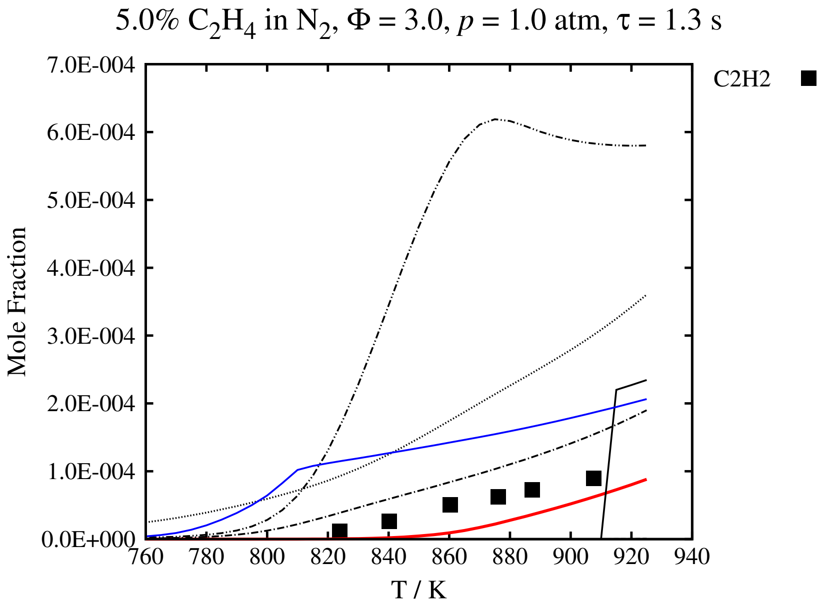
5.0% C_2H_4 in N_2, Φ = 3.0, p = 1.0 atm, τ = 1.3 s



(b)

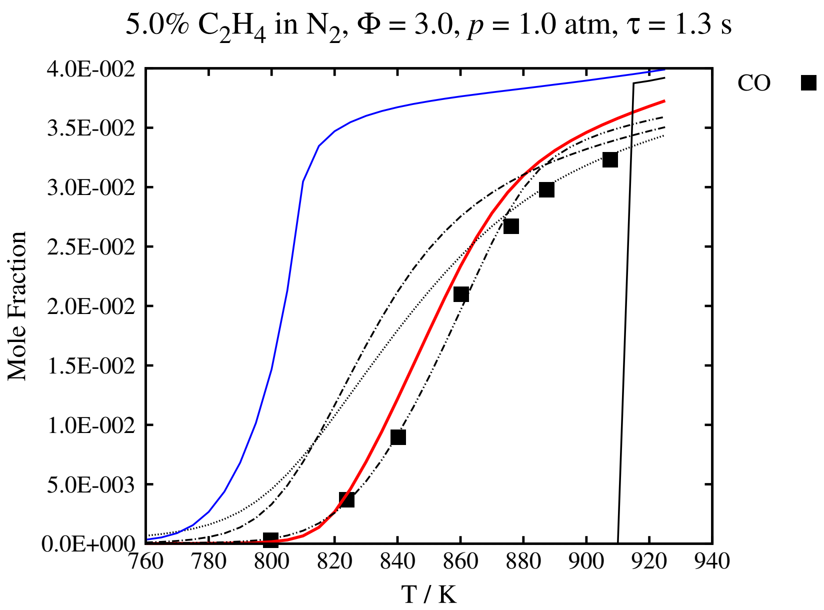


(c)



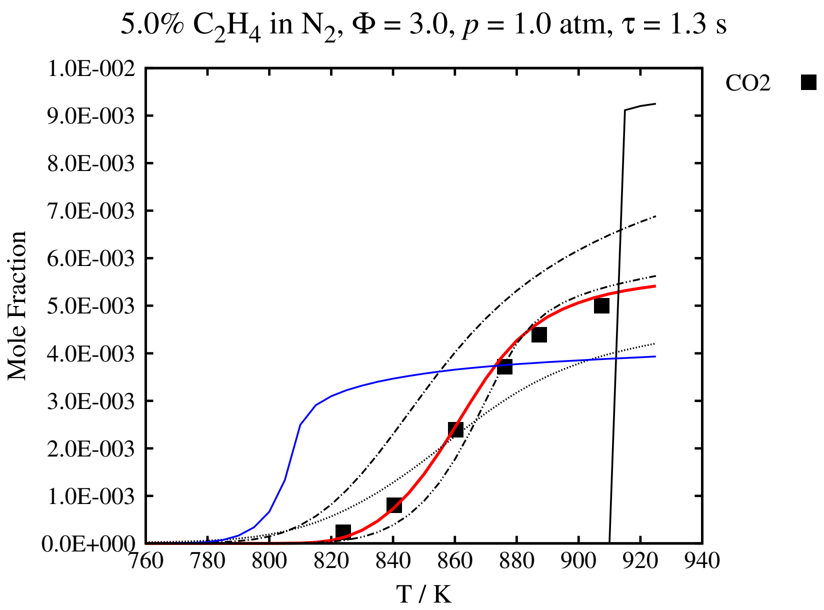
(d)

S33 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [33] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



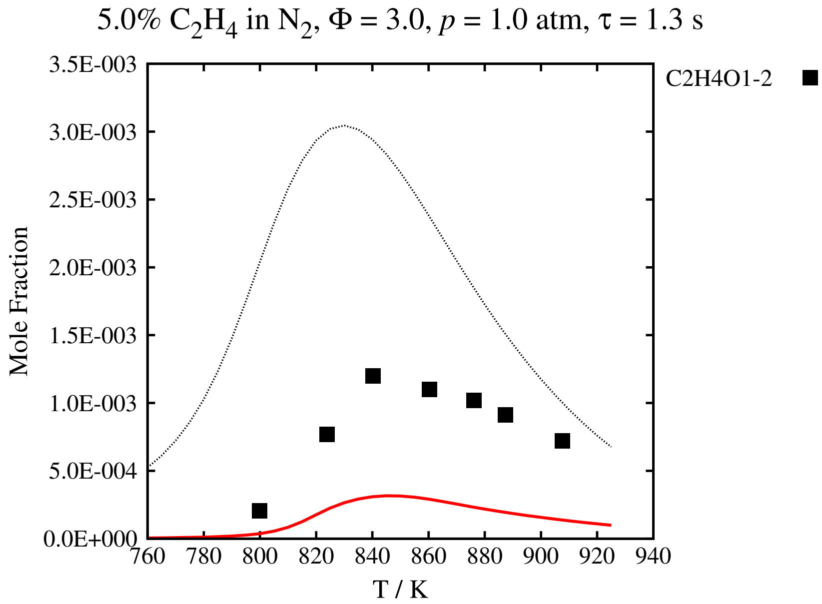
5.0% C2H4 in N2, Φ = 3.0, p = 1.0 atm, τ = 1.3 s
CO
Mole Fraction
T / K
0.0E+000
5.0E-003
1.0E-002
1.5E-002
2.0E-002
2.5E-002
3.0E-002
3.5E-002
4.0E-002
760
780
800
820
840
860
880
900
920
940

(a)



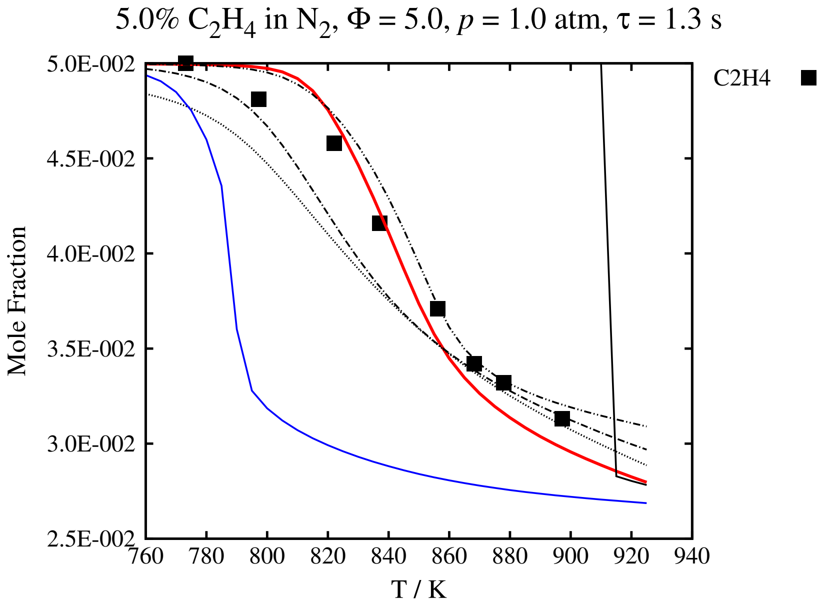
5.0% C2H4 in N2, Φ = 3.0, p = 1.0 atm, τ = 1.3 s
CO2
Mole Fraction
T / K
0.0E+000
1.0E-003
2.0E-003
3.0E-003
4.0E-003
5.0E-003
6.0E-003
7.0E-003
8.0E-003
9.0E-003
1.0E-002
760
780
800
820
840
860
880
900
920
940

(b)

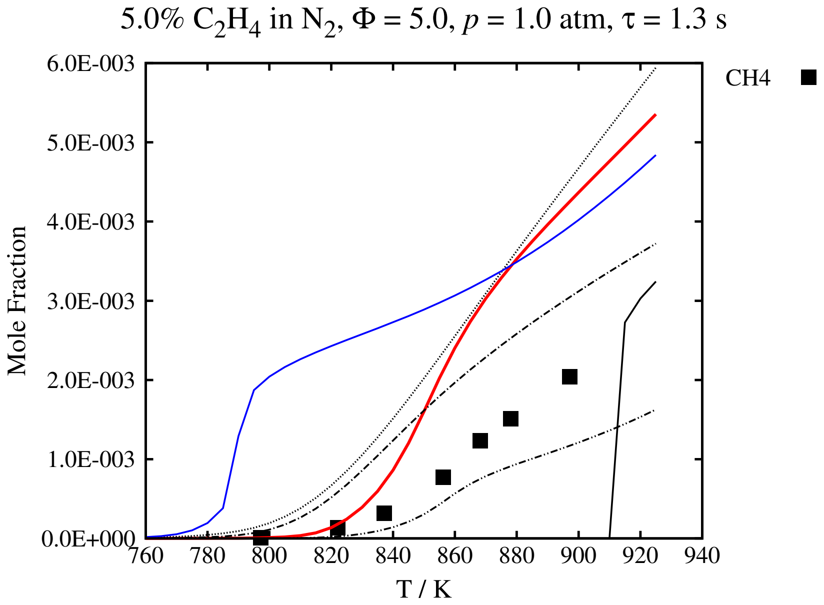


(c)

S34 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [33] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

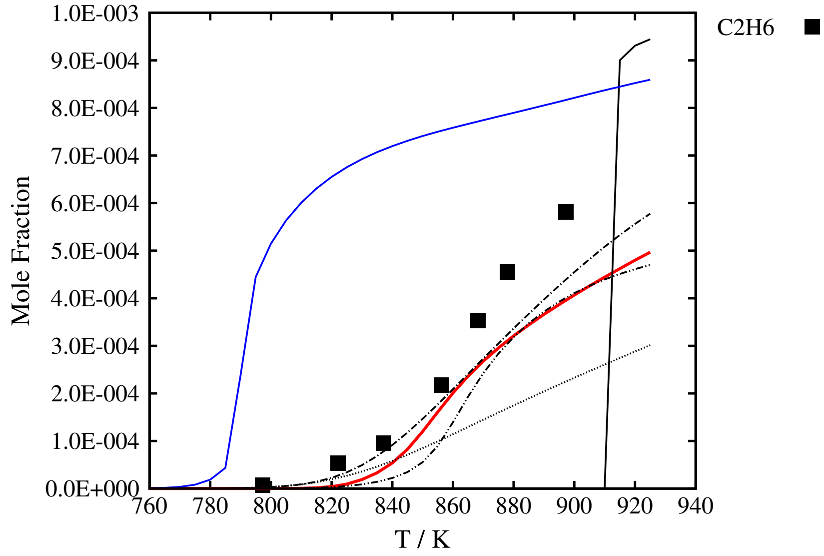

5.0% C2H4 in N2, Φ = 5.0, p = 1.0 atm, τ = 1.3 s
C2H4
Mole Fraction
5.0E-002
4.5E-002
4.0E-002
3.5E-002
3.0E-002
2.5E-002
760 780 800 820 840 860 880 900 920 940
T / K

(a)


5.0% C2H4 in N2, Φ = 5.0, p = 1.0 atm, τ = 1.3 s
CH4
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
760 780 800 820 840 860 880 900 920 940
T / K

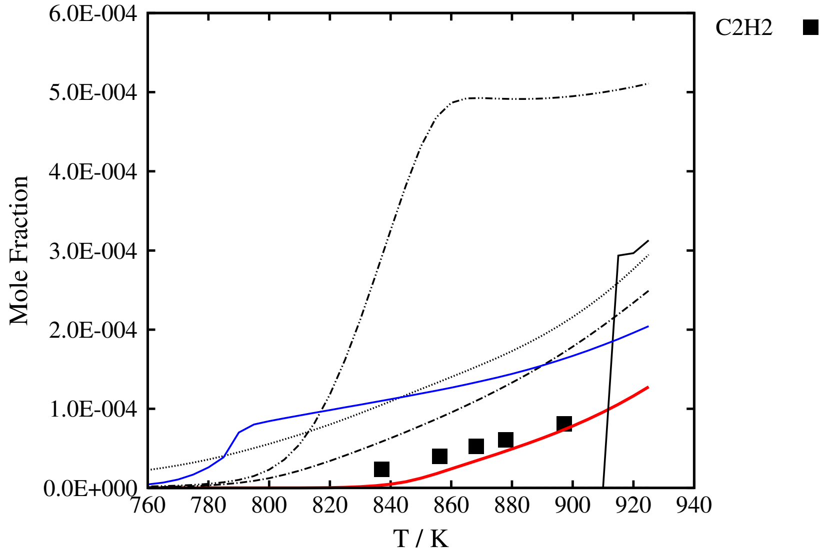
(b)

5.0% C_2H_4 in N_2, Φ = 5.0, p = 1.0 atm, τ = 1.3 s

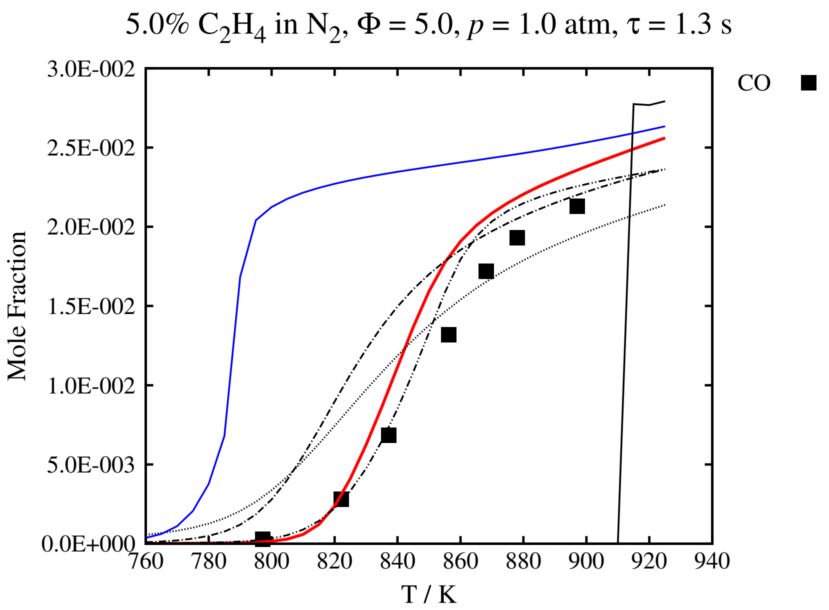


(c)

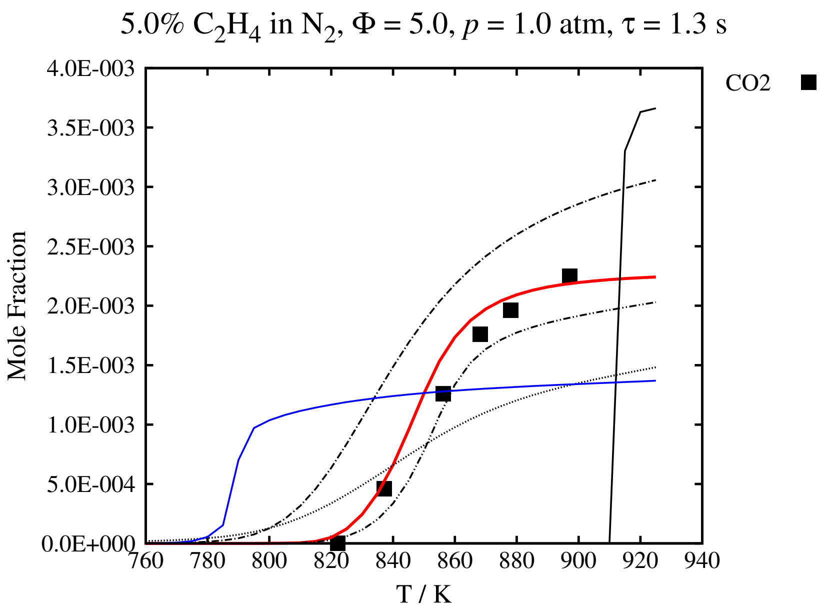
5.0% C_2H_4 in N_2, Φ = 5.0, p = 1.0 atm, τ = 1.3 s



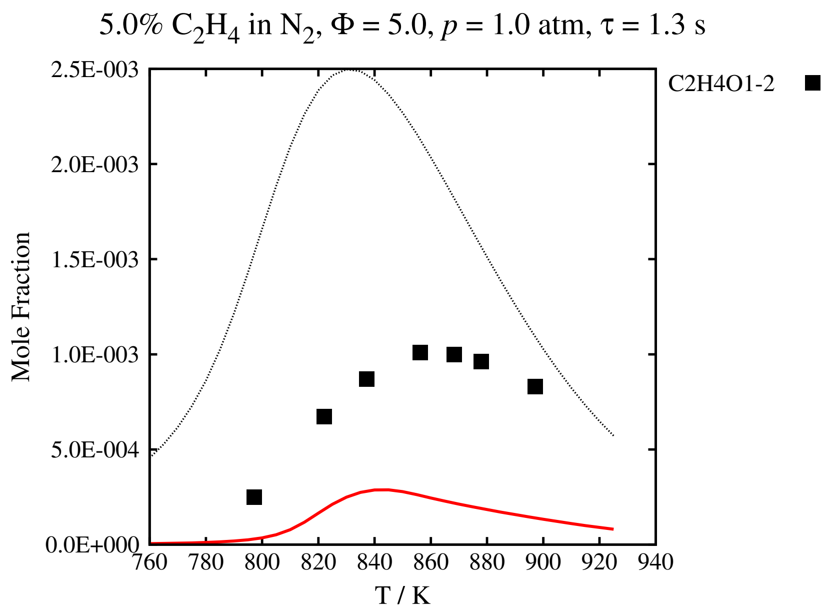
(d)


5.0% C_2H_4 in N_2, Φ = 5.0, p = 1.0 atm, τ = 1.3 s
CO
Mole Fraction
T / K
3.0E-002
2.5E-002
2.0E-002
1.5E-002
1.0E-002
5.0E-003
0.0E+000
760
780
800
820
840
860
880
900
920
940

(e)

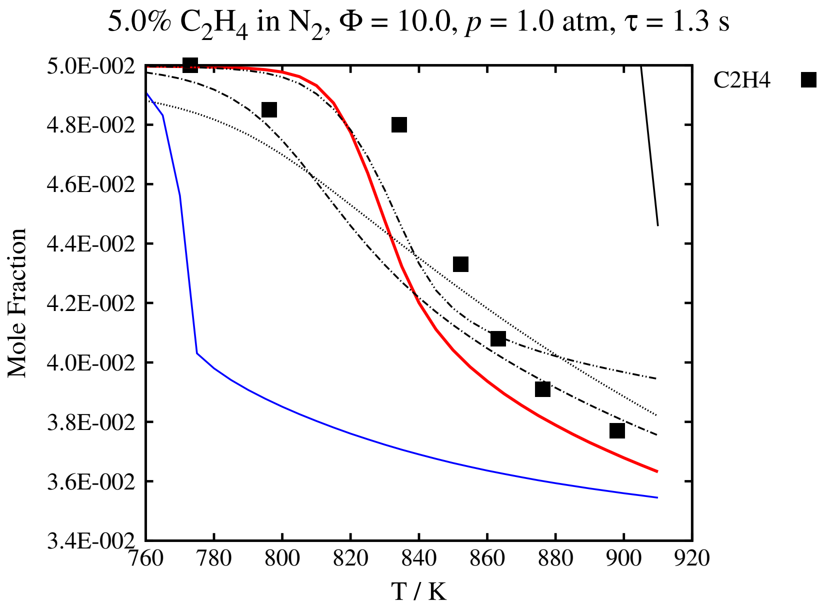

5.0% C_2H_4 in N_2, Φ = 5.0, p = 1.0 atm, τ = 1.3 s
CO2
Mole Fraction
T / K
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
760
780
800
820
840
860
880
900
920
940

(f)



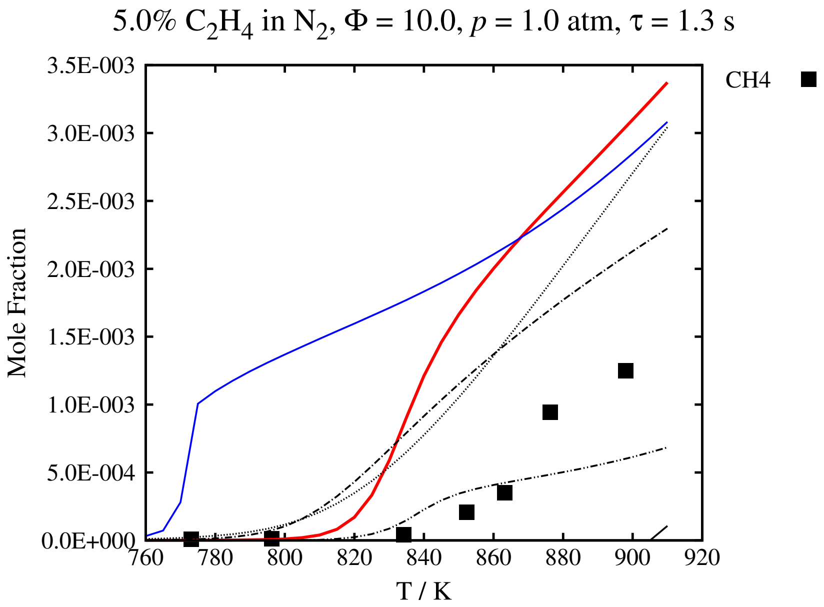
(g)

S35 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [33] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



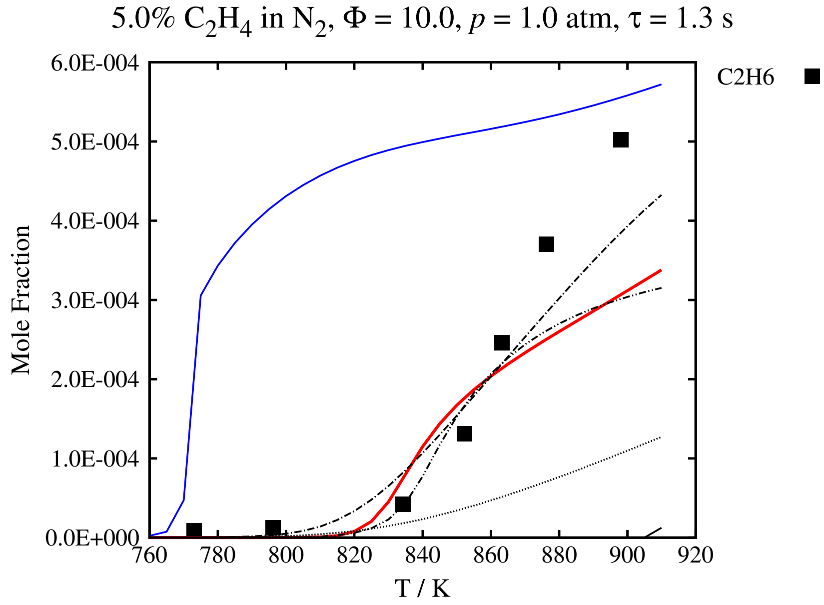
5.0% C_2H_4 in N_2, Φ = 10.0, p = 1.0 atm, τ = 1.3 s
C2H4
Mole Fraction
5.0E-002
4.8E-002
4.6E-002
4.4E-002
4.2E-002
4.0E-002
3.8E-002
3.6E-002
3.4E-002
760
780
800
820
840
860
880
900
920
T / K

(a)

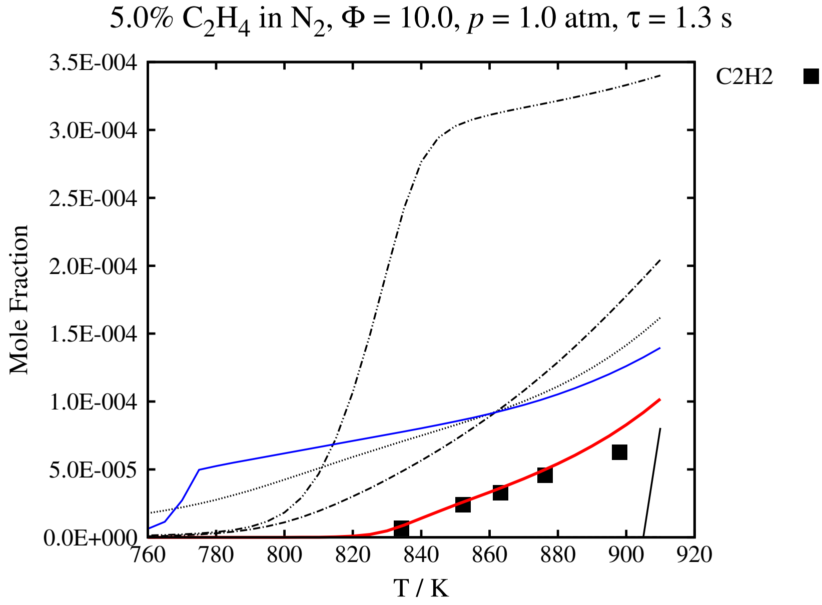


5.0% C_2H_4 in N_2, Φ = 10.0, p = 1.0 atm, τ = 1.3 s
CH4
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
760
780
800
820
840
860
880
900
920
T / K

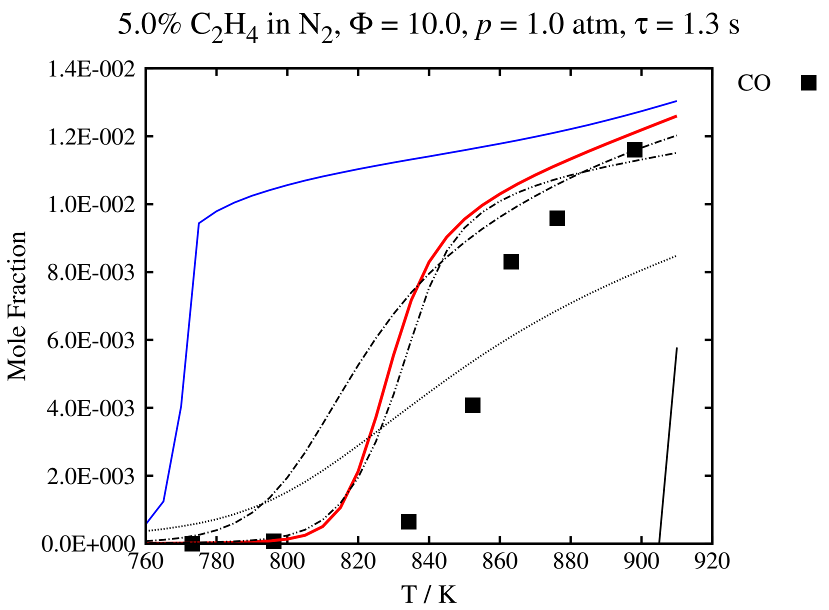
(b)


5.0% C_2H_4 in N_2, Φ = 10.0, p = 1.0 atm, τ = 1.3 s
C2H6
Mole Fraction
T / K
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
760
780
800
820
840
860
880
900
920

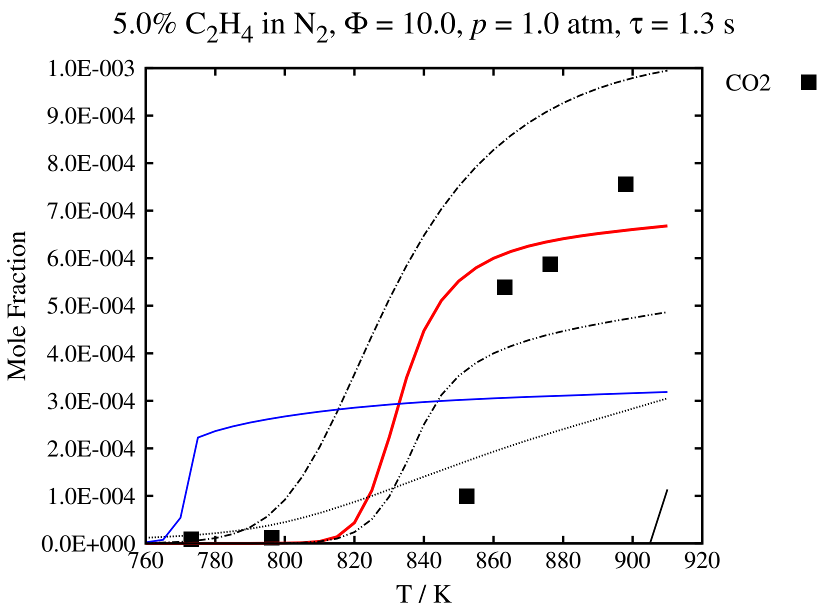
(c)


5.0% C_2H_4 in N_2, Φ = 10.0, p = 1.0 atm, τ = 1.3 s
C2H2
Mole Fraction
T / K
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
760
780
800
820
840
860
880
900
920

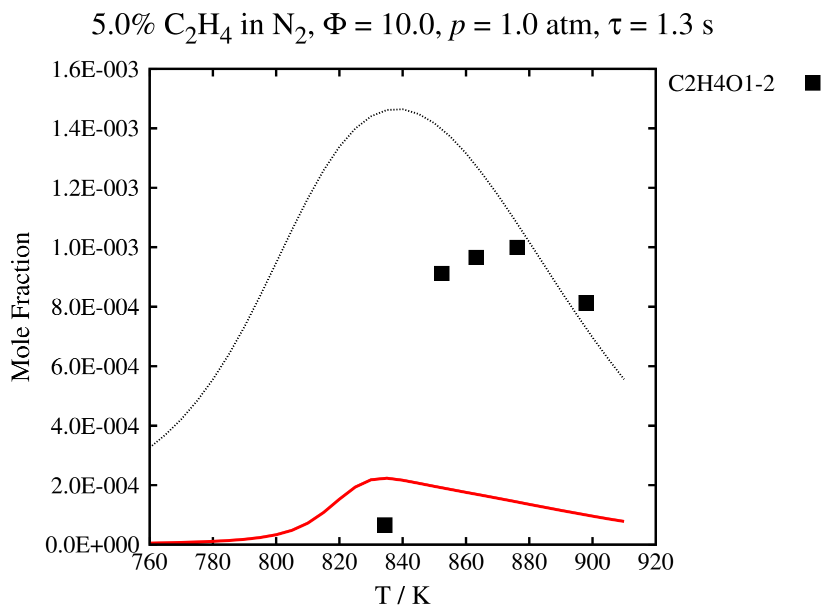
(d)


5.0% C_2H_4 in N_2, Φ = 10.0, p = 1.0 atm, τ = 1.3 s
CO
Mole Fraction
1.4E-002
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
760
780
800
820
840
860
880
900
920
T / K

(e)

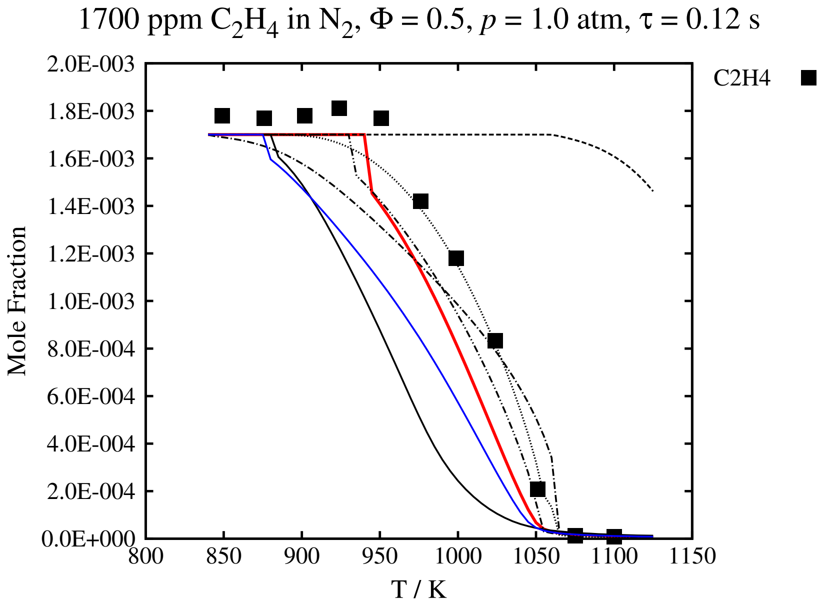

5.0% C_2H_4 in N_2, Φ = 10.0, p = 1.0 atm, τ = 1.3 s
CO2
Mole Fraction
1.0E-003
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
760
780
800
820
840
860
880
900
920
T / K

(f)

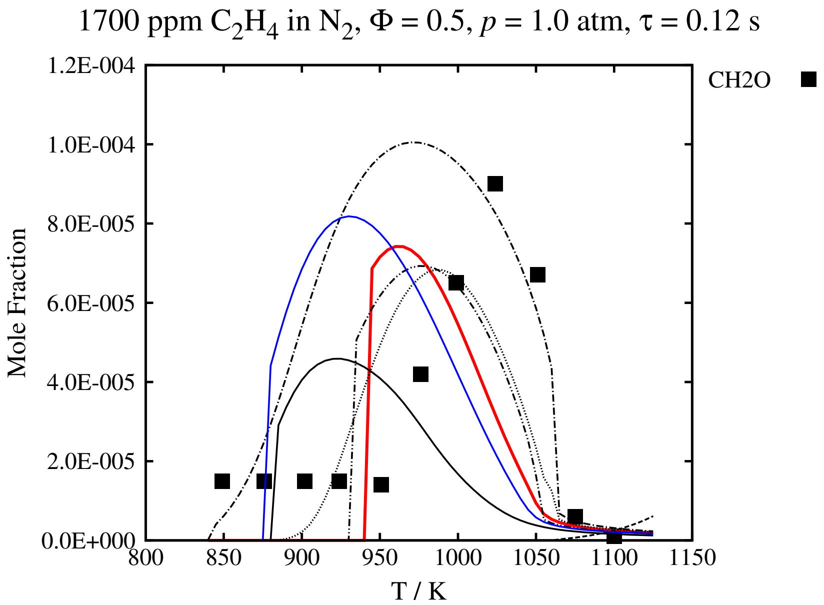


(g)

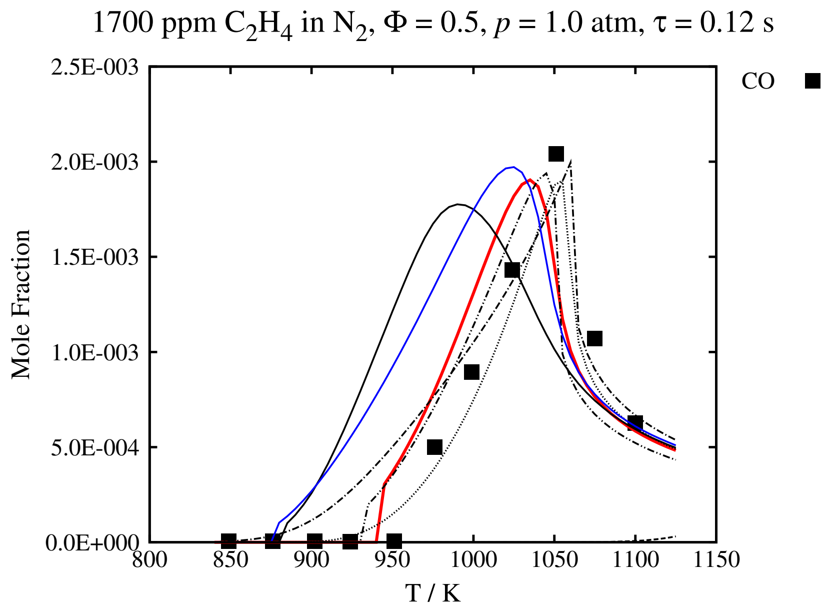
S36 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [33] lines are model predictions. —— AramcoMech 1.3, —— GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, —— USC II.


1700 ppm C2H4 in N2, Φ = 0.5, p = 1.0 atm, τ = 0.12 s
C2H4
Mole Fraction
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
800
850
900
950
1000
1050
1100
1150
T / K

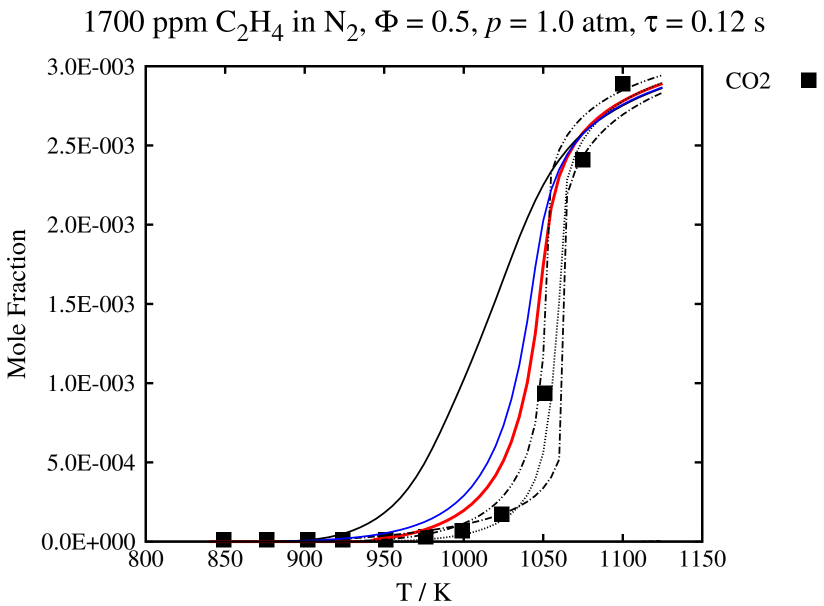
(a)


1700 ppm C2H4 in N2, Φ = 0.5, p = 1.0 atm, τ = 0.12 s
CH2O
Mole Fraction
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
800
850
900
950
1000
1050
1100
1150
T / K

(b)

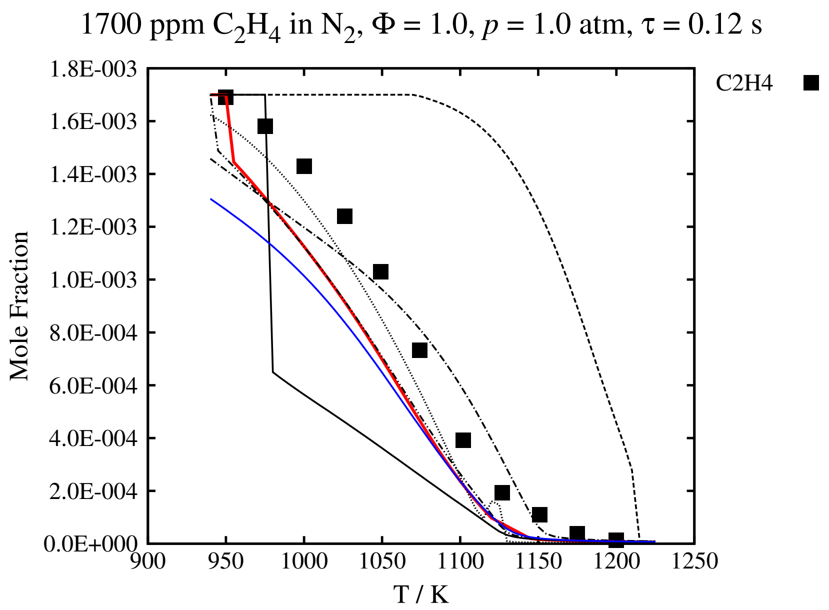


(c)

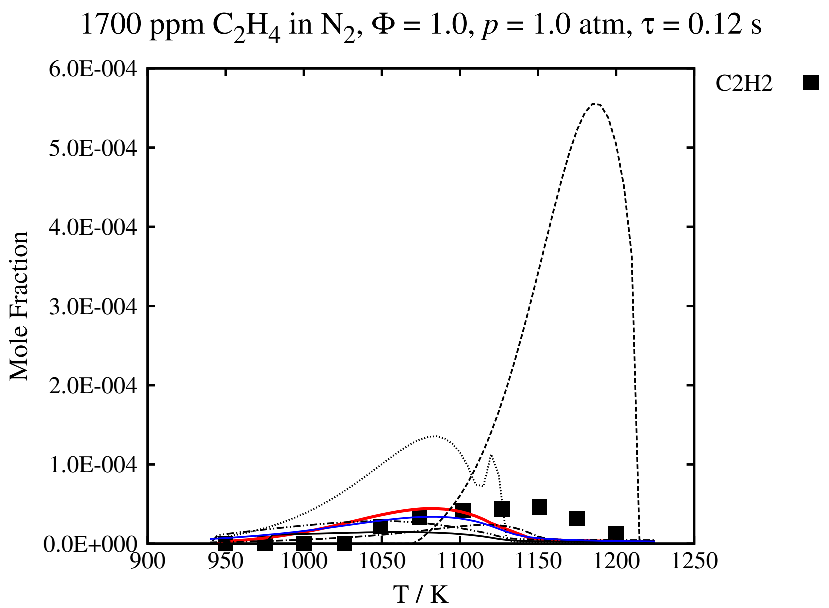


(d)

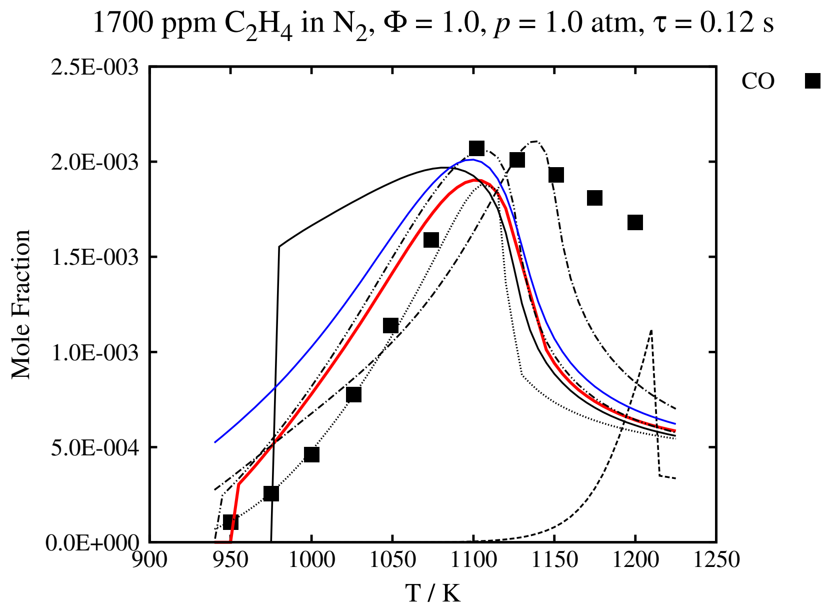
S37 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [34] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


1700 ppm C_2H_4 in N_2, Φ = 1.0, p = 1.0 atm, τ = 0.12 s
C2H4
Mole Fraction
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
900
950
1000
1050
1100
1150
1200
1250
T / K

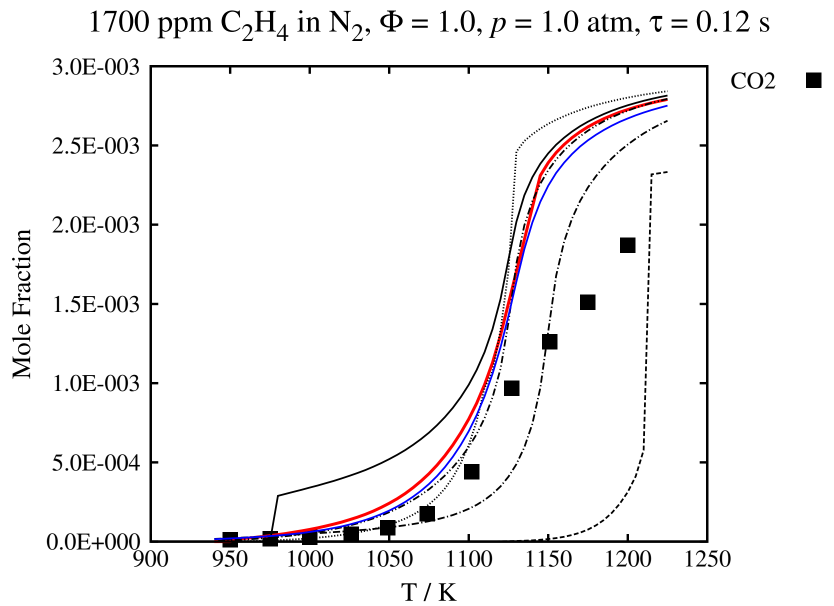
(a)


1700 ppm C_2H_4 in N_2, Φ = 1.0, p = 1.0 atm, τ = 0.12 s
C2H2
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
900
950
1000
1050
1100
1150
1200
1250
T / K

(b)

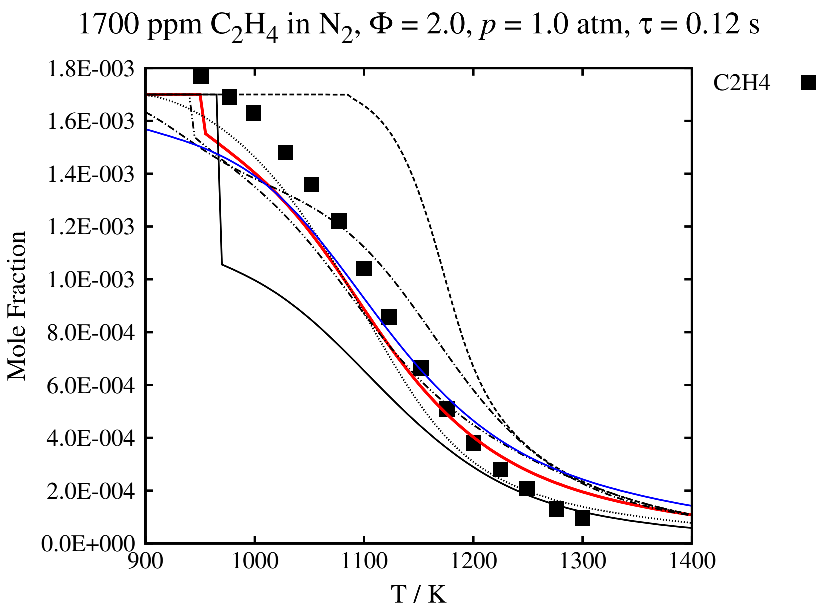


(c)

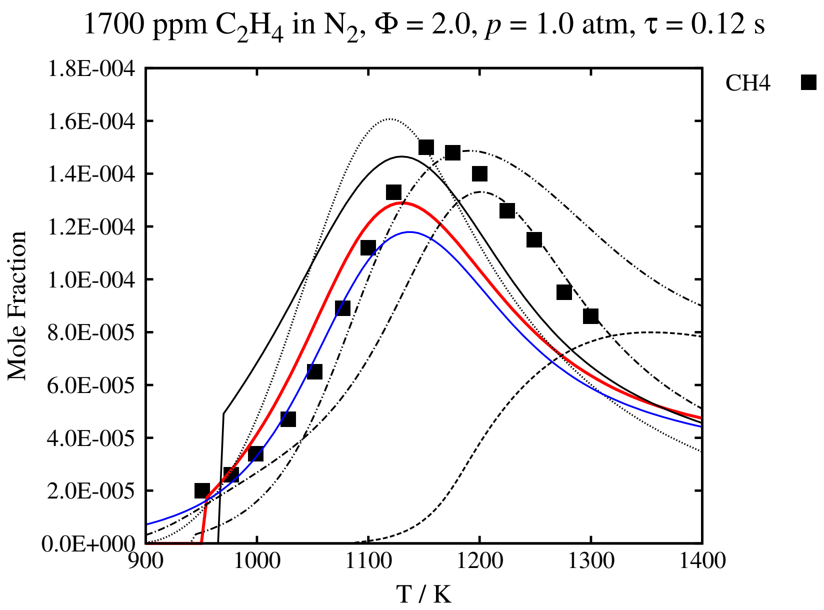


(d)

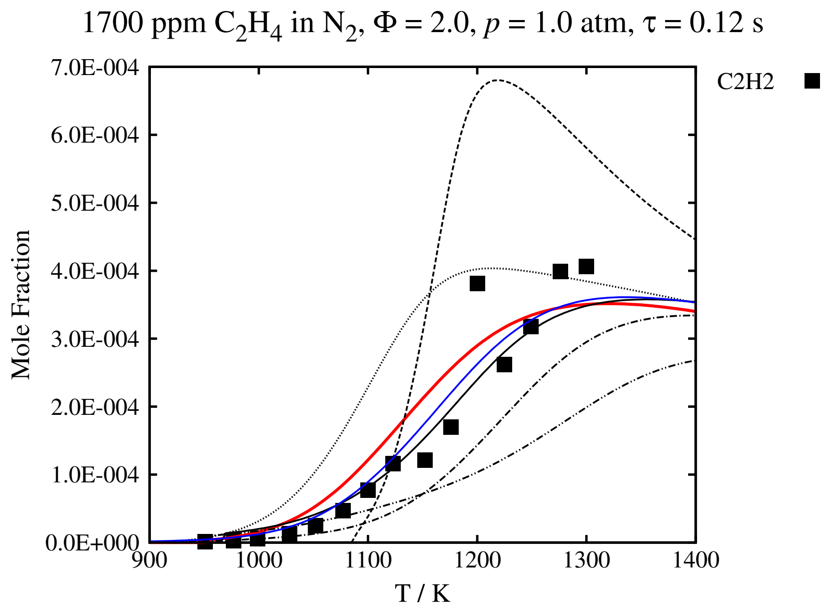
S38 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [34] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

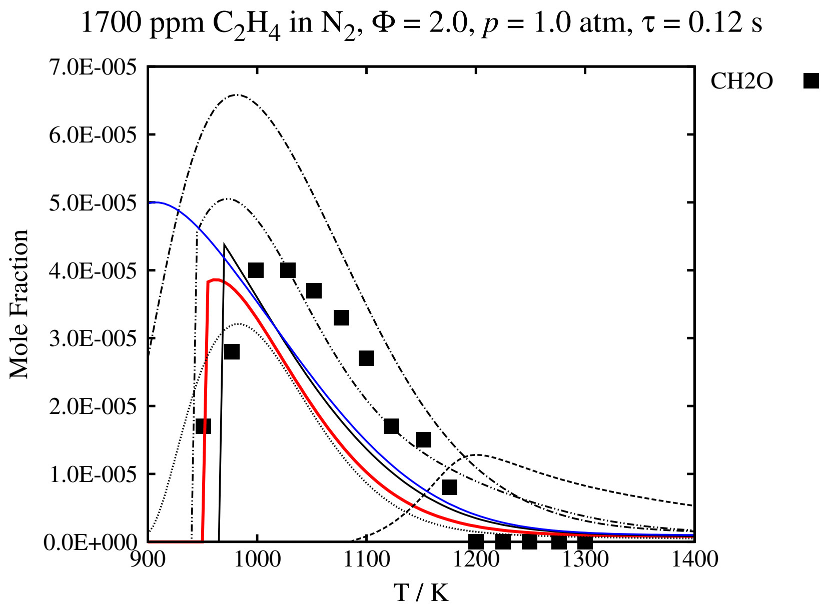

1700 ppm C_2H_4 in N_2, Φ = 2.0, p = 1.0 atm, τ = 0.12 s
C2H4
Mole Fraction
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
900
1000
1100
1200
1300
1400
T / K

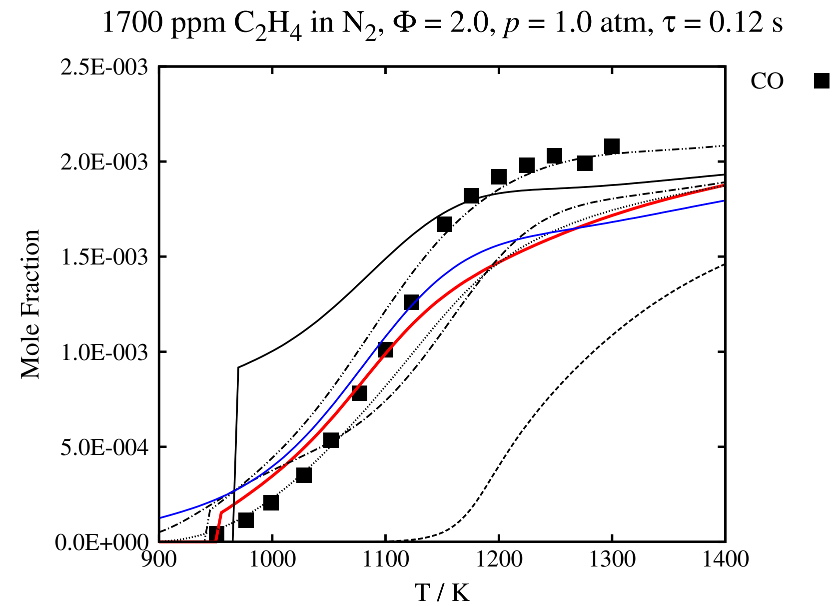
(a)


1700 ppm C_2H_4 in N_2, Φ = 2.0, p = 1.0 atm, τ = 0.12 s
CH4
Mole Fraction
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
900
1000
1100
1200
1300
1400
T / K

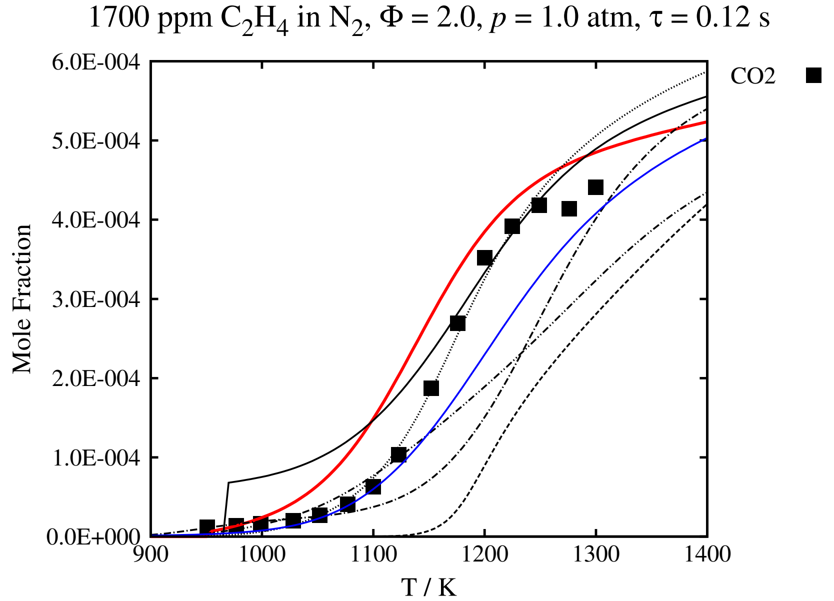
(b)


1700 ppm C_2H_4 in N_2, $\Phi = 2.0$, $p = 1.0$ atm, $\tau = 0.12$ s
Mole Fraction
T / K
C2H2
(c)


1700 ppm C_2H_4 in N_2, $\Phi = 2.0$, $p = 1.0$ atm, $\tau = 0.12$ s
Mole Fraction
T / K
CH2O
(d)

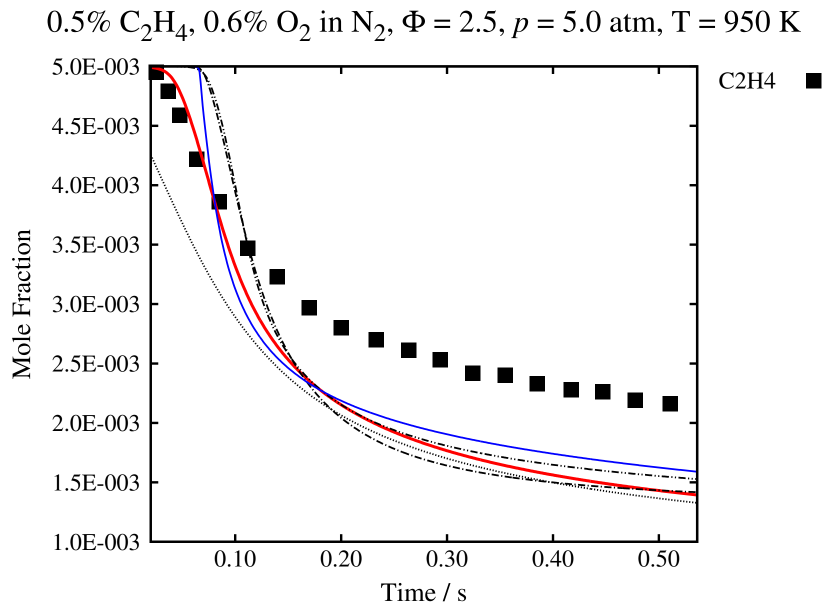


(e)

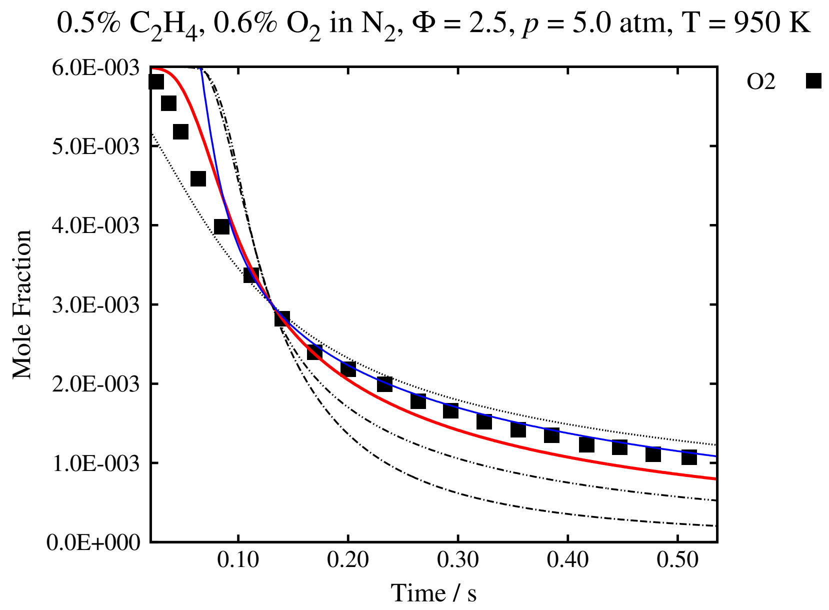


(f)

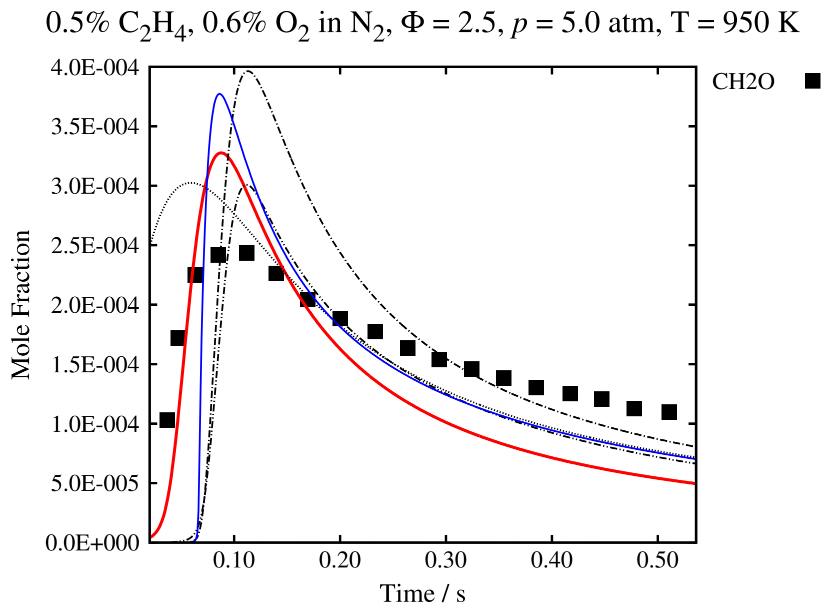
S39 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [34] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.5% C2H4, 0.6% O2 in N2, Φ = 2.5, p = 5.0 atm, T = 950 K
C2H4
Mole Fraction
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
0.10
0.20
0.30
0.40
0.50
Time / s

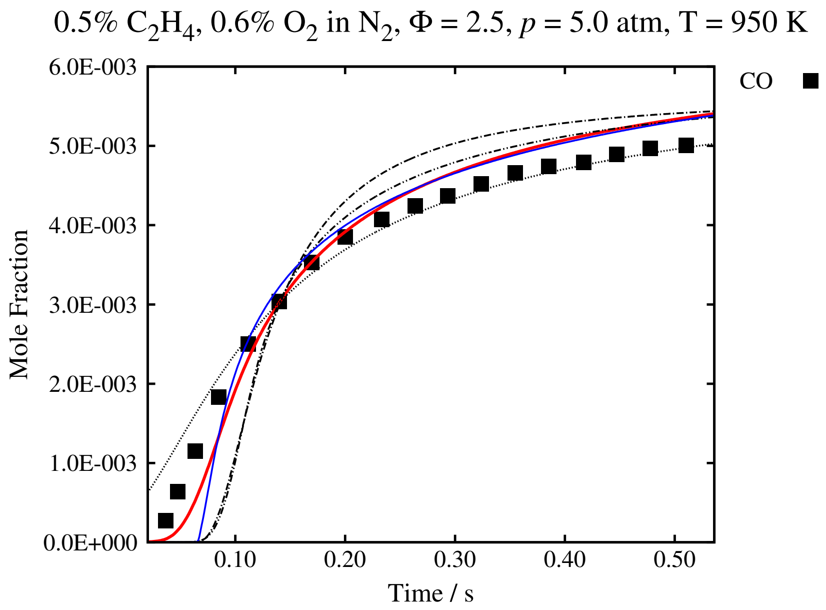
(a)


0.5% C2H4, 0.6% O2 in N2, Φ = 2.5, p = 5.0 atm, T = 950 K
O2
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.10
0.20
0.30
0.40
0.50
Time / s

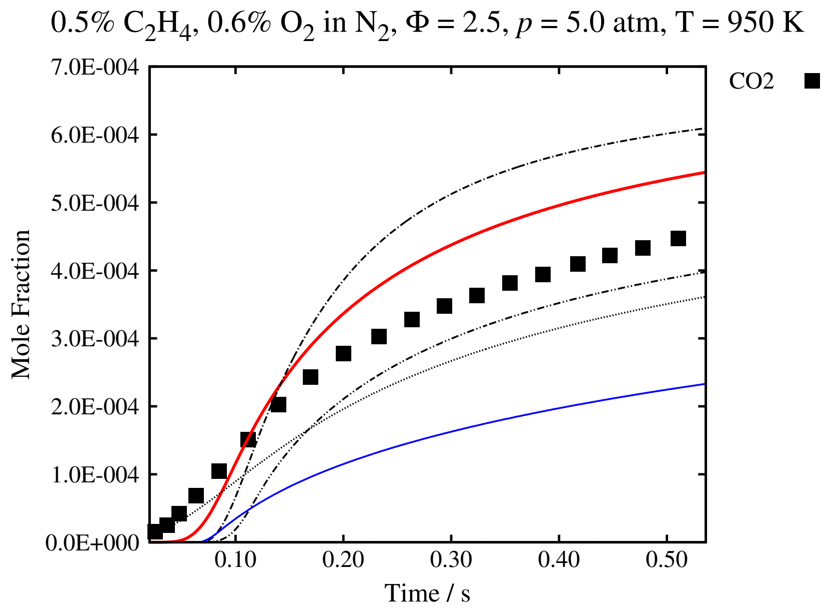
(b)


0.5% C_2H_4, 0.6% O_2 in N_2, Φ = 2.5, p = 5.0 atm, T = 950 K
CH2O
Mole Fraction
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.10
0.20
0.30
0.40
0.50
Time / s

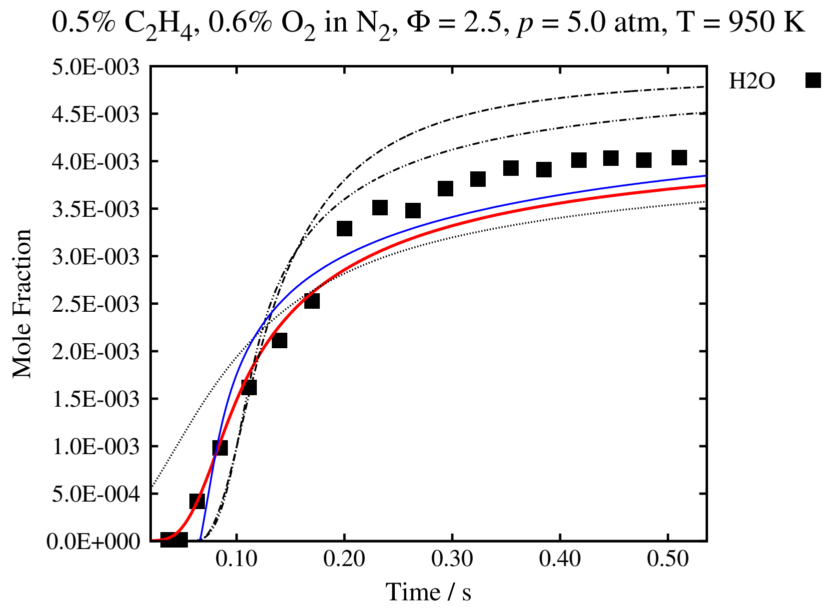
(c)


0.5% C_2H_4, 0.6% O_2 in N_2, Φ = 2.5, p = 5.0 atm, T = 950 K
CO
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.10
0.20
0.30
0.40
0.50
Time / s

(d)

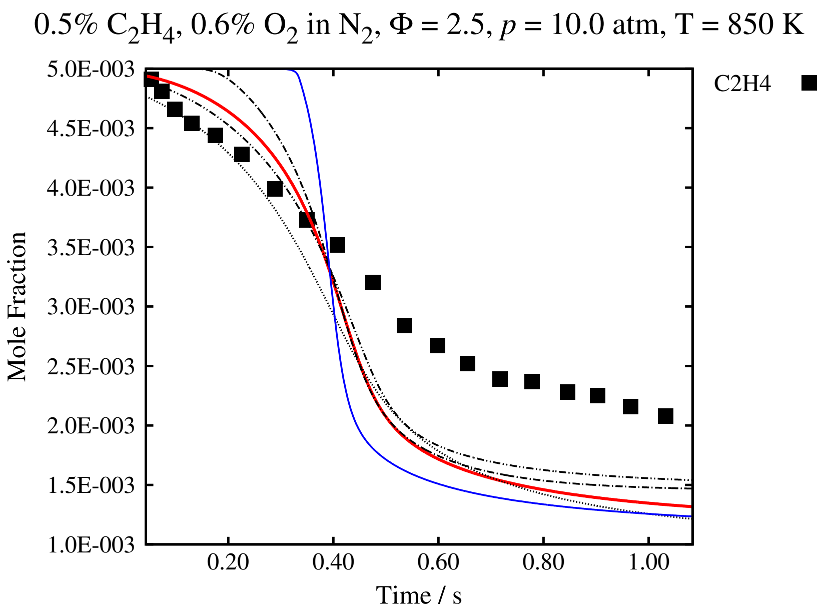


(e)

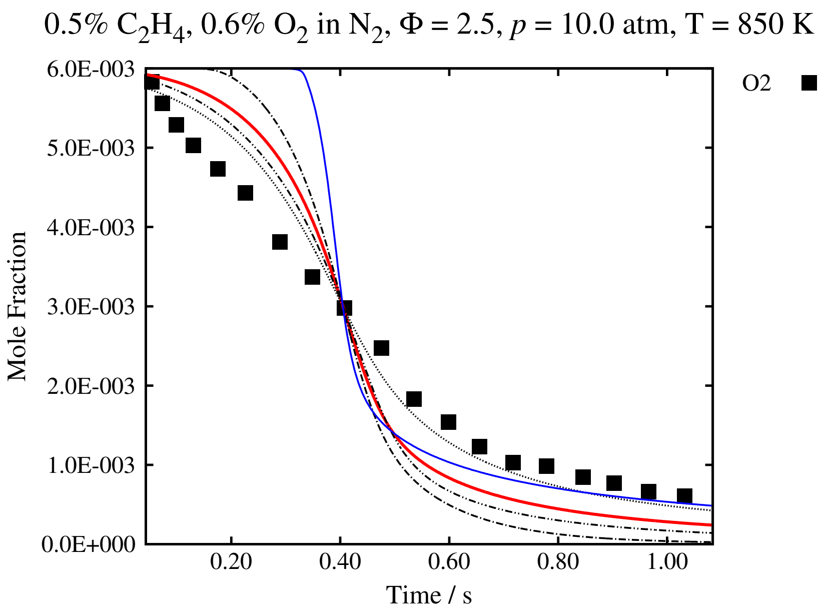


(f)

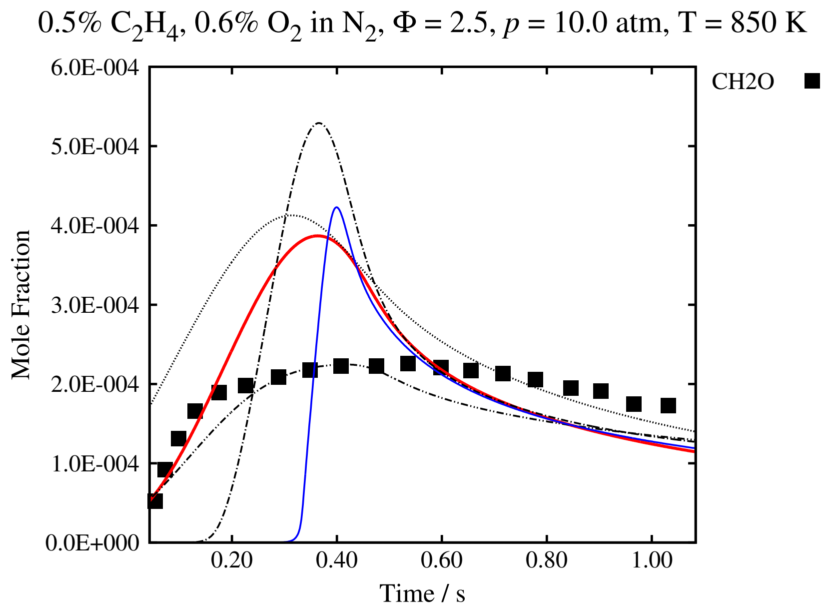
S40 Flow reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [35] lines are model predictions. Model predictions are shifted in order to match 50% oxygen consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.5% C_2H_4, 0.6% O_2 in N_2, Φ = 2.5, p = 10.0 atm, T = 850 K
C2H4
Mole Fraction
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
0.20
0.40
0.60
0.80
1.00
Time / s

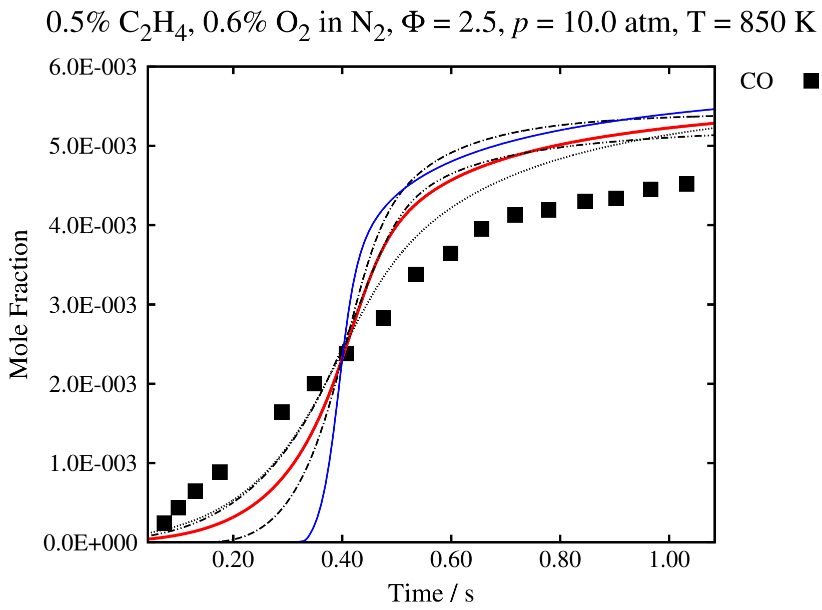
(a)


0.5% C_2H_4, 0.6% O_2 in N_2, Φ = 2.5, p = 10.0 atm, T = 850 K
O2
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.20
0.40
0.60
0.80
1.00
Time / s

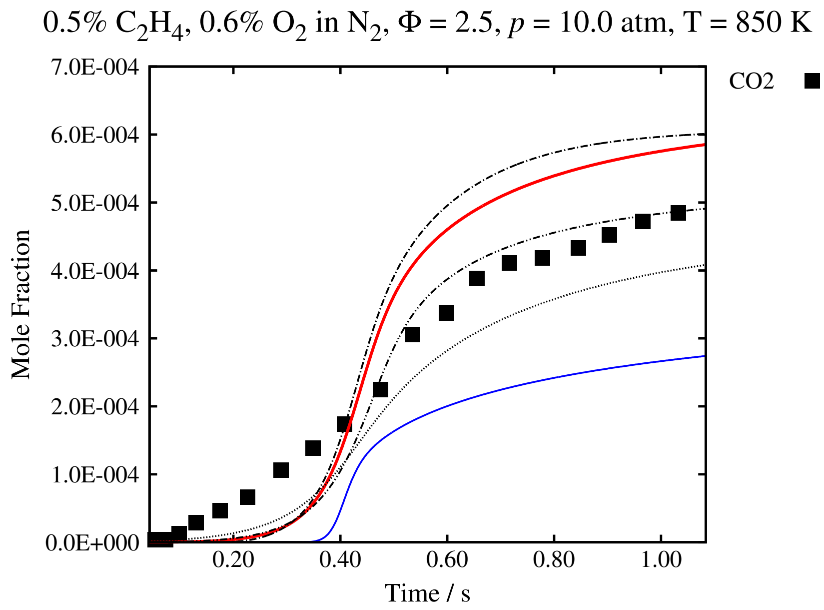
(b)


0.5% C_2H_4, 0.6% O_2 in N_2, Φ = 2.5, p = 10.0 atm, T = 850 K
CH2O
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.20
0.40
0.60
0.80
1.00
Time / s

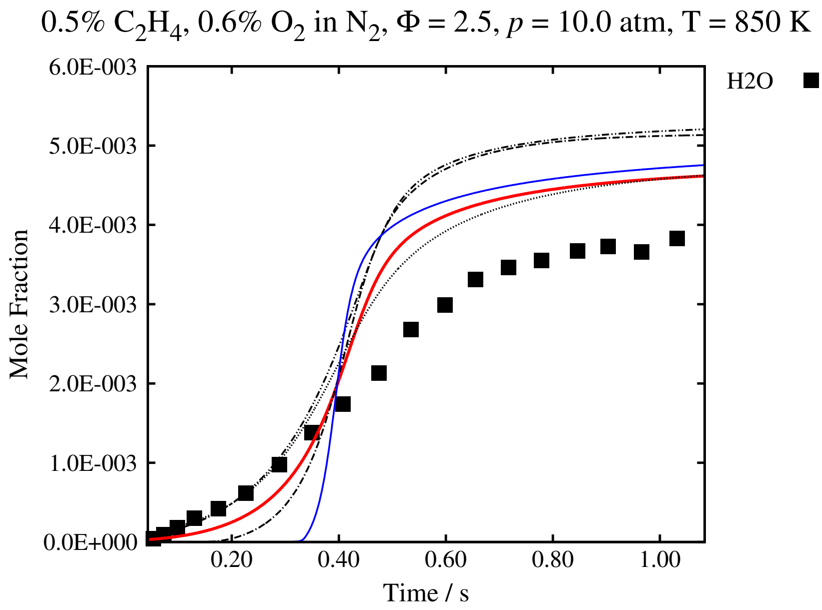
(c)


0.5% C_2H_4, 0.6% O_2 in N_2, Φ = 2.5, p = 10.0 atm, T = 850 K
CO
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.20
0.40
0.60
0.80
1.00
Time / s

(d)

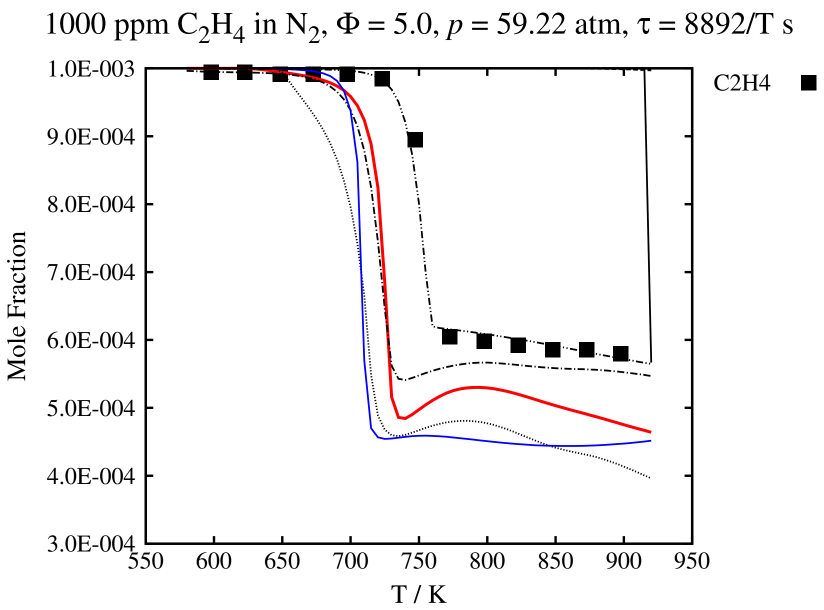


(e)

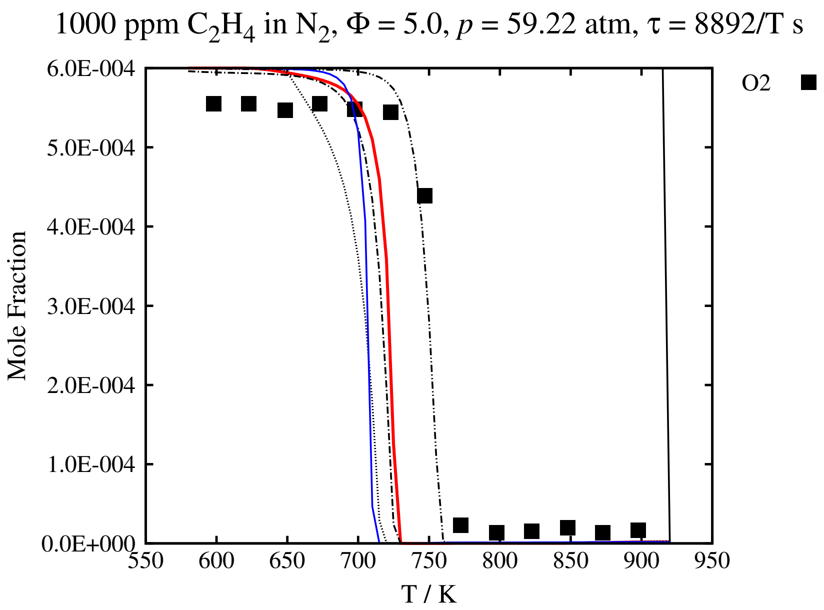


(f)

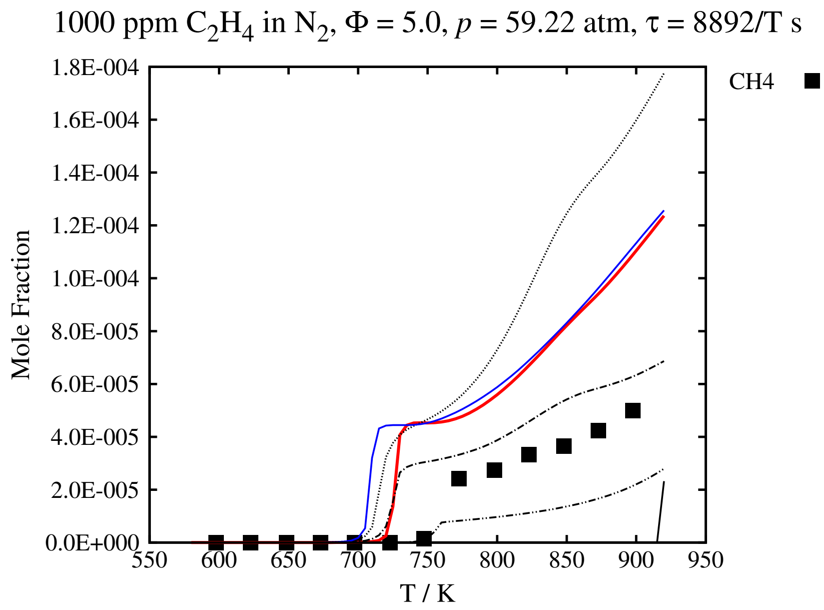
S41 Flow reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [35] lines are model predictions. Model predictions are shifted in order to match 50% oxygen consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


1000 ppm C_2H_4 in N_2, Φ = 5.0, p = 59.22 atm, τ = 8892/T s
C2H4
Mole Fraction
1.0E-003
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
550
600
650
700
750
800
850
900
950
T / K

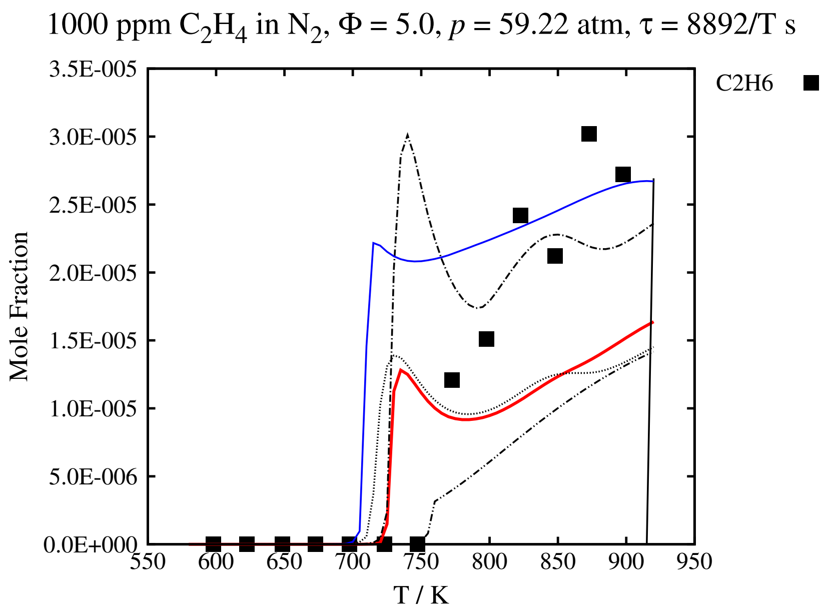
(a)


1000 ppm C_2H_4 in N_2, Φ = 5.0, p = 59.22 atm, τ = 8892/T s
O2
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
550
600
650
700
750
800
850
900
950
T / K

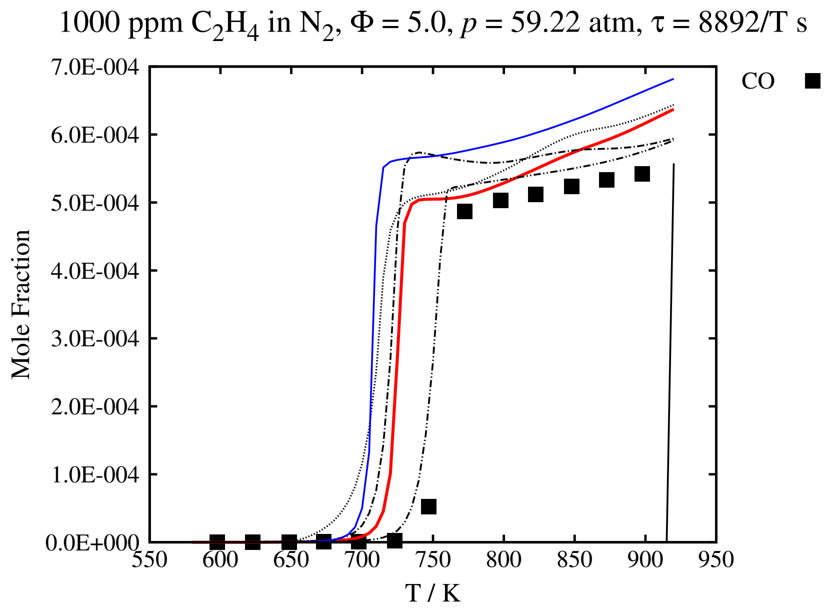
(b)


1000 ppm C_2H_4 in N_2, Φ = 5.0, *p* = 59.22 atm, τ = 8892/T s
CH4
Mole Fraction
T / K
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
550
600
650
700
750
800
850
900
950

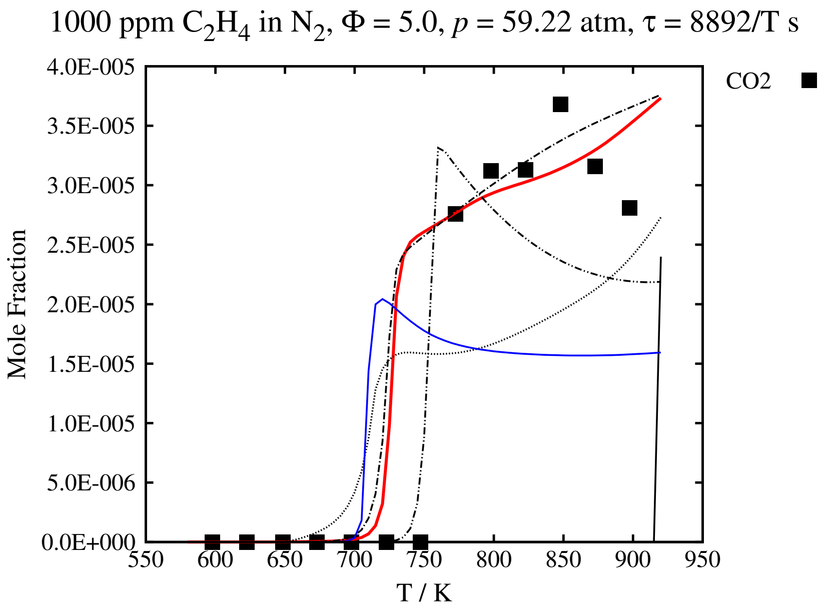
(c)


1000 ppm C_2H_4 in N_2, Φ = 5.0, *p* = 59.22 atm, τ = 8892/T s
C2H6
Mole Fraction
T / K
3.5E-005
3.0E-005
2.5E-005
2.0E-005
1.5E-005
1.0E-005
5.0E-006
0.0E+000
550
600
650
700
750
800
850
900
950

(d)

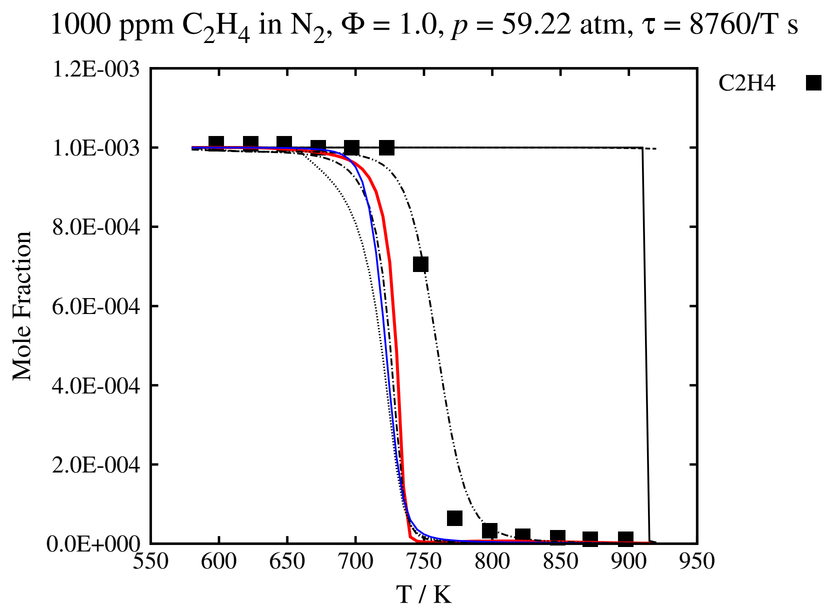


(e)

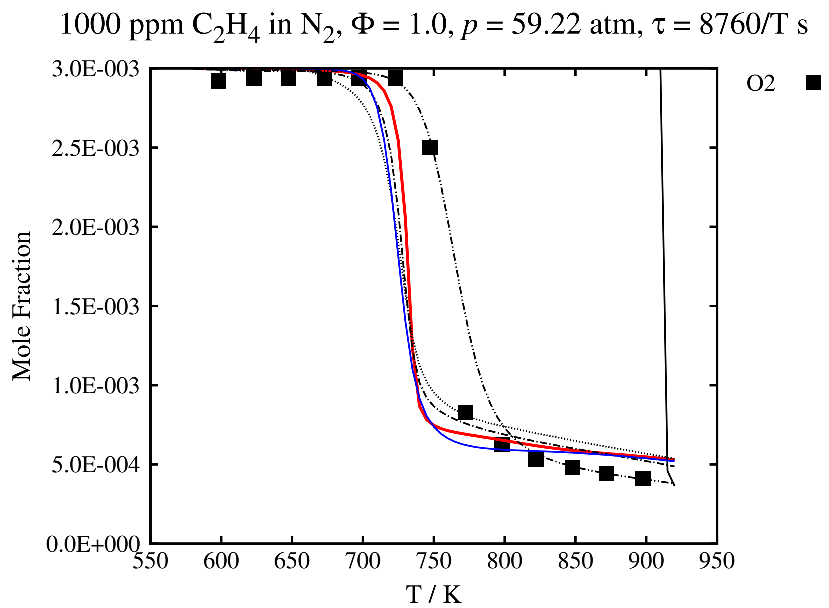


(f)

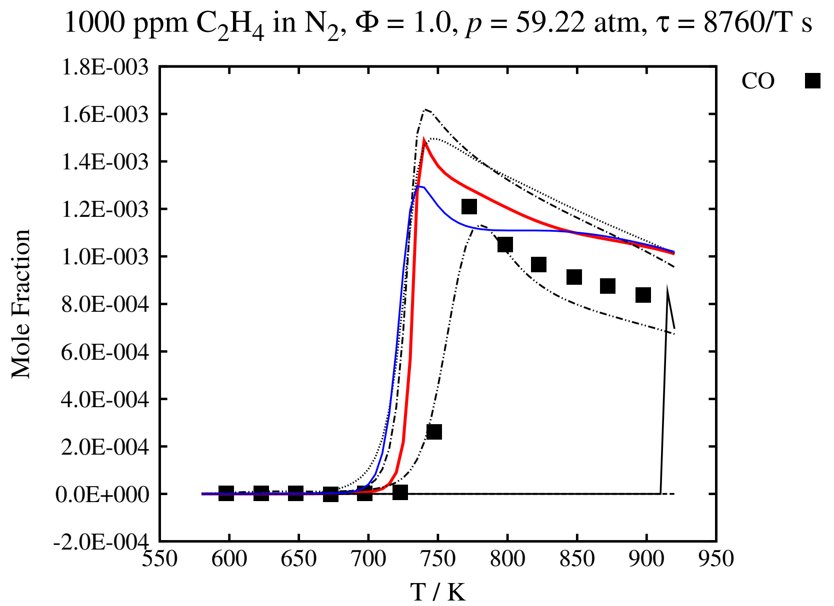
S42 Flow reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [36] lines are model predictions. —— AramcoMech 1.3, —— GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, —— USC II.


1000 ppm C_2H_4 in N_2, Φ = 1.0, p = 59.22 atm, τ = 8760/T s
C2H4
Mole Fraction
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
550 600 650 700 750 800 850 900 950
T / K

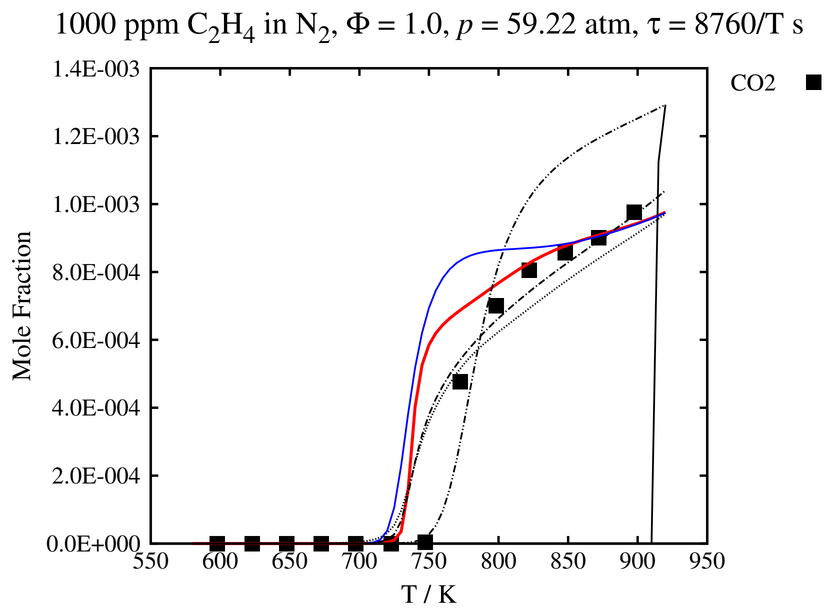
(a)


1000 ppm C_2H_4 in N_2, Φ = 1.0, p = 59.22 atm, τ = 8760/T s
O2
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
550 600 650 700 750 800 850 900 950
T / K

(b)

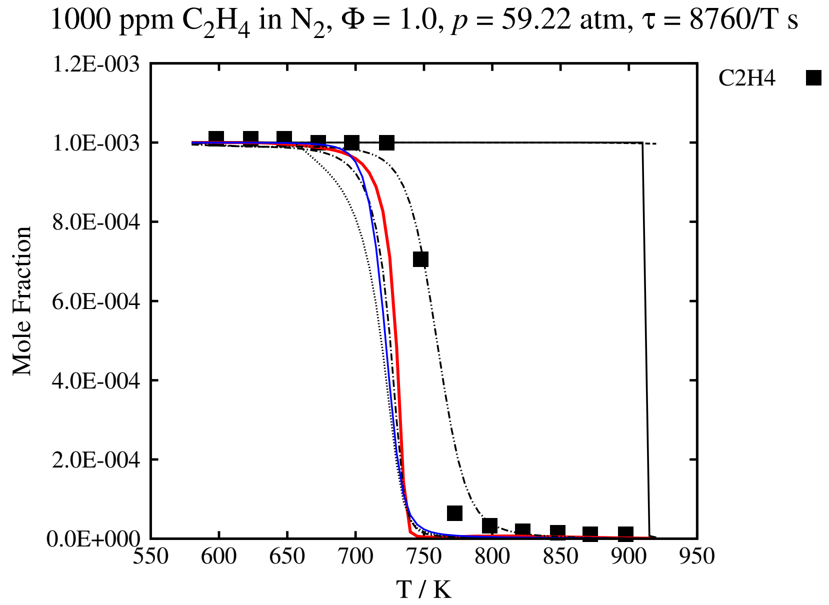


(c)



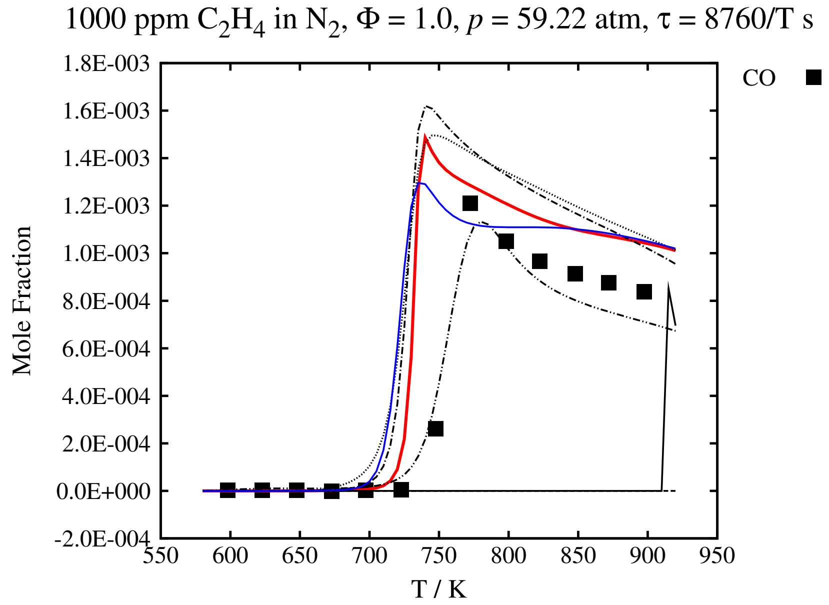
(d)

S43 Flow reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [36] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



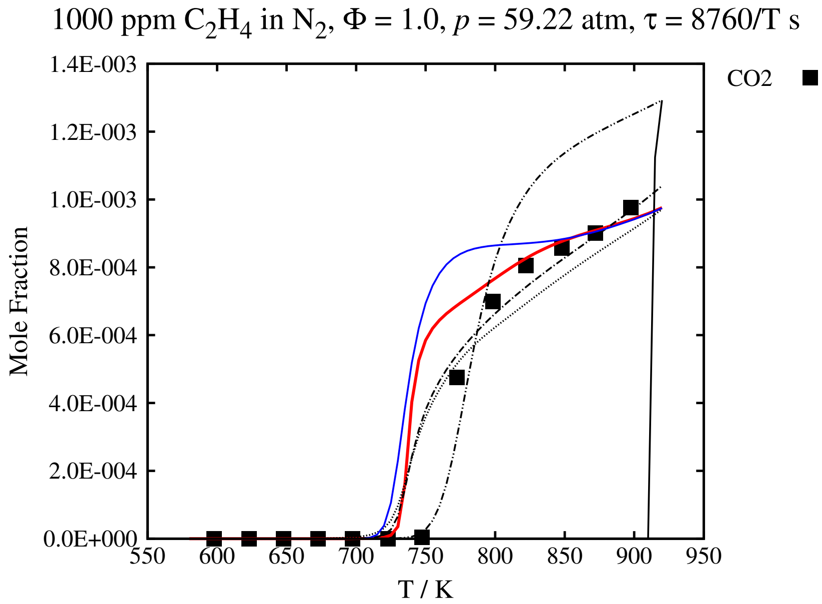
1000 ppm C_2H_4 in N_2, Φ = 1.0, p = 59.22 atm, τ = 8760/T s
C2H4
Mole Fraction
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
550
600
650
700
750
800
850
900
950
T / K

(a)



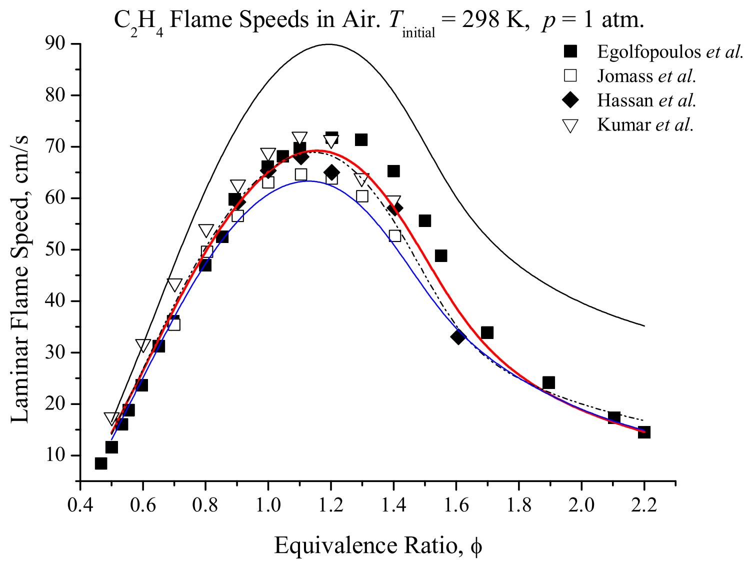
1000 ppm C_2H_4 in N_2, Φ = 1.0, p = 59.22 atm, τ = 8760/T s
CO
Mole Fraction
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
-2.0E-004
550
600
650
700
750
800
850
900
950
T / K

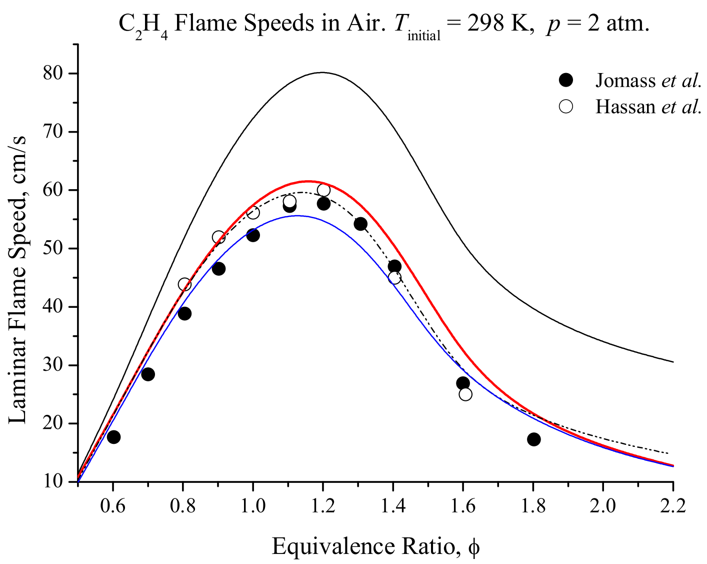
(b)

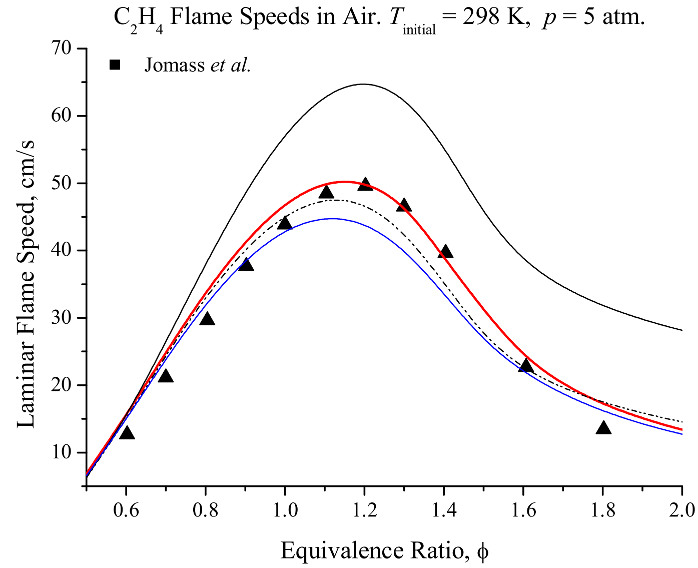


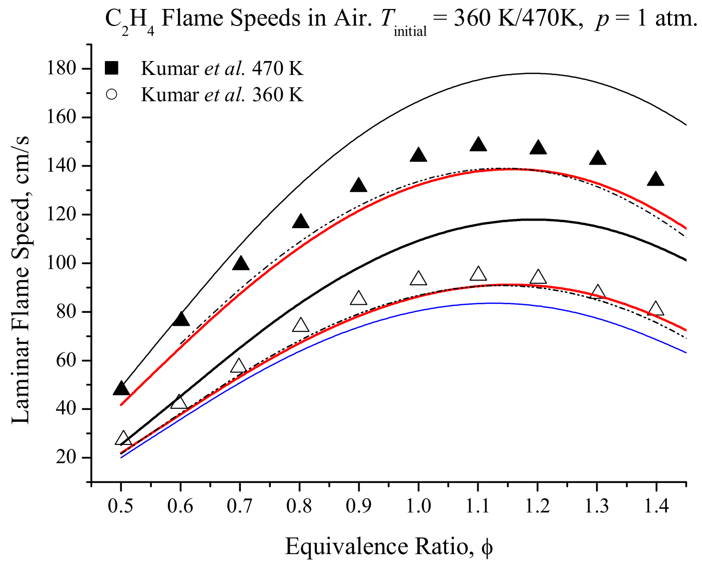
(c)

S44 Flow reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [36] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

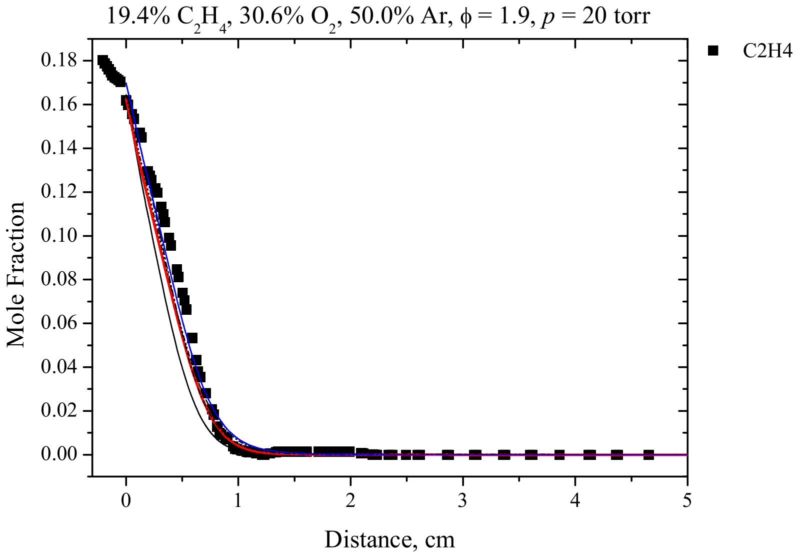

C$_2$H$_4$ Flame Speeds in Air. T_{initial} = 298 K, p = 1 atm.
Laminar Flame Speed, cm/s
Equivalence Ratio, ϕ
Egolfopoulos *et al.*
Jomass *et al.*
Hassan *et al.*
Kumar *et al.*
90
80
70
60
50
40
30
20
10
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2


C$_2$H$_4$ Flame Speeds in Air. T_{initial} = 298 K, p = 2 atm.
Laminar Flame Speed, cm/s
Equivalence Ratio, ϕ
Jomass *et al.*
Hassan *et al.*
80
70
60
50
40
30
20
10
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2

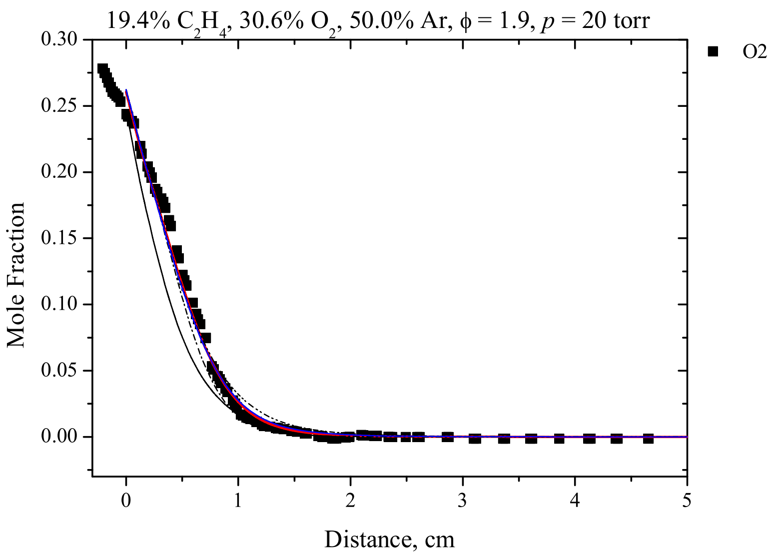




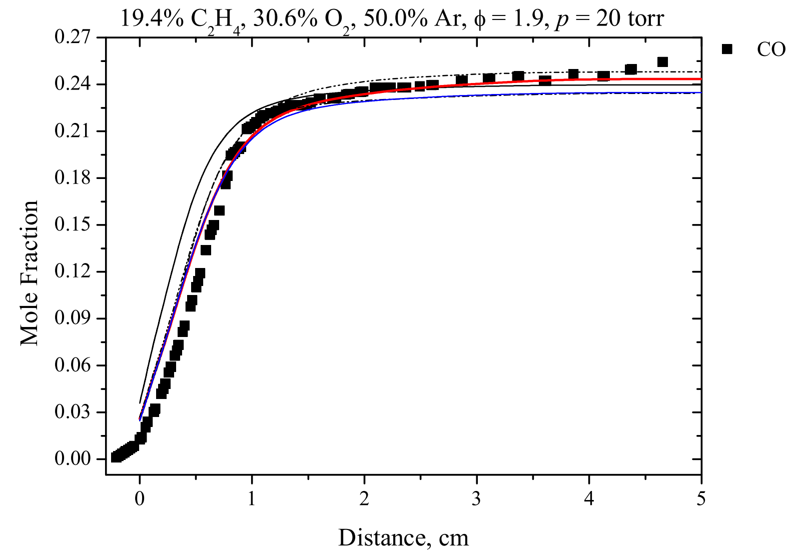
S45 Laminar flame speed measurements ethylene/air mixtures. Symbols are experimental data [19, 24, 37, 38] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

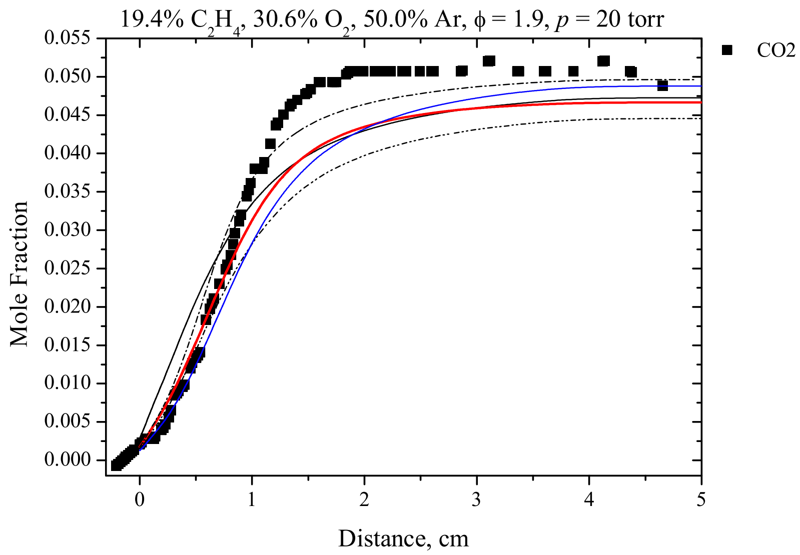


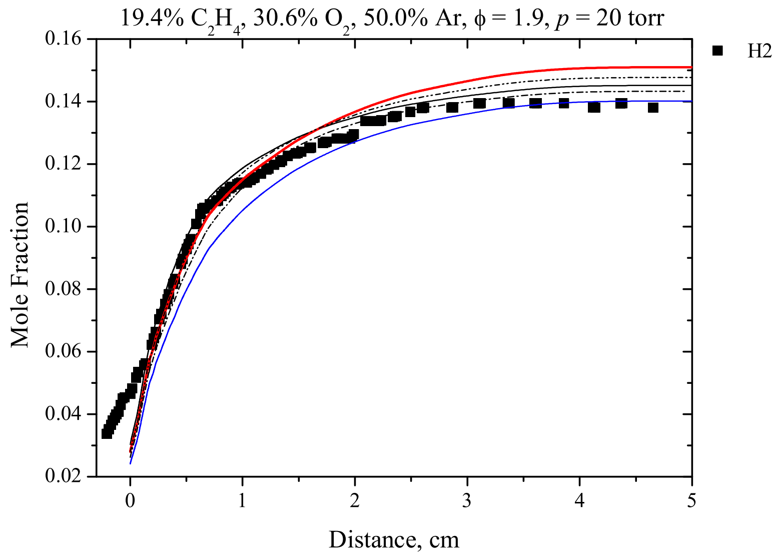
19.4% C2H4, 30.6% O2, 50.0% Ar, ϕ = 1.9, p = 20 torr
C2H4
Mole Fraction
Distance, cm
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0
1
2
3
4
5

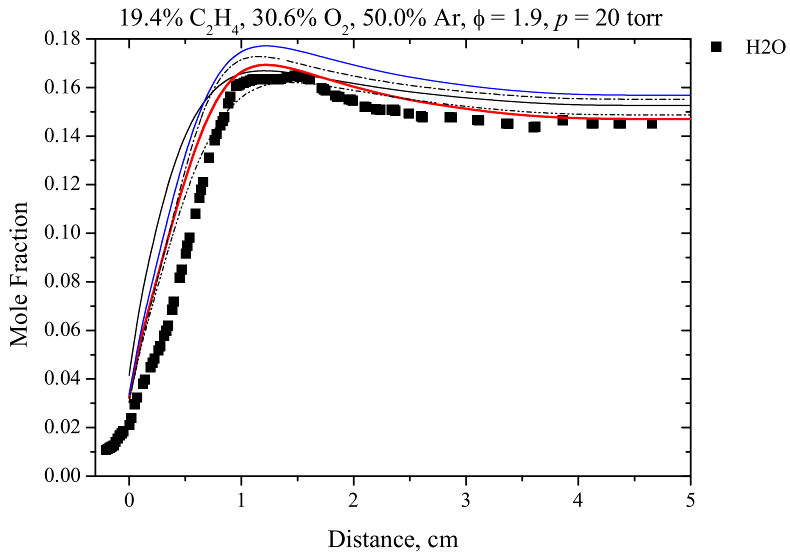


19.4% C2H4, 30.6% O2, 50.0% Ar, ϕ = 1.9, p = 20 torr
O2
Mole Fraction
Distance, cm
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
1
2
3
4
5


19.4% C2H4, 30.6% O2, 50.0% Ar, ϕ = 1.9, p = 20 torr
CO
Mole Fraction
Distance, cm
0.27
0.24
0.21
0.18
0.15
0.12
0.09
0.06
0.03
0.00
0
1
2
3
4
5


19.4% C2H4, 30.6% O2, 50.0% Ar, ϕ = 1.9, p = 20 torr
CO2
Mole Fraction
Distance, cm
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
0
1
2
3
4
5

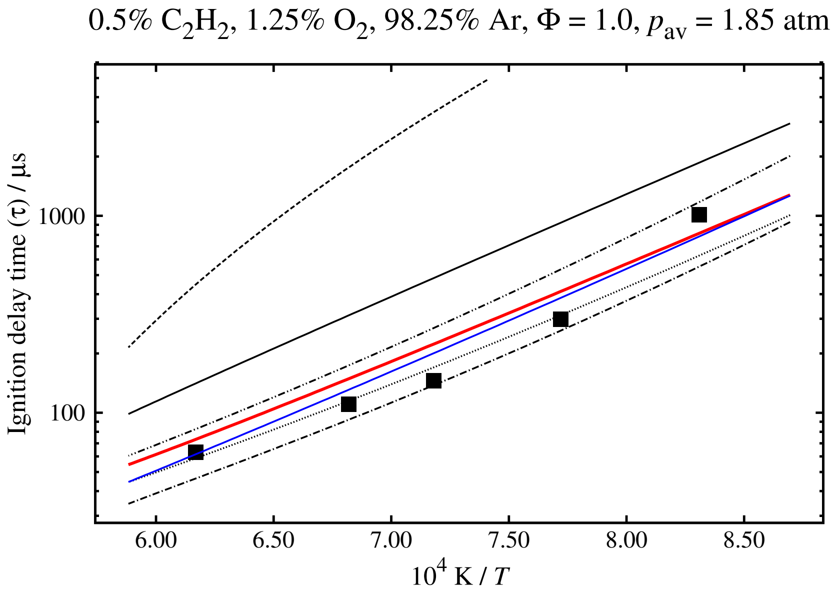




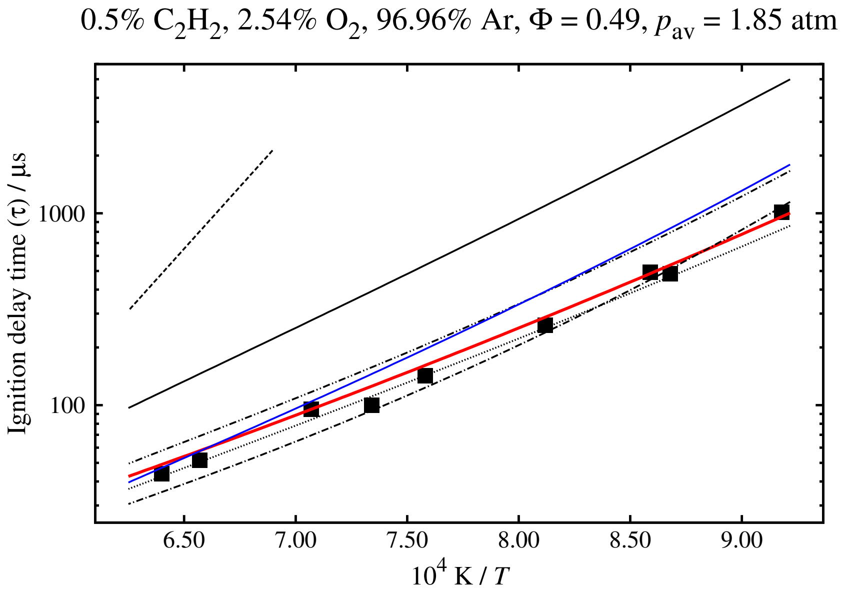
S46 Flame species profiles of ethylene/oxygen/argon mixtures. Experimental data has been shifted by 0.2054 cm which is within experimental uncertainty. Symbols are experimental data [39] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

2.4. Acetylene

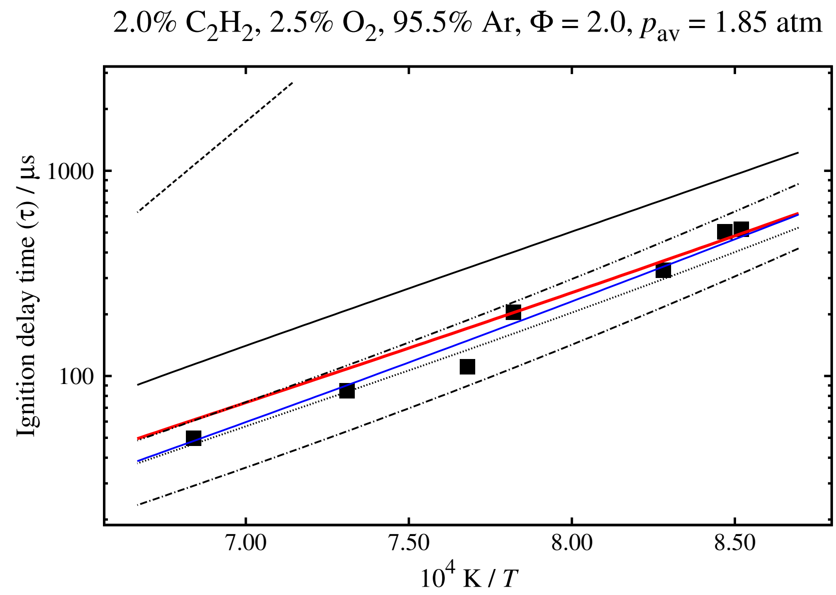
2.4.1. Shock Tube



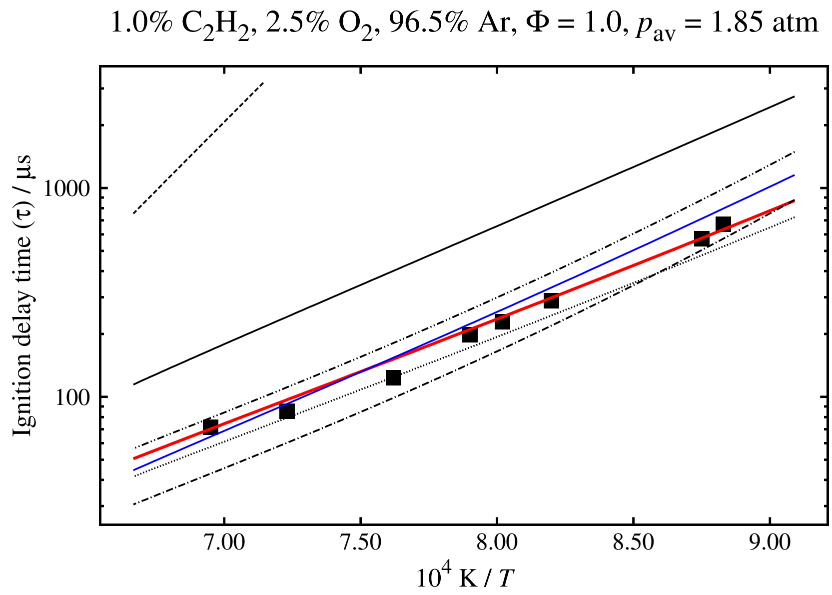
(a)



(b)

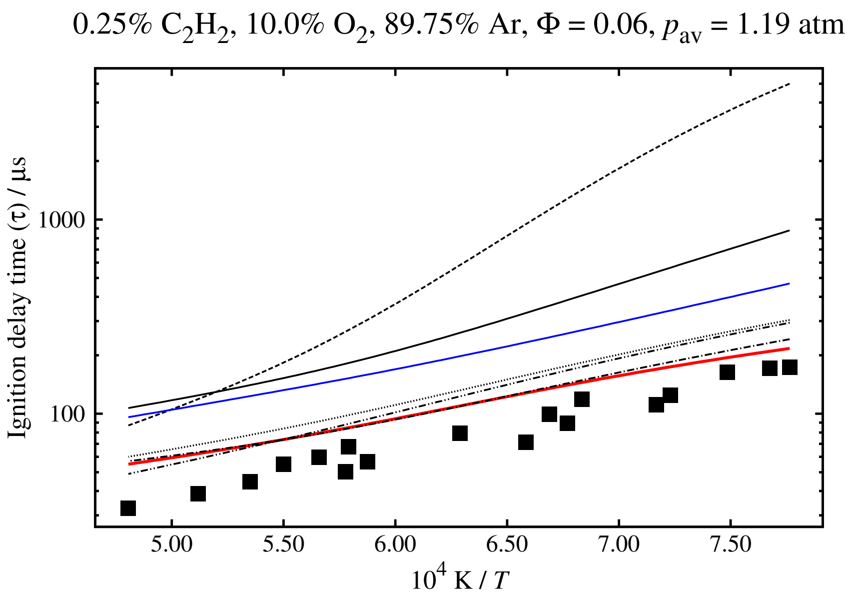


(c)

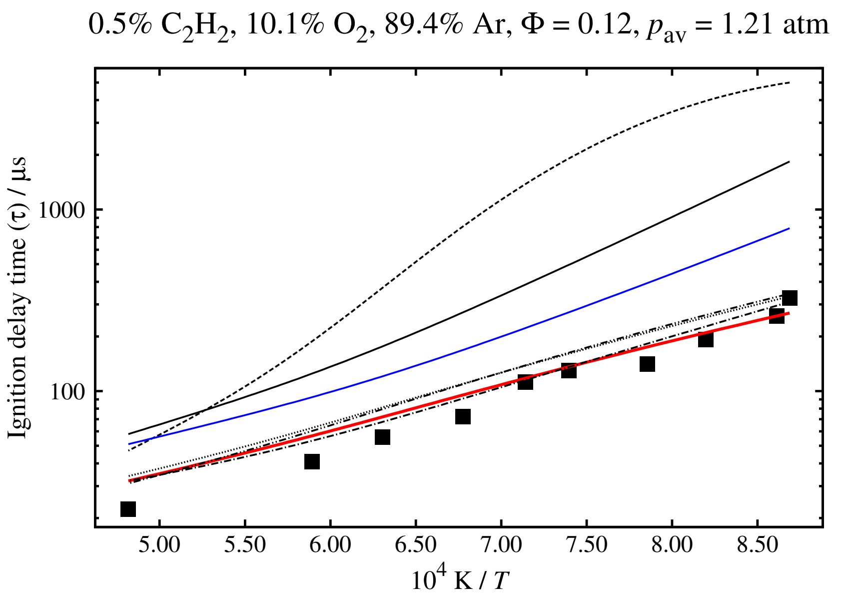


(d)

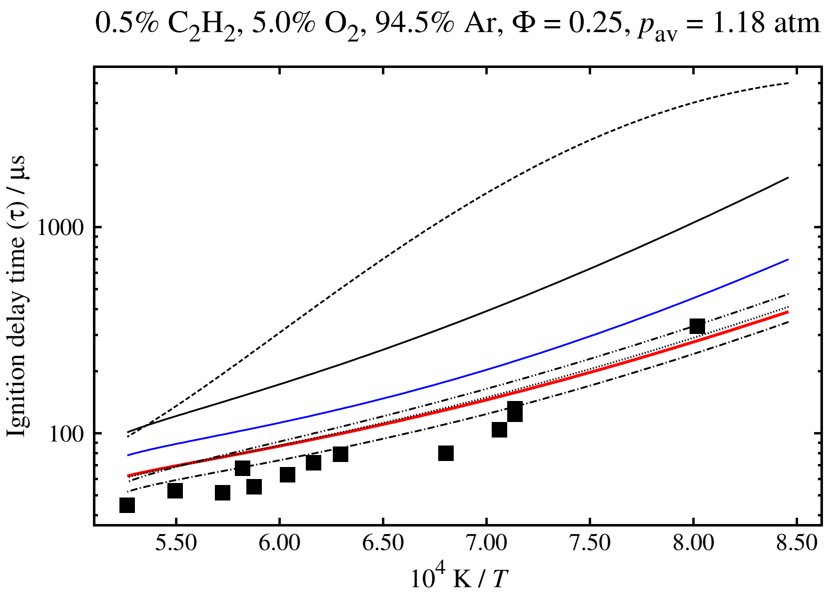
S47 Shock tube ignition delay times of acetylene/oxygen/argon mixtures. Symbols are experimental data [40] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.25% C2H2, 10.0% O2, 89.75% Ar, Φ = 0.06, pav = 1.19 atm
Ignition delay time (τ) / μs
1000
100
5.00
5.50
6.00
6.50
7.00
7.50
10⁴ K / T

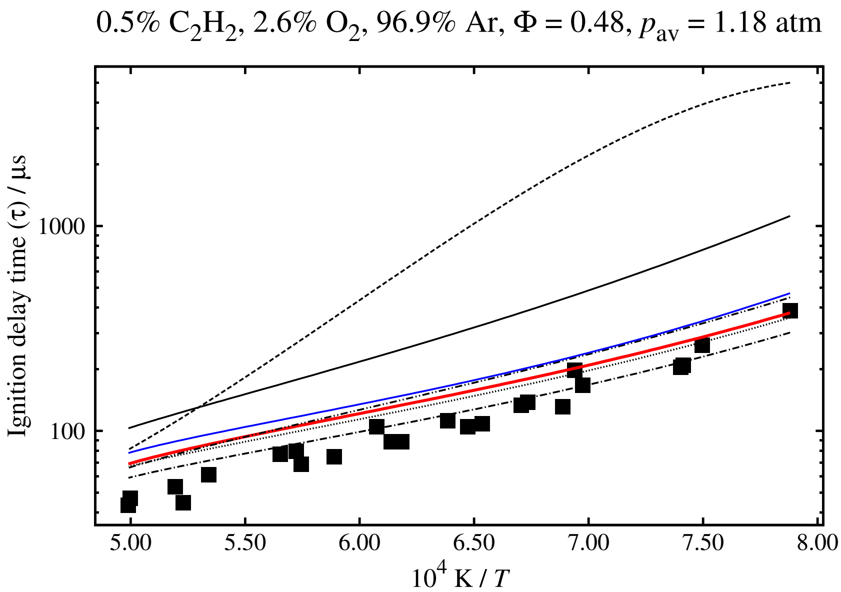
(a)


0.5% C2H2, 10.1% O2, 89.4% Ar, Φ = 0.12, pav = 1.21 atm
Ignition delay time (τ) / μs
1000
100
5.00
5.50
6.00
6.50
7.00
7.50
8.00
8.50
10⁴ K / T

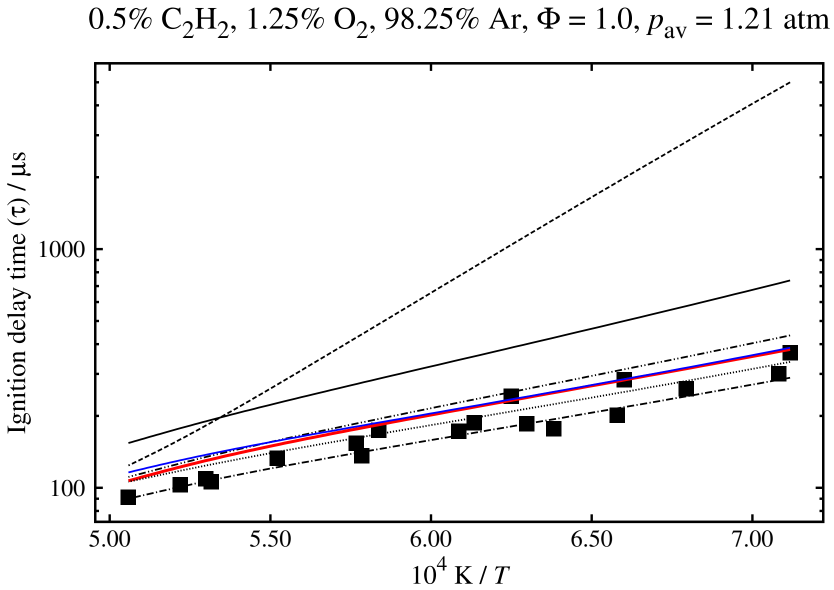
(b)


0.5% C_2H_2, 5.0% O_2, 94.5% Ar, $\Phi = 0.25$, $p_{av} = 1.18$ atm
Ignition delay time (τ) / µs
1000
100
5.50
6.00
6.50
7.00
7.50
8.00
8.50
10^4 K / T

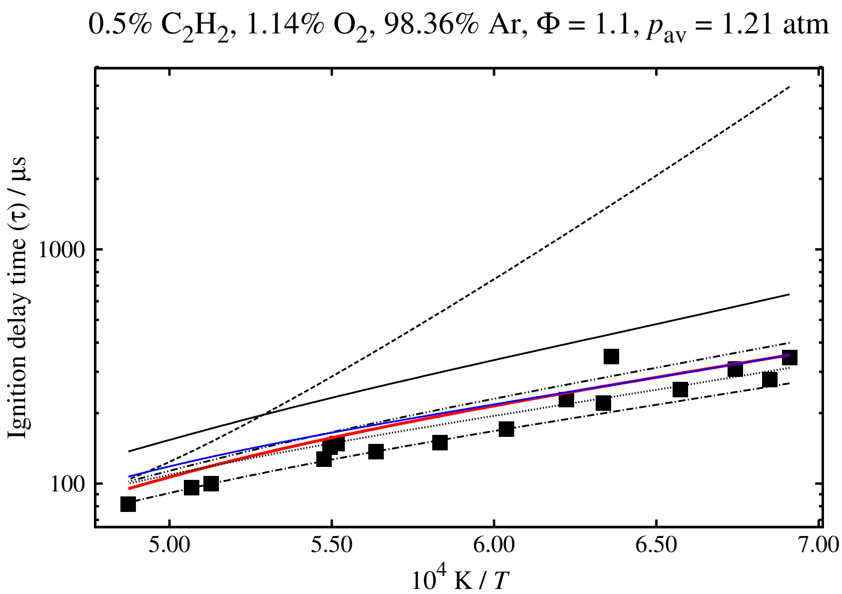
(c)


0.5% C_2H_2, 2.6% O_2, 96.9% Ar, $\Phi = 0.48$, $p_{av} = 1.18$ atm
Ignition delay time (τ) / µs
1000
100
5.00
5.50
6.00
6.50
7.00
7.50
8.00
10^4 K / T

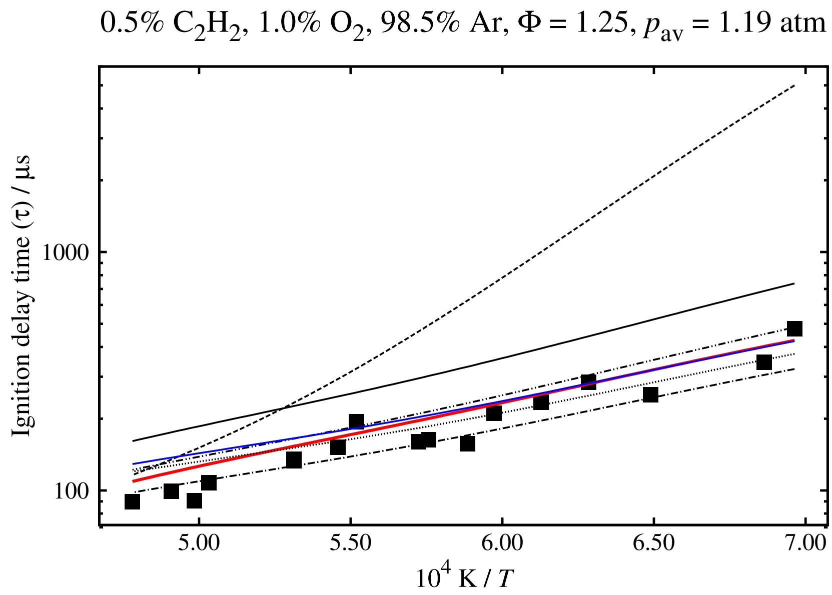
(d)


0.5% C2H2, 1.25% O2, 98.25% Ar, Φ = 1.0, pav = 1.21 atm
Ignition delay time (τ) / µs
1000
100
5.00
5.50
6.00
6.50
7.00
10^4 K / T

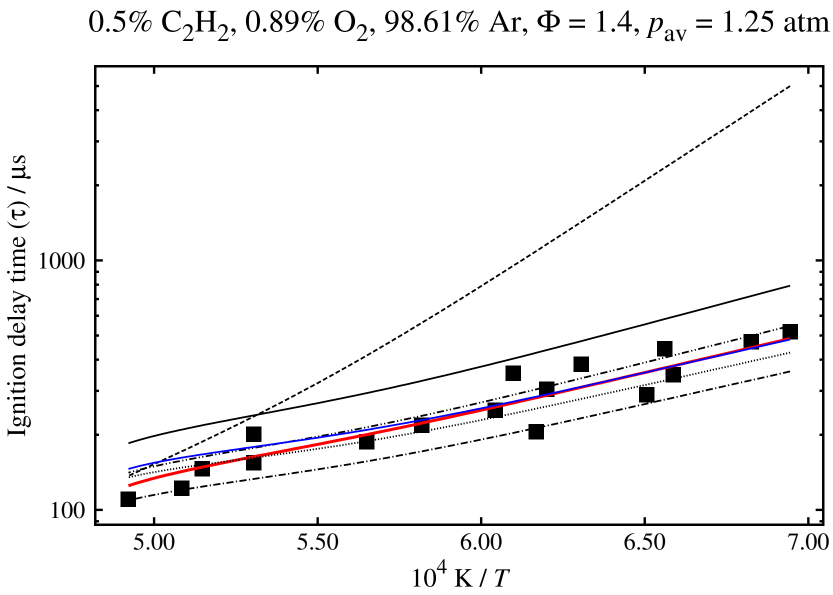
(e)


0.5% C2H2, 1.14% O2, 98.36% Ar, Φ = 1.1, pav = 1.21 atm
Ignition delay time (τ) / µs
1000
100
5.00
5.50
6.00
6.50
7.00
10^4 K / T

(f)

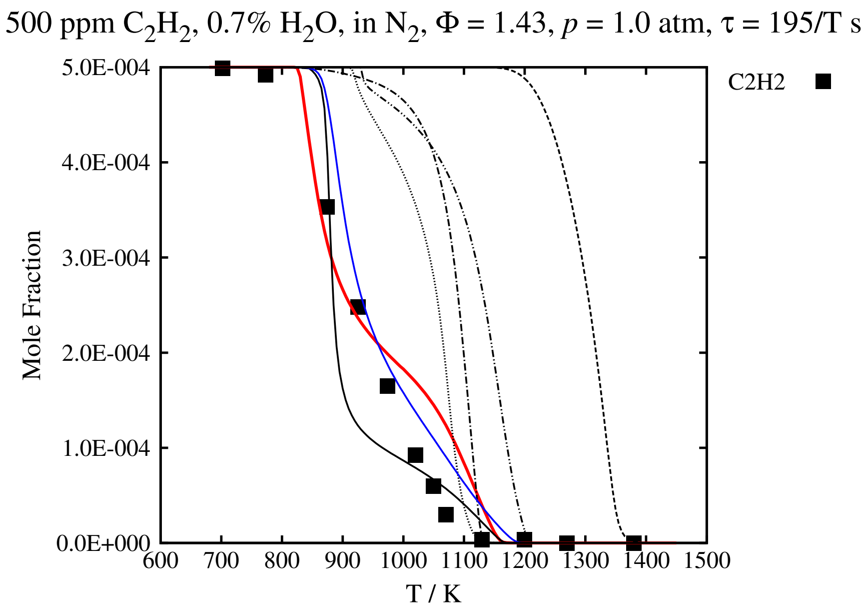


(g)

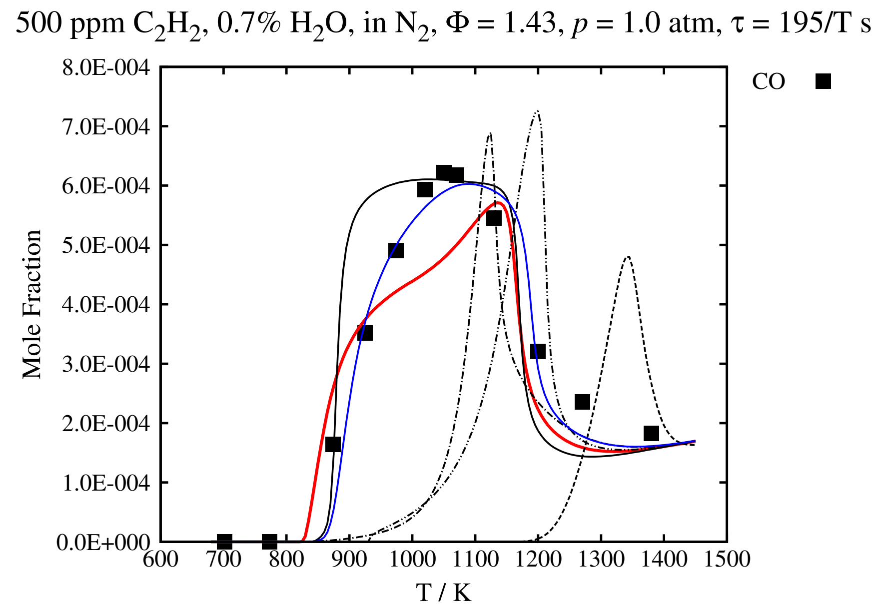


(h)

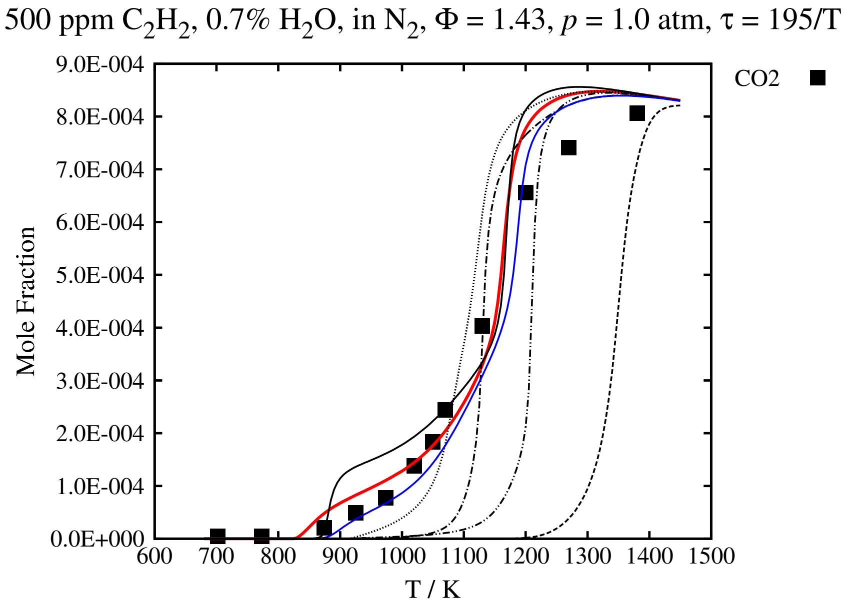
S48 Shock tube ignition delay times of acetylene/oxygen/argon mixtures. Symbols are experimental data [41] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


500 ppm C2H2, 0.7% H2O, in N2, Φ = 1.43, p = 1.0 atm, τ = 195/T s
C2H2
Mole Fraction
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
600 700 800 900 1000 1100 1200 1300 1400 1500
T / K

(a)


500 ppm C2H2, 0.7% H2O, in N2, Φ = 1.43, p = 1.0 atm, τ = 195/T s
CO
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
600 700 800 900 1000 1100 1200 1300 1400 1500
T / K

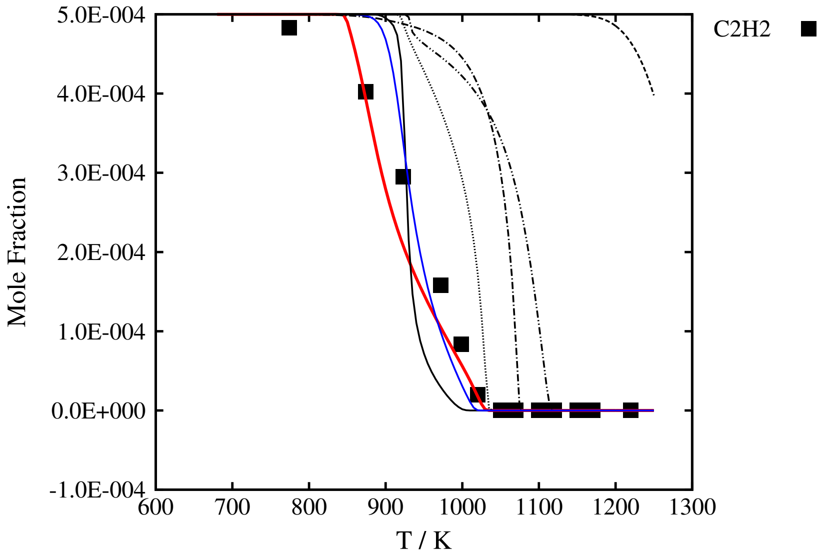
(b)



(c)

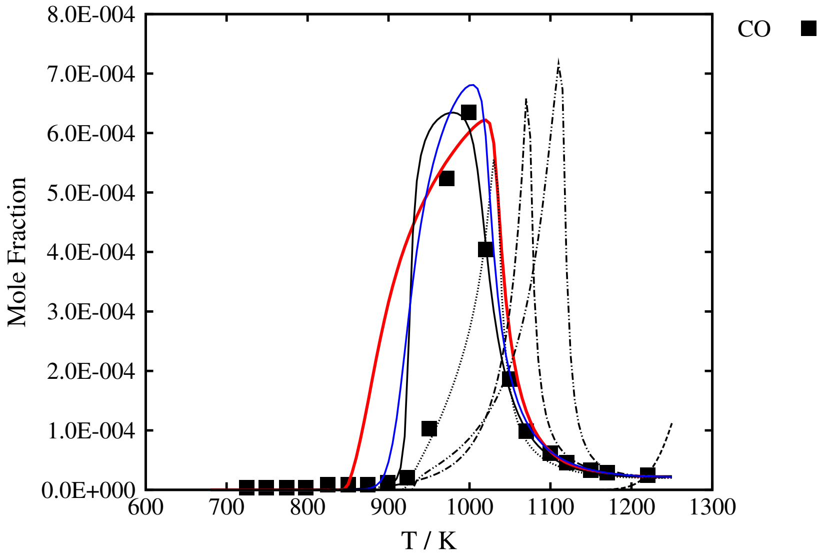
S49 Flow reactor species profiles of acetylene/oxygen/water/nitrogen mixtures. Symbols are experimental data [36] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

500 ppm C_2H_2, 0.7% H_2O, in N_2, $\Phi = 1.0$, $p = 1.0$ atm, $\tau = 195/T$ s

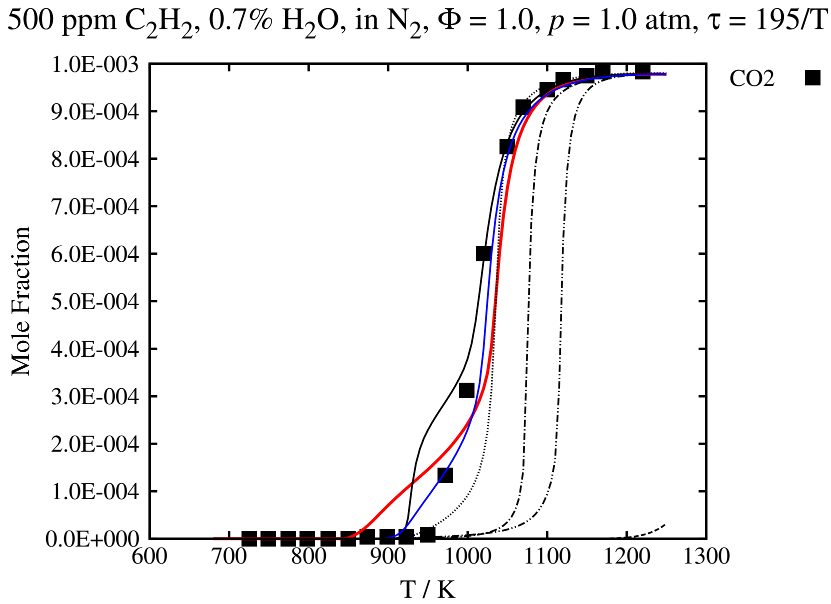


(a)

500 ppm C_2H_2, 0.7% H_2O, in N_2, $\Phi = 1.0$, $p = 1.0$ atm, $\tau = 195/T$ s

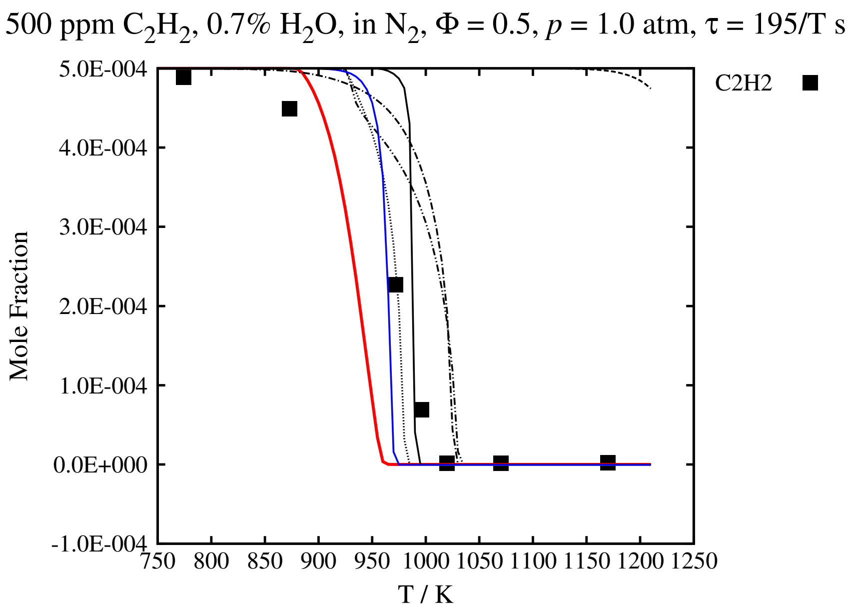


(b)

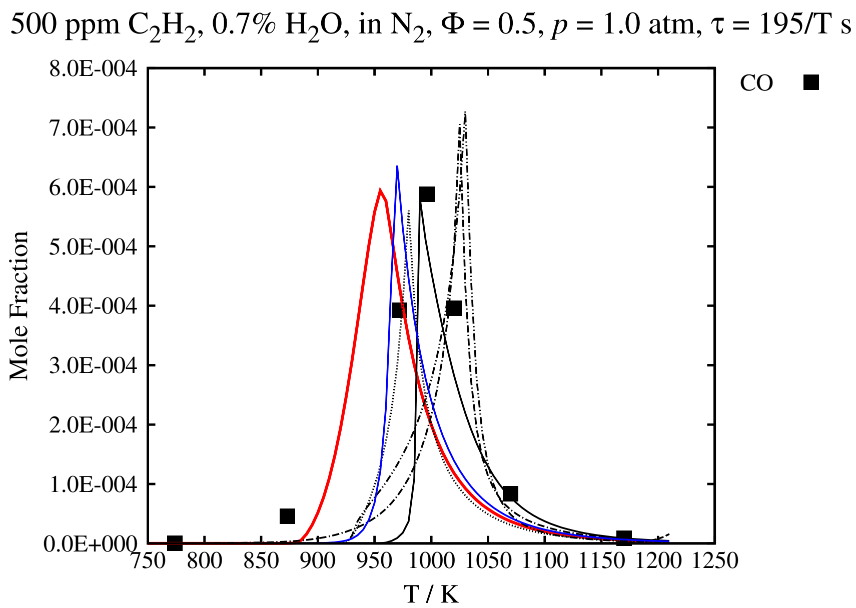


(c)

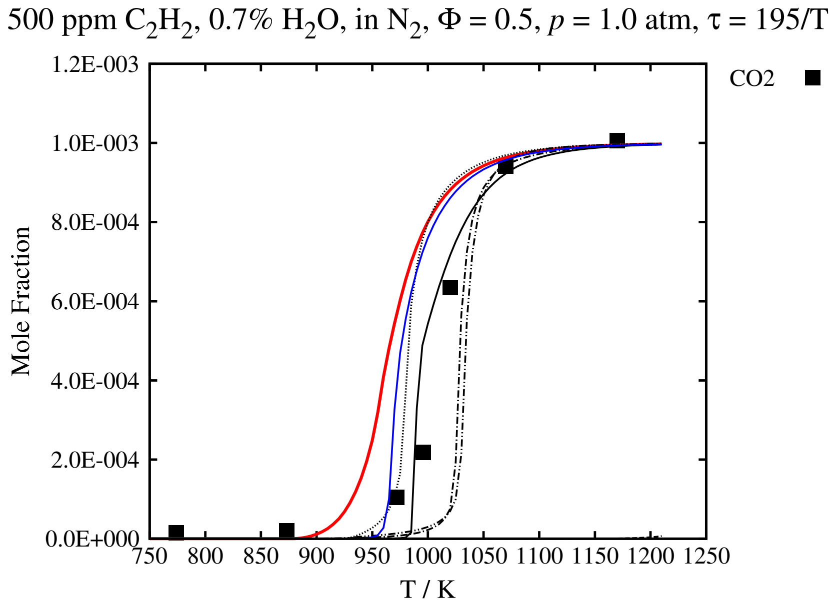
S50 Flow reactor species profiles of acetylene/oxygen/water/nitrogen mixtures. Symbols are experimental data [36] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


500 ppm C_2H_2, 0.7% H_2O, in N_2, Φ = 0.5, p = 1.0 atm, τ = 195/T s
C2H2
Mole Fraction
T / K
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
-1.0E-004
750 800 850 900 950 1000 1050 1100 1150 1200 1250

(a)


500 ppm C_2H_2, 0.7% H_2O, in N_2, Φ = 0.5, p = 1.0 atm, τ = 195/T s
CO
Mole Fraction
T / K
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
750 800 850 900 950 1000 1050 1100 1150 1200 1250

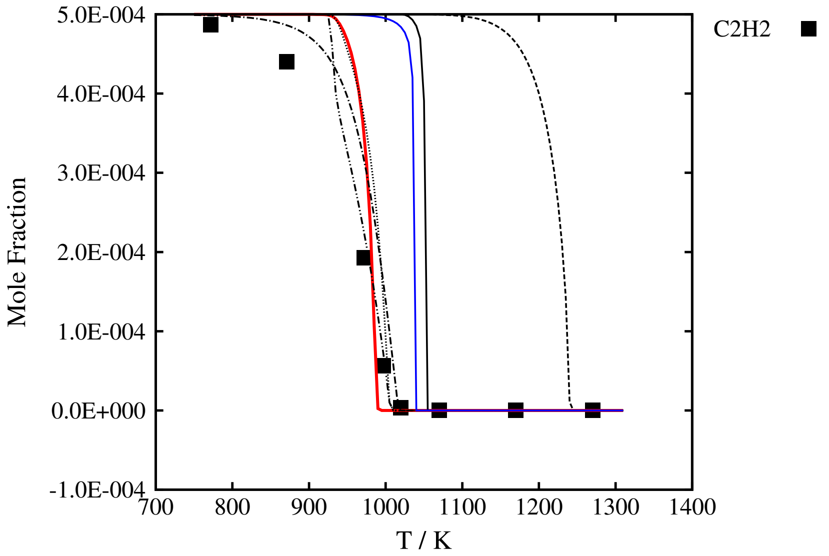
(b)



(c)

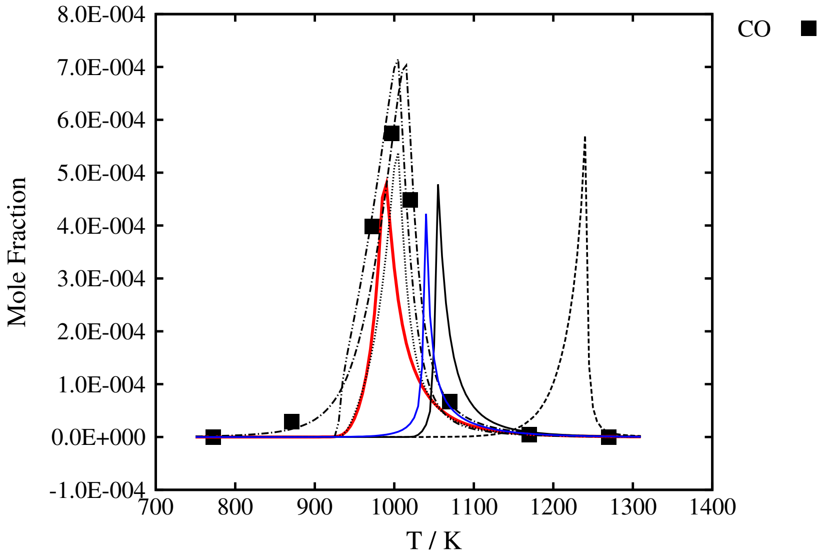
S51 Flow reactor species profiles of acetylene/oxygen/water/nitrogen mixtures. Symbols are experimental data [36] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

500 ppm C_2H_2, 0.7% H_2O, in N_2, $\Phi = 0.05$, $p = 1.0$ atm, $\tau = 195/T$ s

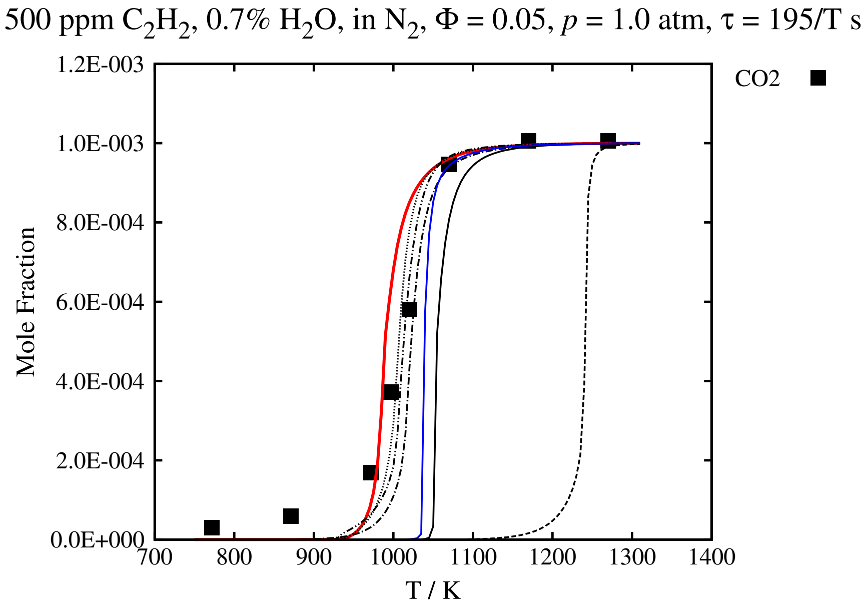


(a)

500 ppm C_2H_2, 0.7% H_2O, in N_2, $\Phi = 0.05$, $p = 1.0$ atm, $\tau = 195/T$ s



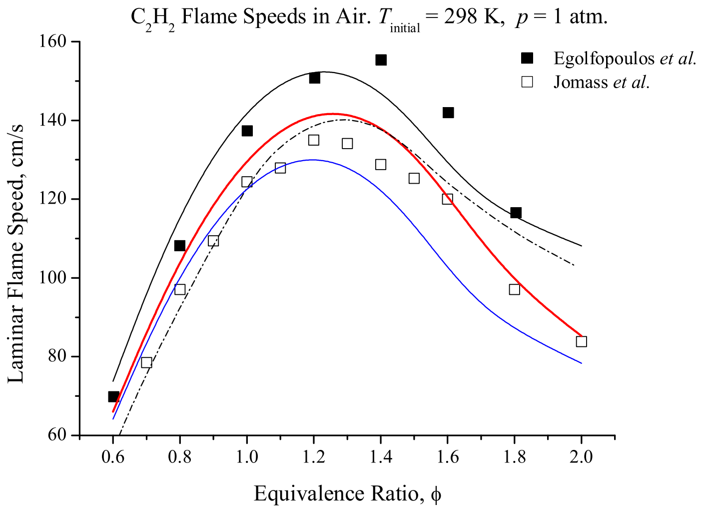
(b)

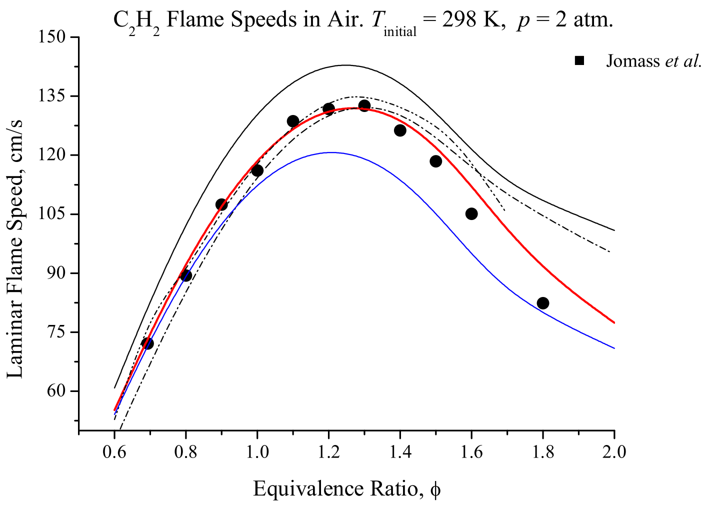


(c)

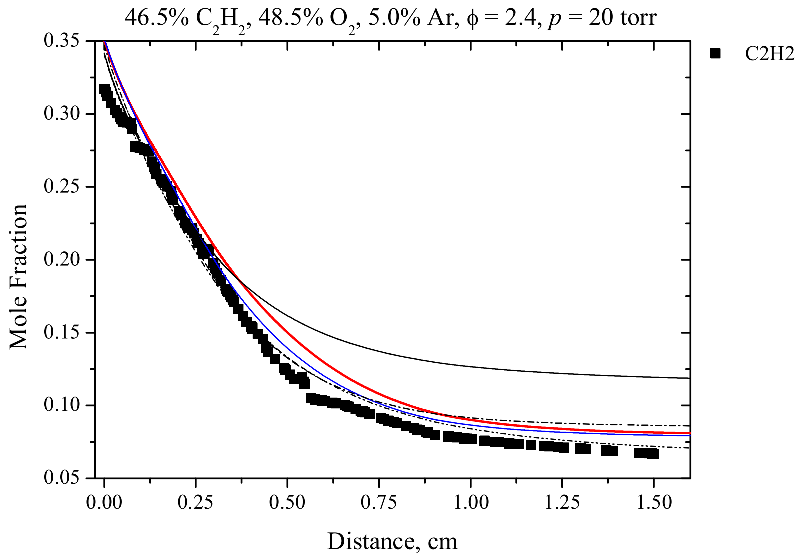
S52 Flow reactor species profiles of acetylene/oxygen/water/nitrogen mixtures. Symbols are experimental data [36] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

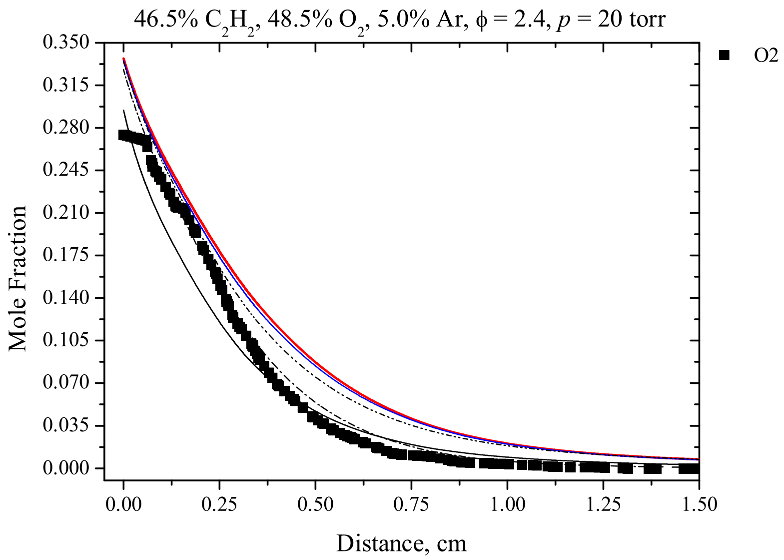
2.4.3. Flame Speed

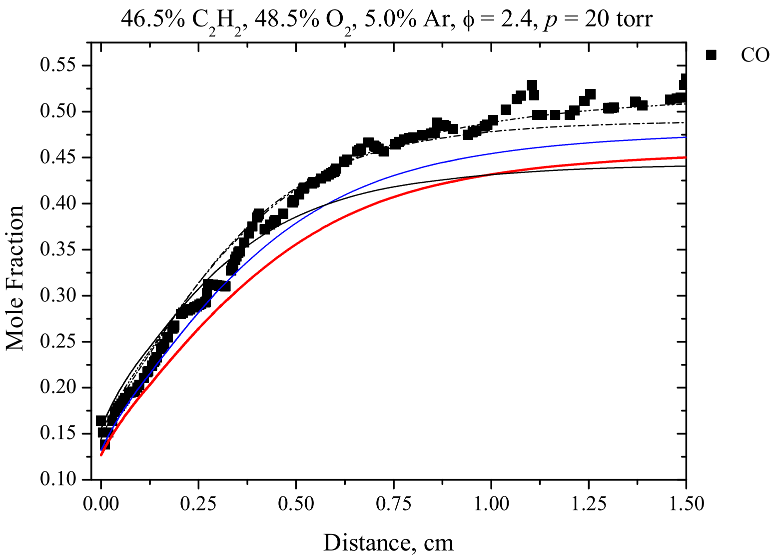


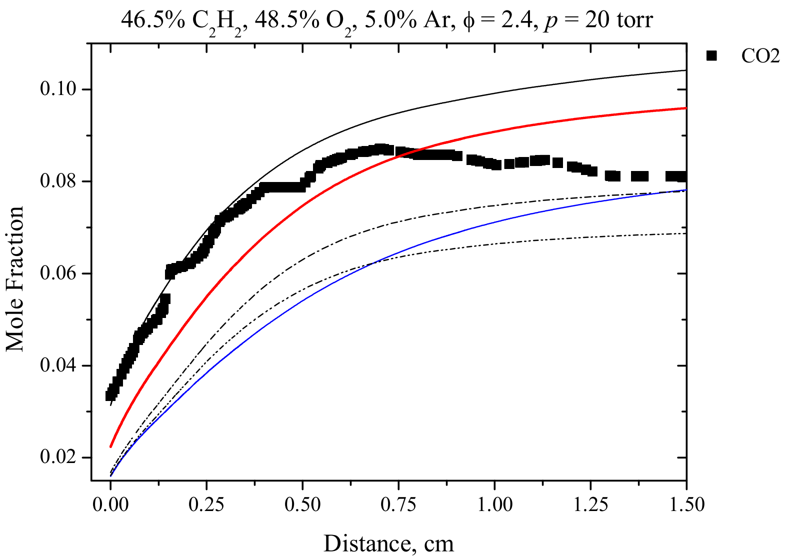


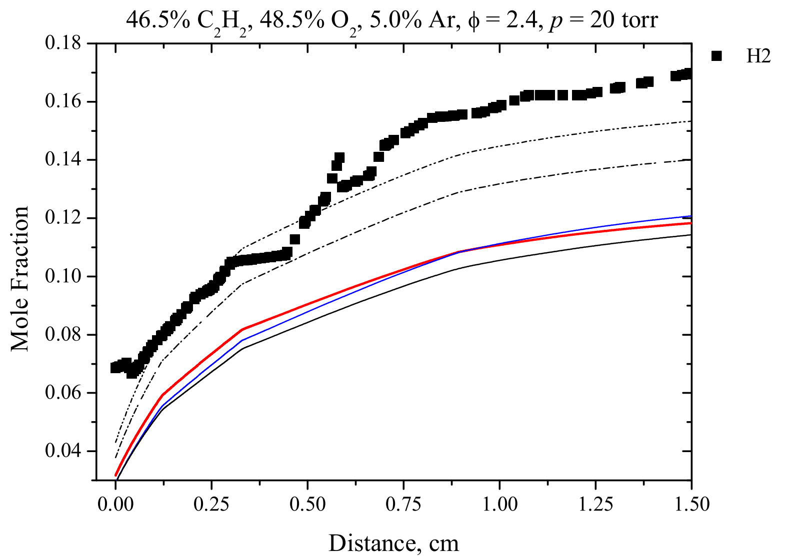
S53 Laminar flame speed measurements acetylene/air mixtures. Symbols are experimental data [24, 37] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, — USC II.

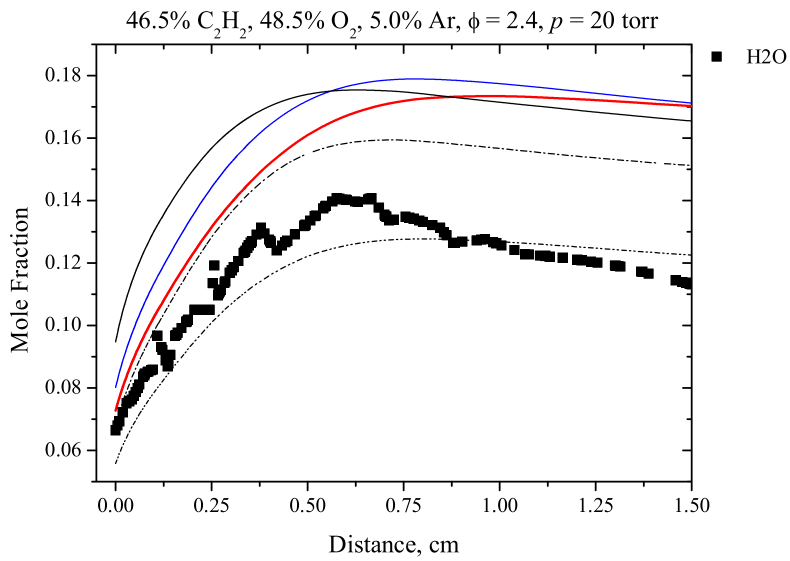

46.5% C2H2, 48.5% O2, 5.0% Ar, ϕ = 2.4, p = 20 torr
C2H2
Mole Fraction
Distance, cm
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.25
0.50
0.75
1.00
1.25
1.50


46.5% C2H2, 48.5% O2, 5.0% Ar, ϕ = 2.4, p = 20 torr
O2
Mole Fraction
Distance, cm
0.350
0.315
0.280
0.245
0.210
0.175
0.140
0.105
0.070
0.035
0.000
0.00
0.25
0.50
0.75
1.00
1.25
1.50


46.5% C2H2, 48.5% O2, 5.0% Ar, ϕ = 2.4, p = 20 torr
CO
Mole Fraction
Distance, cm
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
0.55
0.00
0.25
0.50
0.75
1.00
1.25
1.50


46.5% C2H2, 48.5% O2, 5.0% Ar, ϕ = 2.4, p = 20 torr
CO2
Mole Fraction
Distance, cm
0.02
0.04
0.06
0.08
0.10
0.00
0.25
0.50
0.75
1.00
1.25
1.50

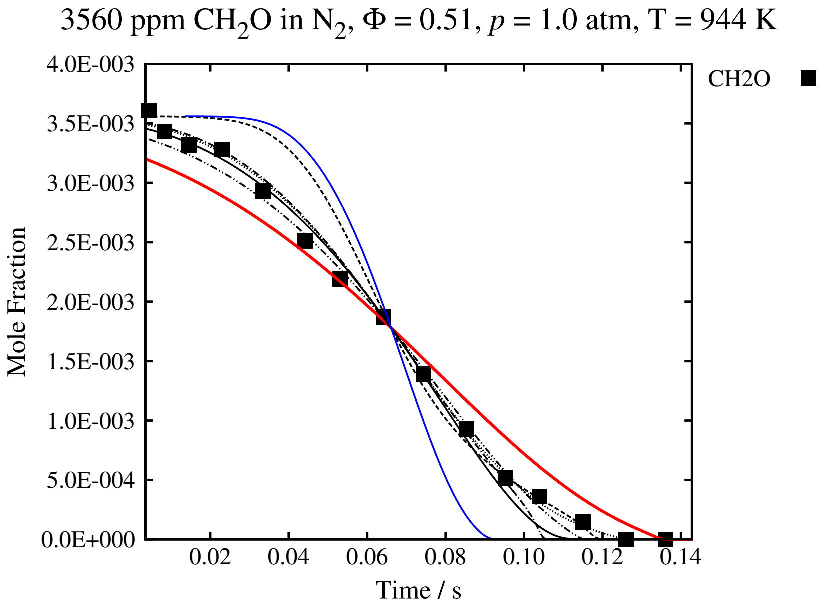




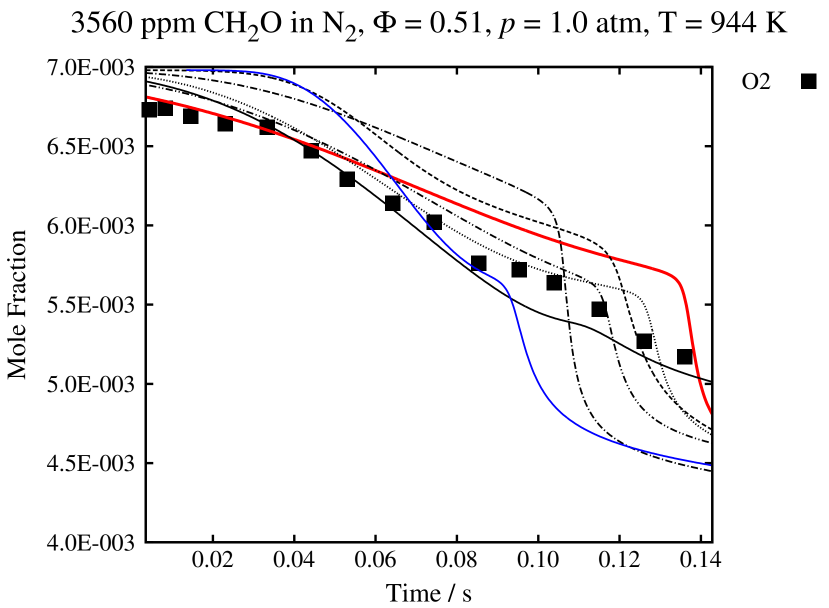
S54 Flame species profiles of acetylene/oxygen/argon mixtures. Symbols are experimental data [43] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

2.5. Formaldehyde

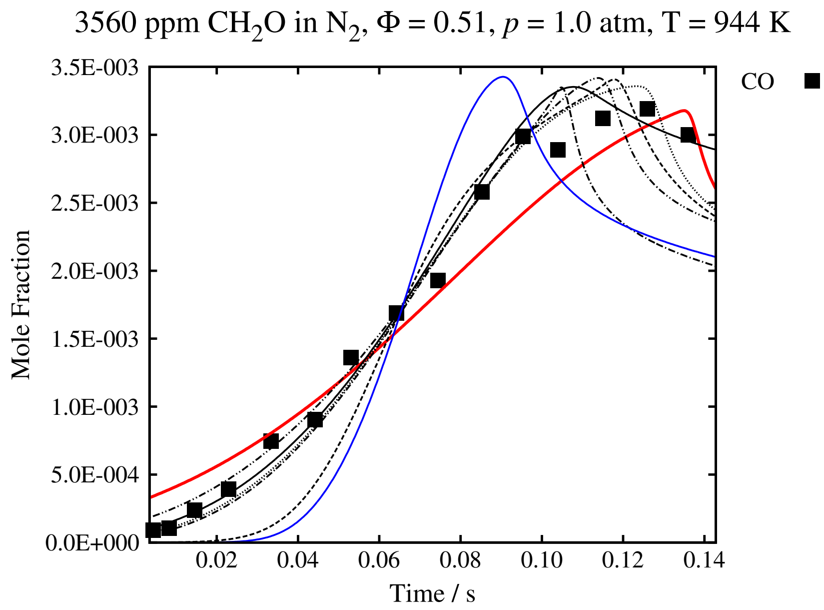
2.5.1. Flow Reactor



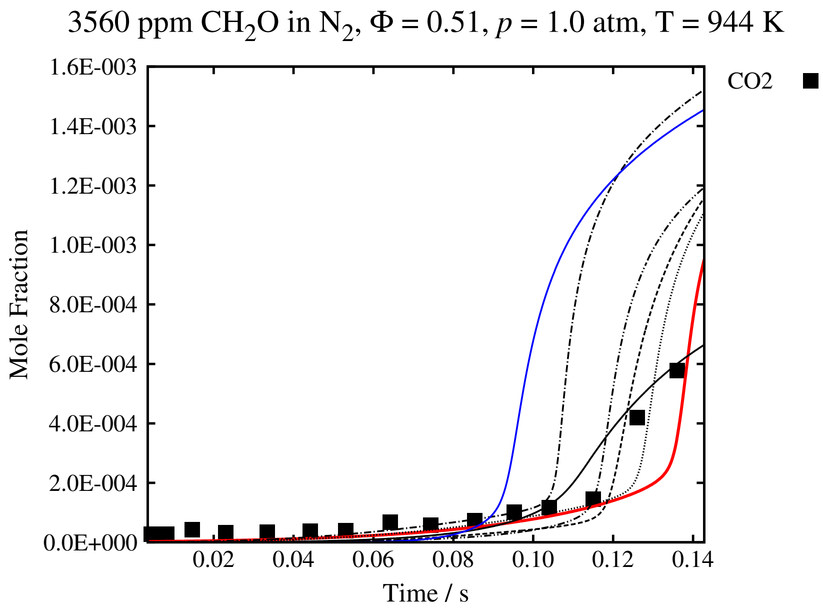
(a)



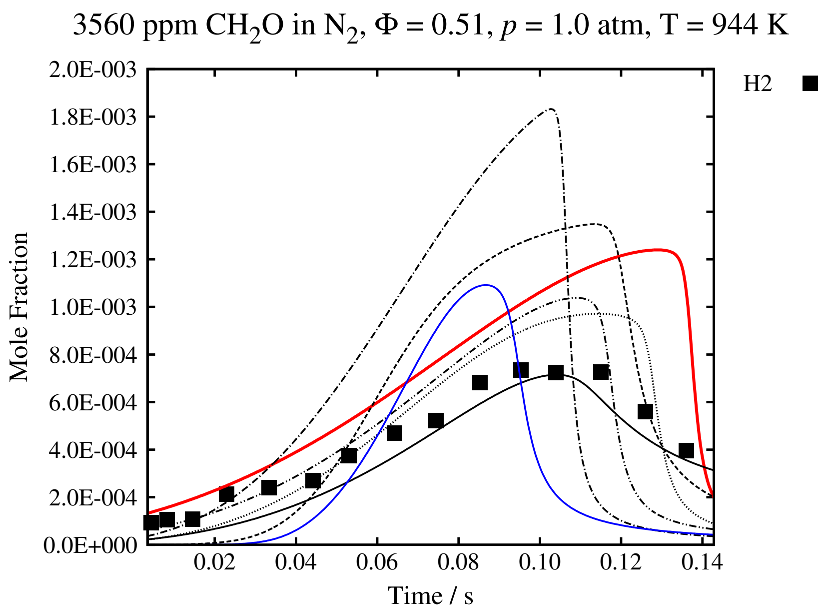
(b)


3560 ppm CH_2O in N_2, Φ = 0.51, p = 1.0 atm, T = 944 K
CO
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

(c)

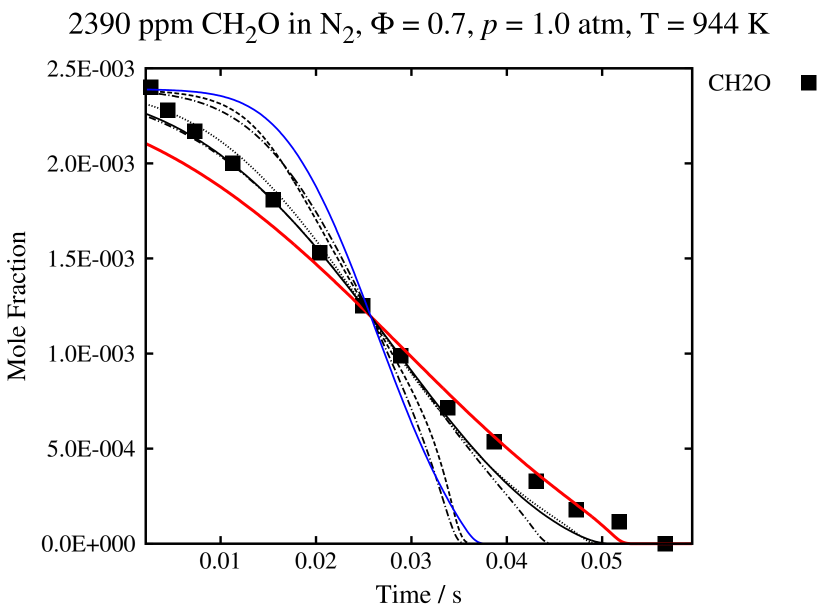

3560 ppm CH_2O in N_2, Φ = 0.51, p = 1.0 atm, T = 944 K
CO2
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

(d)

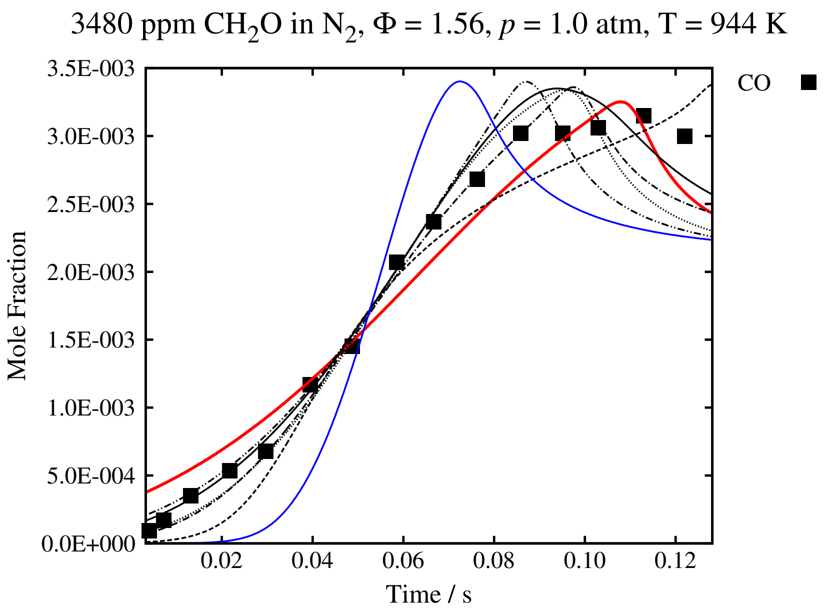


(e)

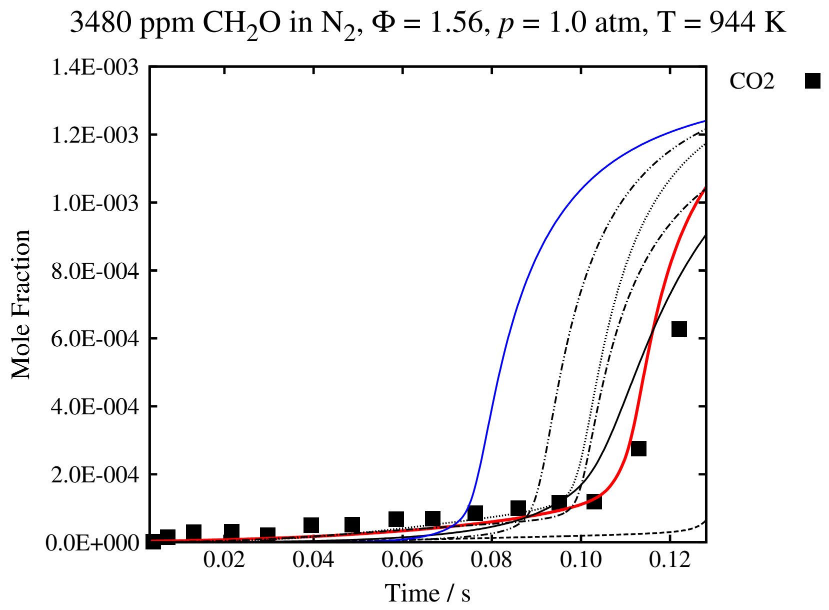
S55 Flow reactor species profiles of formaldehyde/oxygen/nitrogen mixtures. Symbols are experimental data [44] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


2390 ppm CH$_2$O in N$_2$, Φ = 0.7, *p* = 1.0 atm, T = 944 K
CH2O
Mole Fraction
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05
Time / s

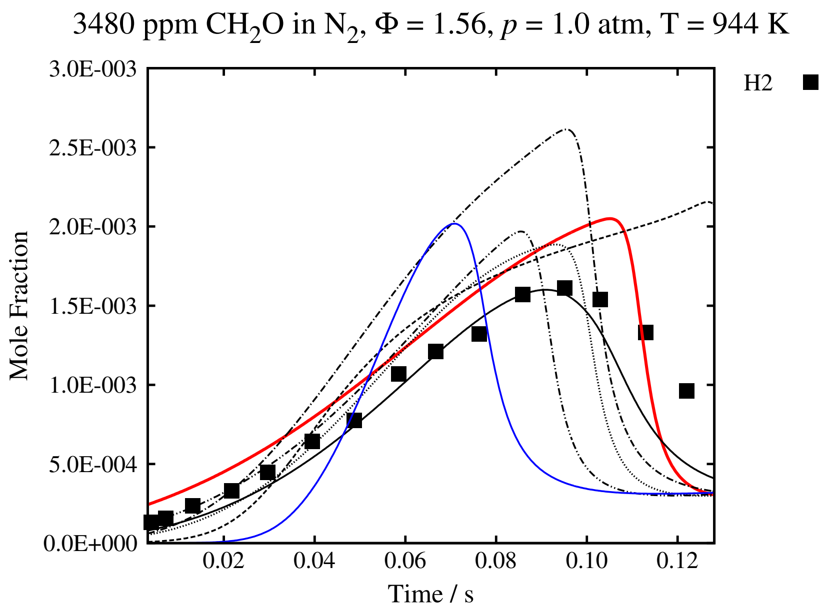
(a)


3480 ppm CH$_2$O in N$_2$, Φ = 1.56, *p* = 1.0 atm, T = 944 K
CO
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

(b)

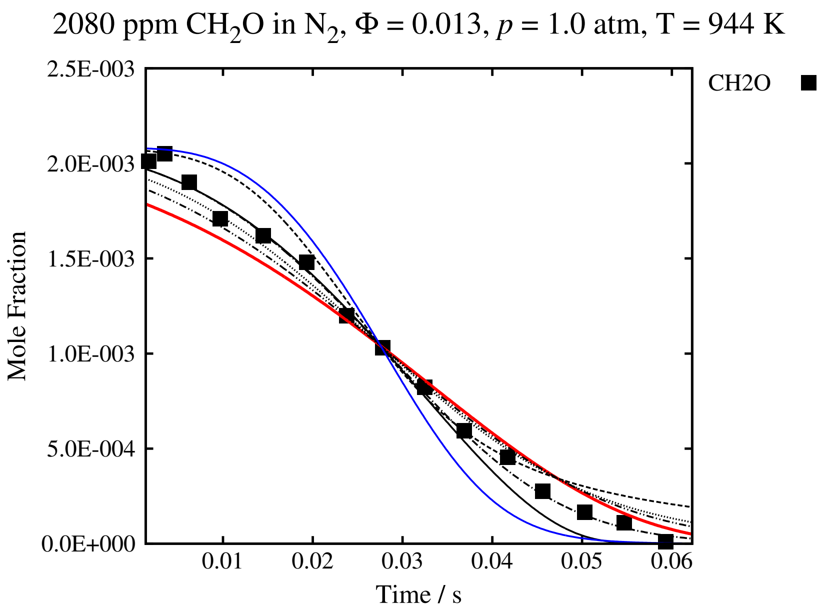


(c)

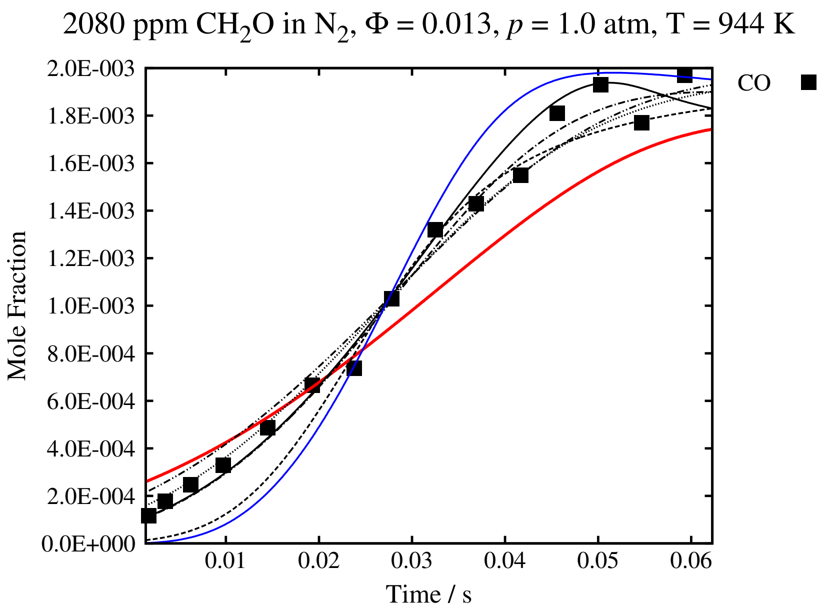


(d)

S56 Flow reactor species profiles of formaldehyde/oxygen/nitrogen mixtures. Symbols are experimental data [44] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

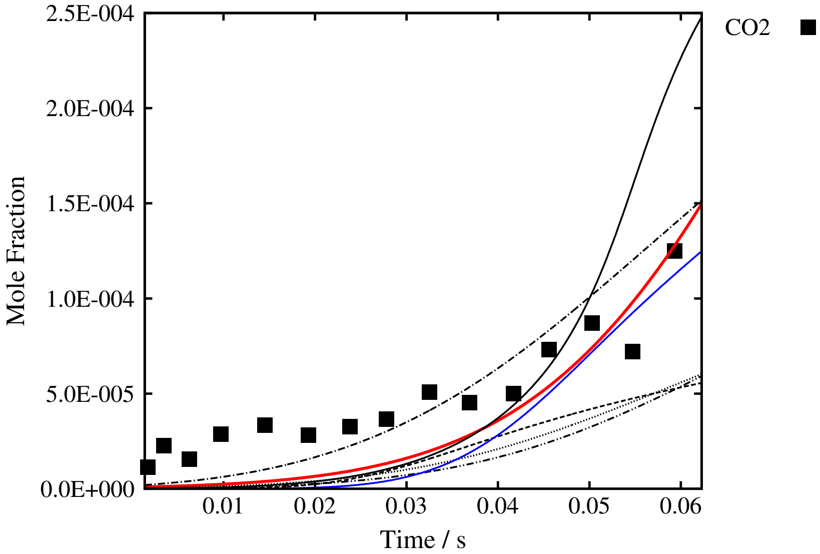

2080 ppm CH2O in N2, Φ = 0.013, p = 1.0 atm, T = 944 K
CH2O
Mole Fraction
Time / s
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06

(a)


2080 ppm CH2O in N2, Φ = 0.013, p = 1.0 atm, T = 944 K
CO
Mole Fraction
Time / s
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06

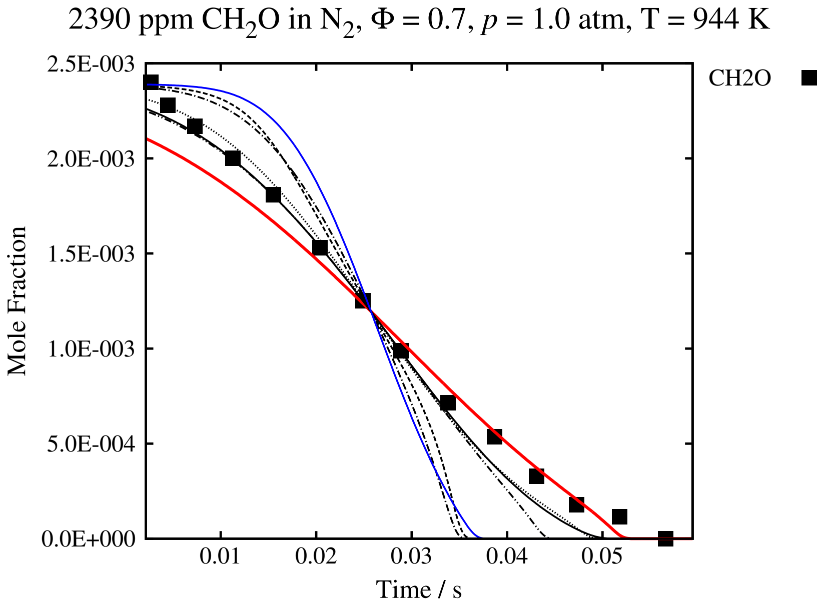
(b)

2080 ppm CH_2O in N_2, $\Phi = 0.013$, $p = 1.0$ atm, T = 944 K

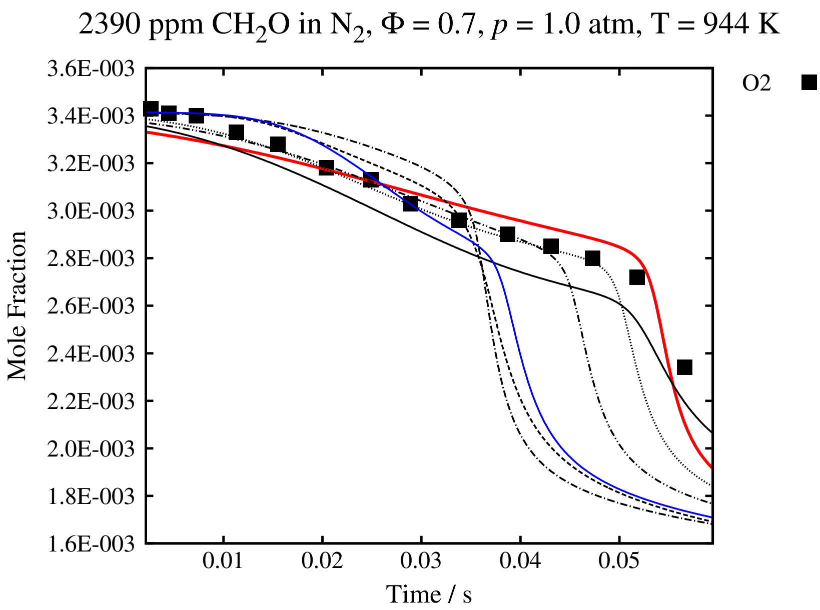


(c)

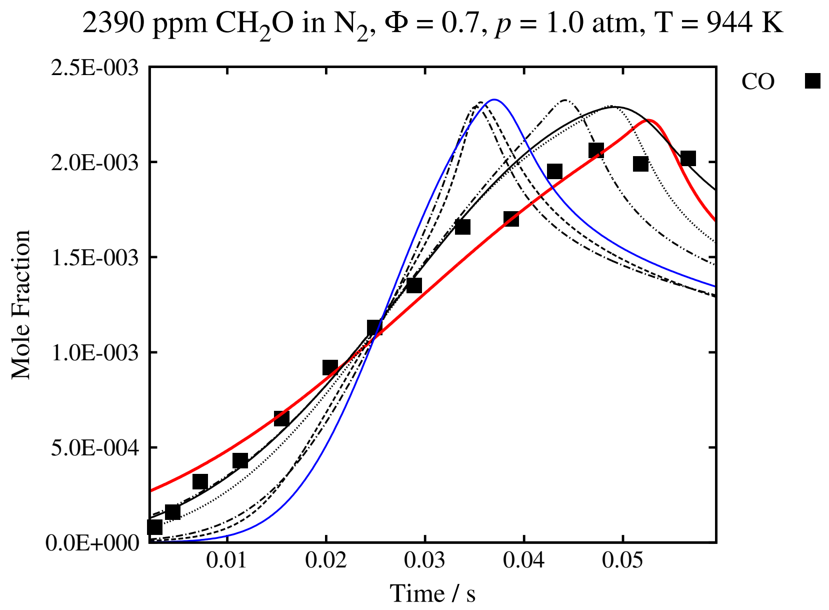
S57 Flow reactor species profiles of formaldehyde/oxygen/nitrogen mixtures. Symbols are experimental data [44] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


2390 ppm CH$_2$O in N$_2$, Φ = 0.7, *p* = 1.0 atm, T = 944 K
CH2O
Mole Fraction
Time / s
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05

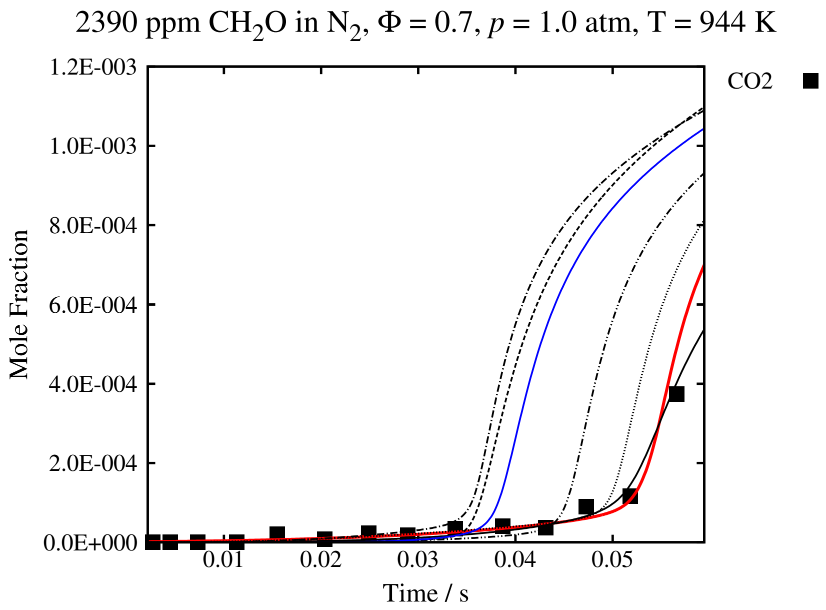
(a)


2390 ppm CH$_2$O in N$_2$, Φ = 0.7, *p* = 1.0 atm, T = 944 K
O2
Mole Fraction
Time / s
3.6E-003
3.4E-003
3.2E-003
3.0E-003
2.8E-003
2.6E-003
2.4E-003
2.2E-003
2.0E-003
1.8E-003
1.6E-003
0.01
0.02
0.03
0.04
0.05

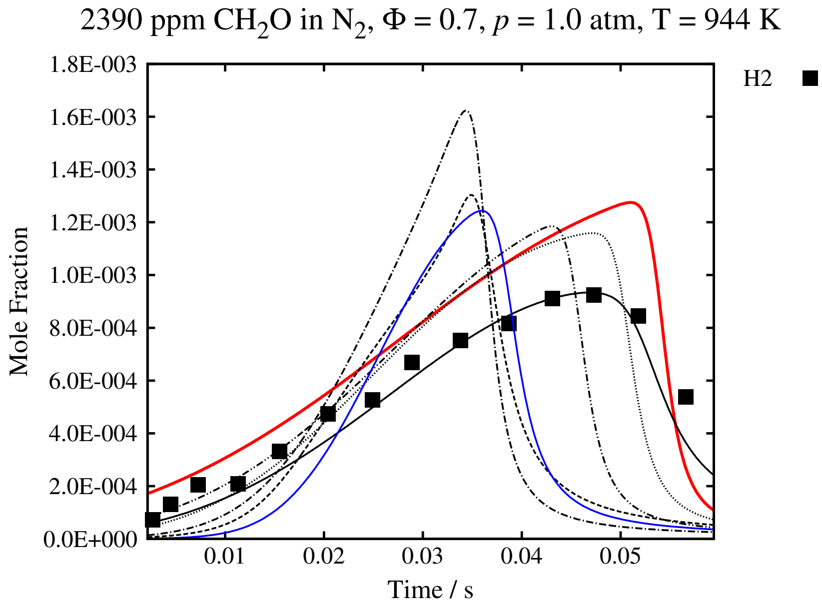
(b)


2390 ppm CH2O in N2, Φ = 0.7, p = 1.0 atm, T = 944 K
CO
Mole Fraction
Time / s
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05

(c)

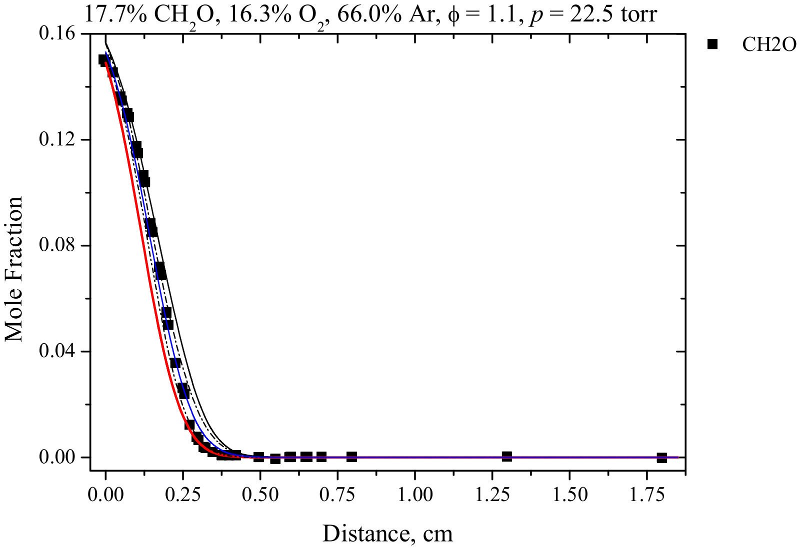

2390 ppm CH2O in N2, Φ = 0.7, p = 1.0 atm, T = 944 K
CO2
Mole Fraction
Time / s
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05

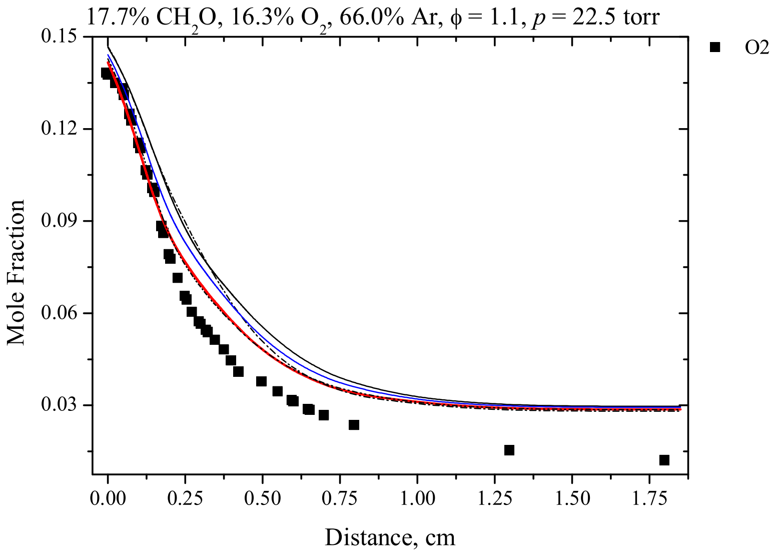
(d)

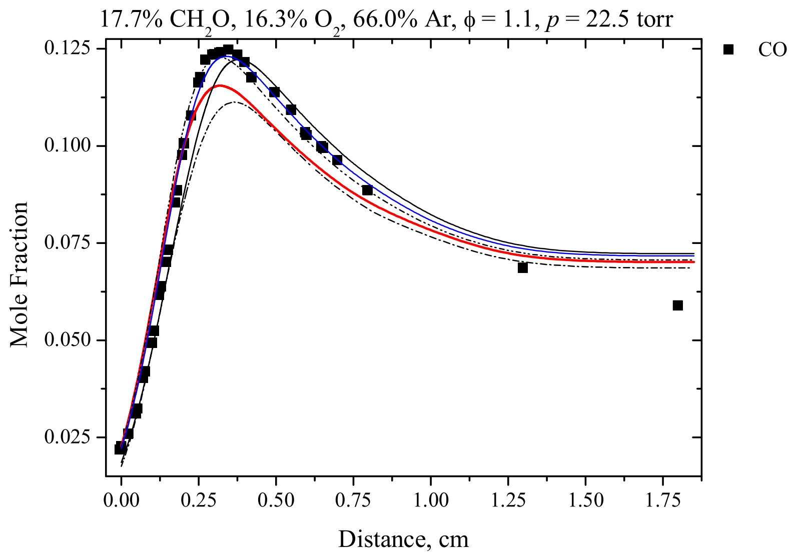


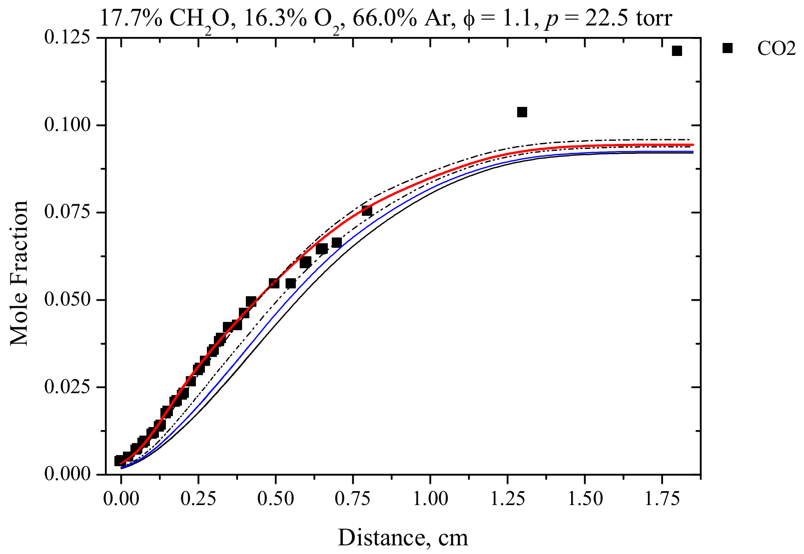
(e)

S58 Flow reactor species profiles of formaldehyde/oxygen/nitrogen mixtures. Symbols are experimental data [44] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


17.7% CH2O, 16.3% O2, 66.0% Ar, ϕ = 1.1, p = 22.5 torr
CH2O
Mole Fraction
Distance, cm
0.16
0.12
0.08
0.04
0.00
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75


17.7% CH2O, 16.3% O2, 66.0% Ar, ϕ = 1.1, p = 22.5 torr
O2
Mole Fraction
Distance, cm
0.15
0.12
0.09
0.06
0.03
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75



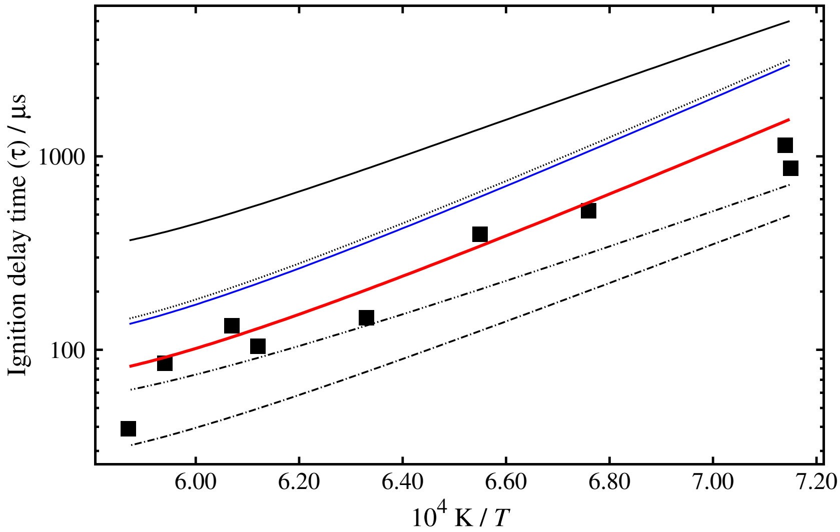


S59 Flame species profiles of formaldehyde/oxygen/argon mixtures. Symbols are experimental data [45] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

2.6. Acetaldehyde

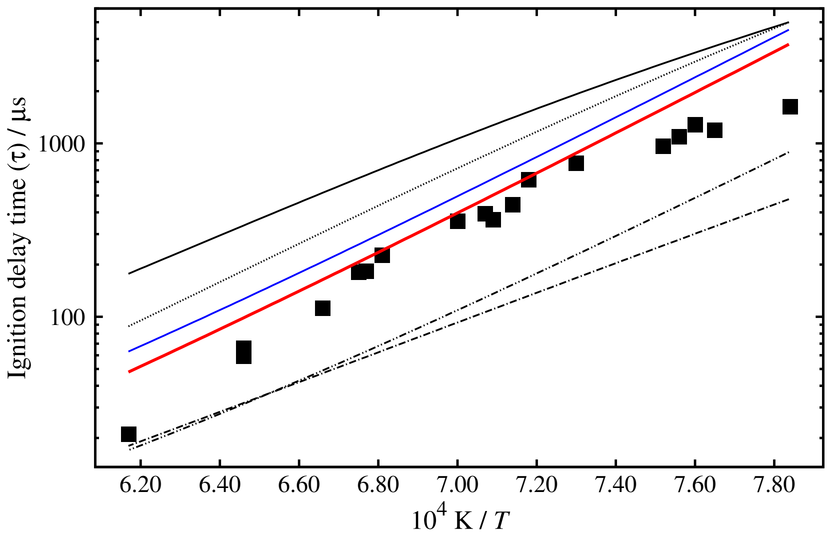
2.6.1. Shock Tube

2.00% CH_3CHO, 2.00% O_2, 96.00% Ar, Φ = 2.50, p_{av} = 2.32 atm

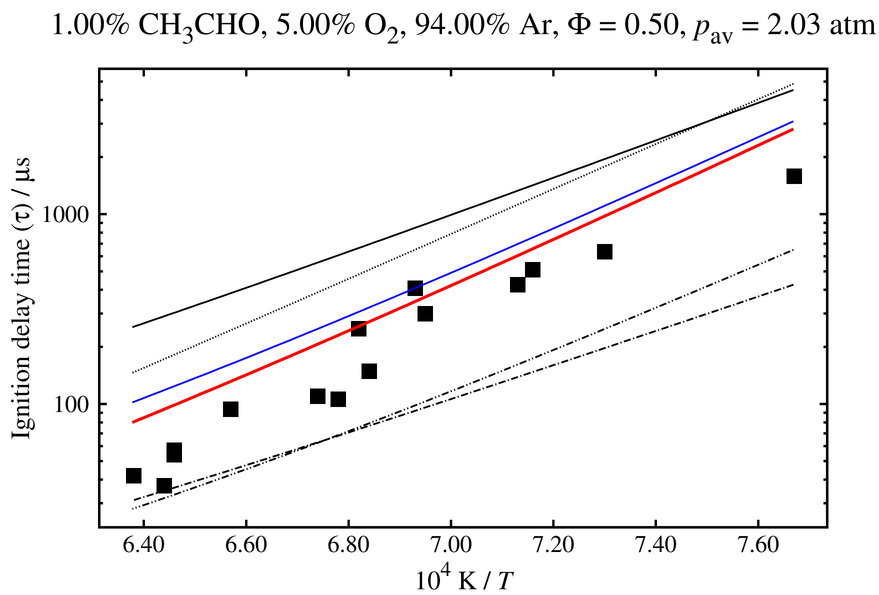


(a)

2.00% CH_3CHO, 5.00% O_2, 93.00% Ar, Φ = 1.00, p_{av} = 2.06 atm

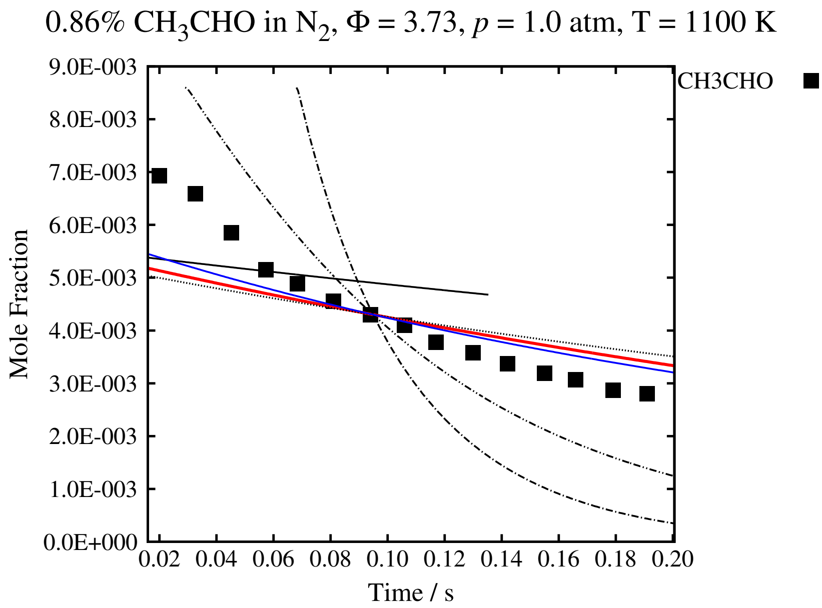


(b)

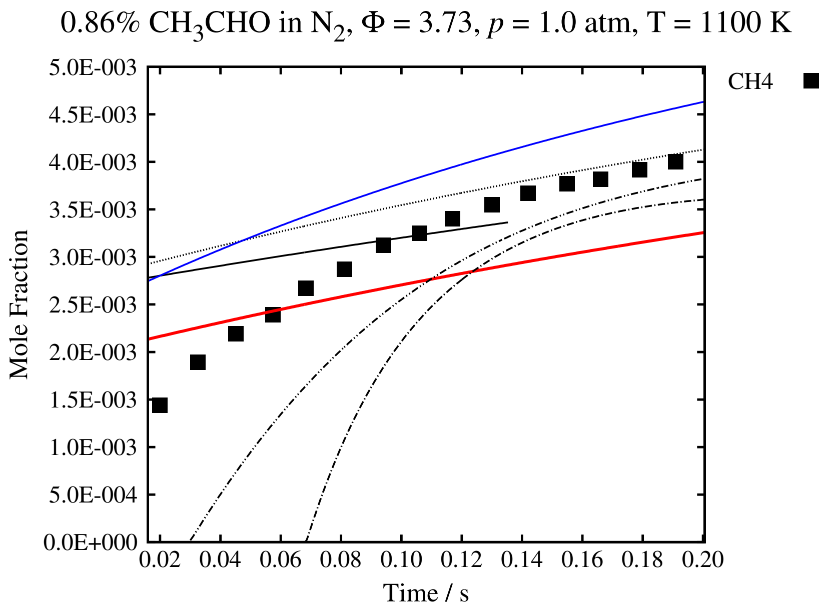


(c)

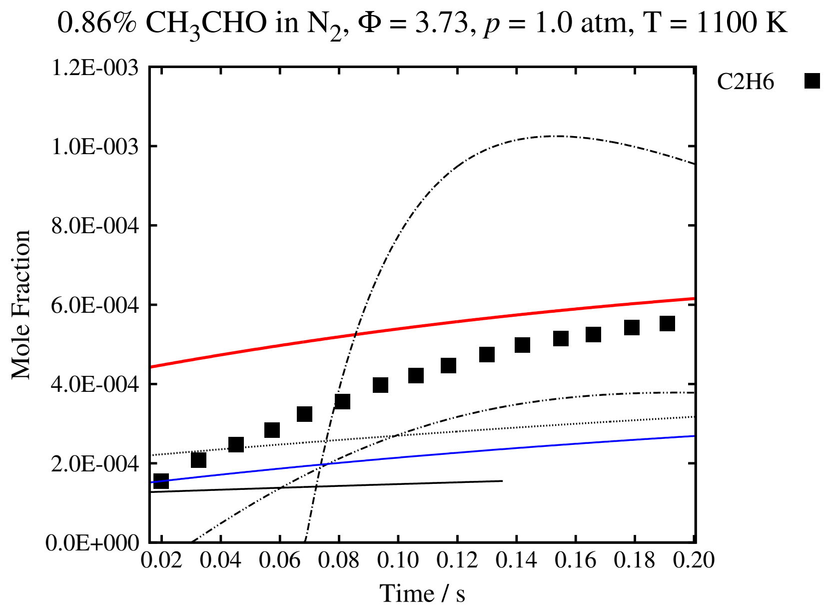
S60 Shock tube ignition delay times of acetaldehyde/oxygen/argon mixtures. Symbols are experimental data [46] lines are model predictions. ── AramcoMech 1.3, ── GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, ── USC II.


0.86% CH_3CHO in N_2, Φ = 3.73, *p* = 1.0 atm, T = 1100 K
CH3CHO
Mole Fraction
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.02 0.04 0.06 0.08 0.10 0.12 0.14 0.16 0.18 0.20
Time / s

(a)

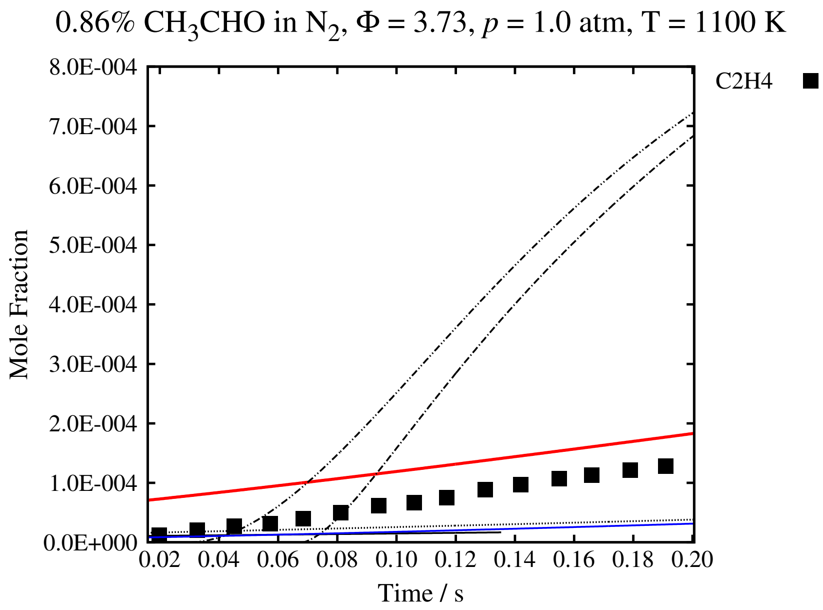

0.86% CH_3CHO in N_2, Φ = 3.73, *p* = 1.0 atm, T = 1100 K
CH4
Mole Fraction
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.02 0.04 0.06 0.08 0.10 0.12 0.14 0.16 0.18 0.20
Time / s

(b)



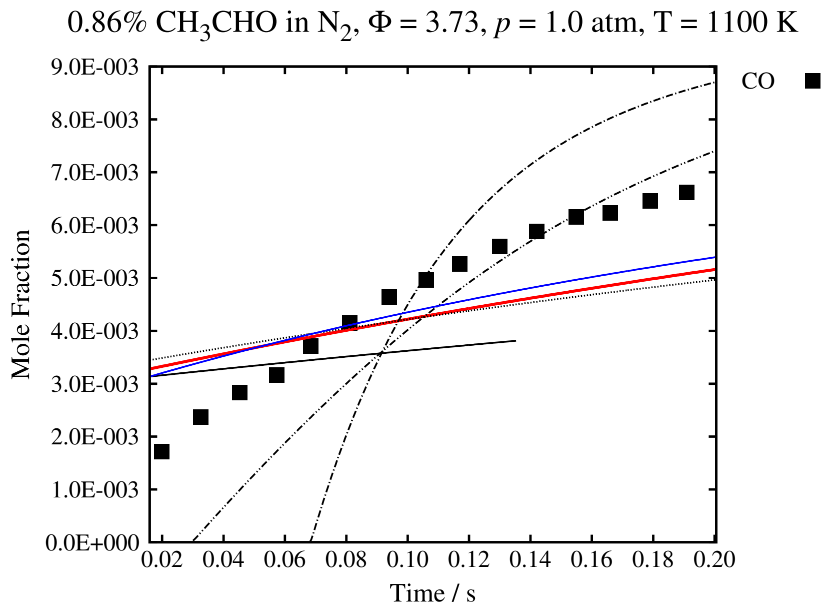
0.86% CH3CHO in N2, Φ = 3.73, p = 1.0 atm, T = 1100 K
C2H6
Mole Fraction
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.02 0.04 0.06 0.08 0.10 0.12 0.14 0.16 0.18 0.20
Time / s

(c)

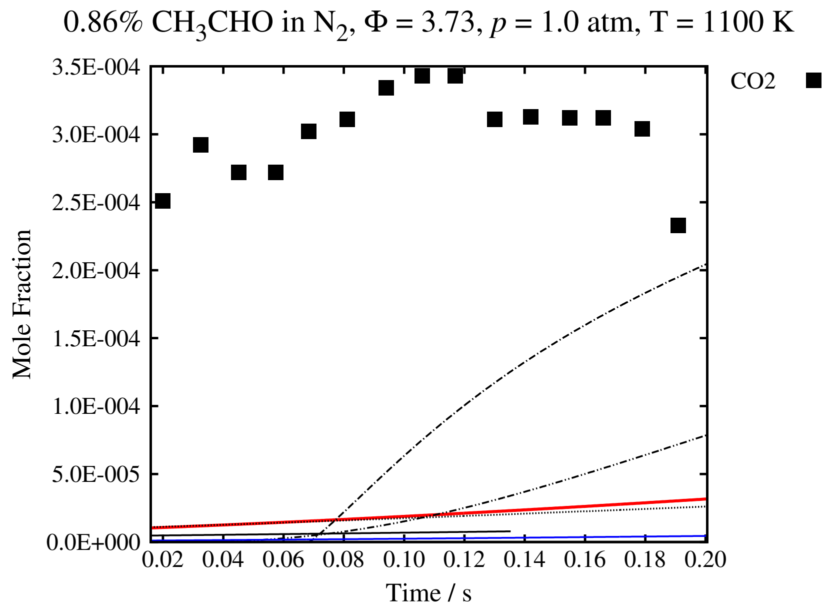


0.86% CH3CHO in N2, Φ = 3.73, p = 1.0 atm, T = 1100 K
C2H4
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.02 0.04 0.06 0.08 0.10 0.12 0.14 0.16 0.18 0.20
Time / s

(d)



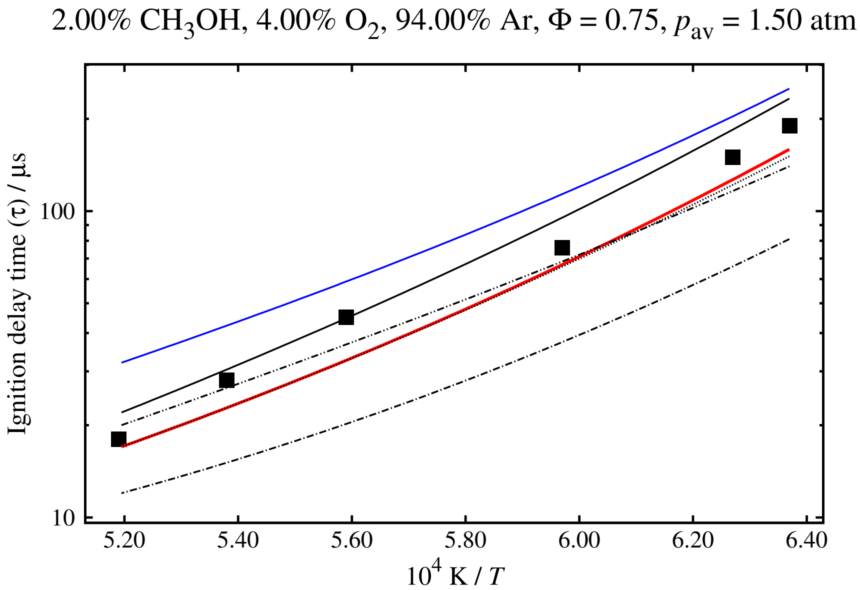
(e)



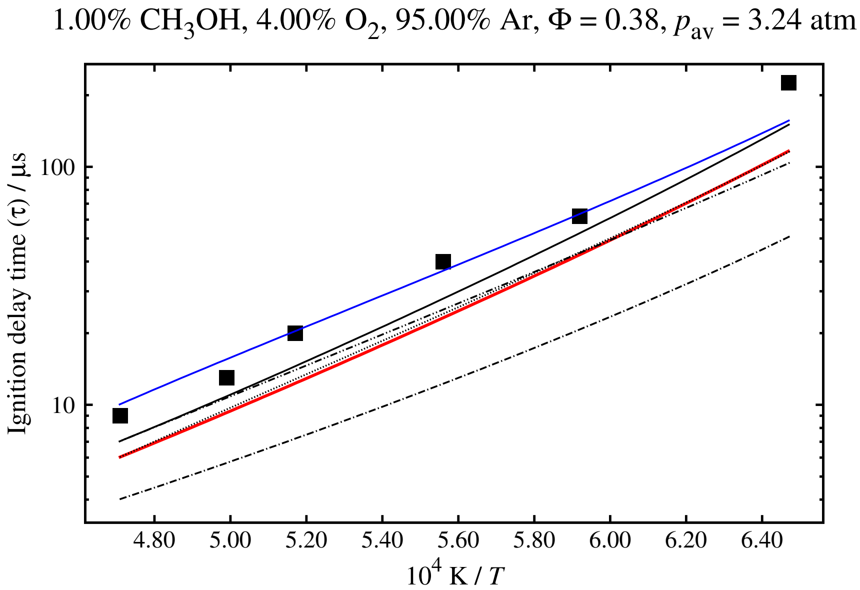
(f)

S61 Flow reactor species profiles of acetaldehyde/oxygen/nitrogen mixtures. Symbols are experimental data [47] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

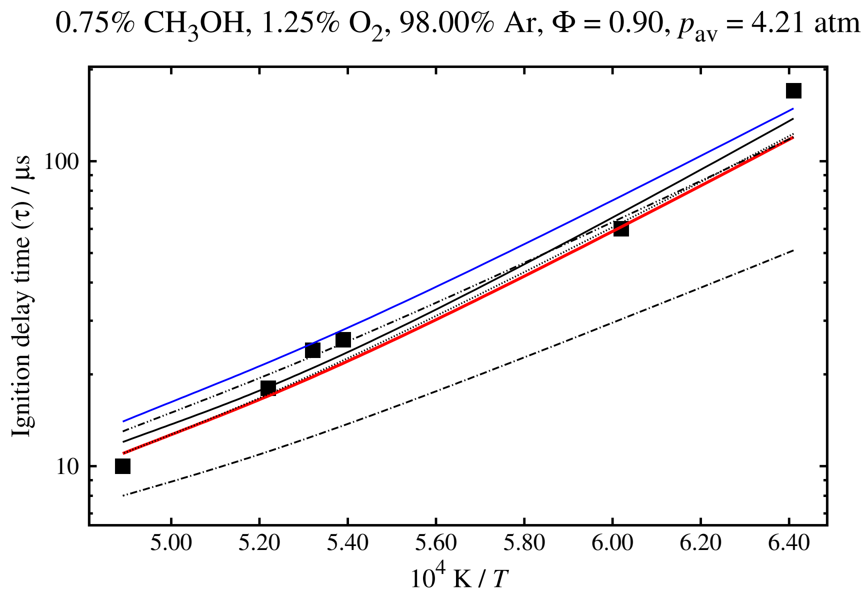
2.7.1. Shock Tube



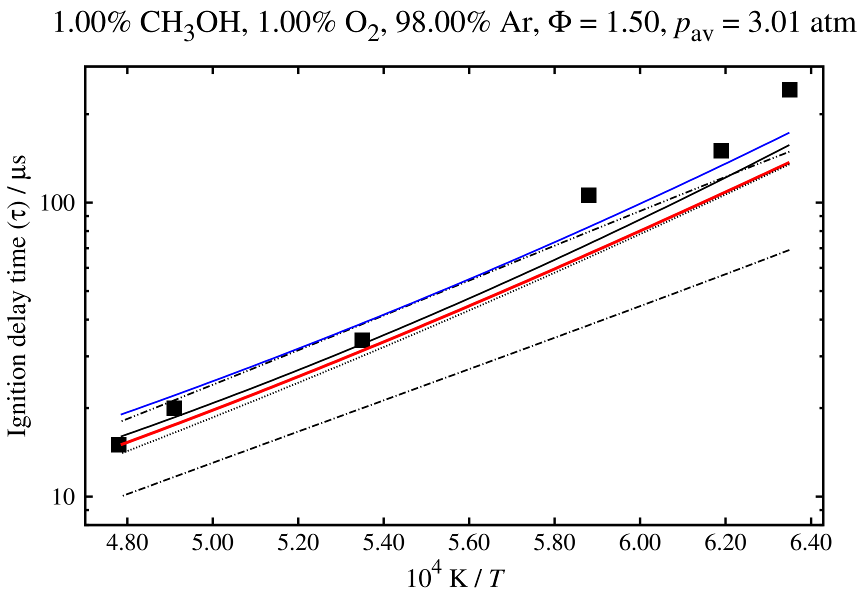
(a)



(b)

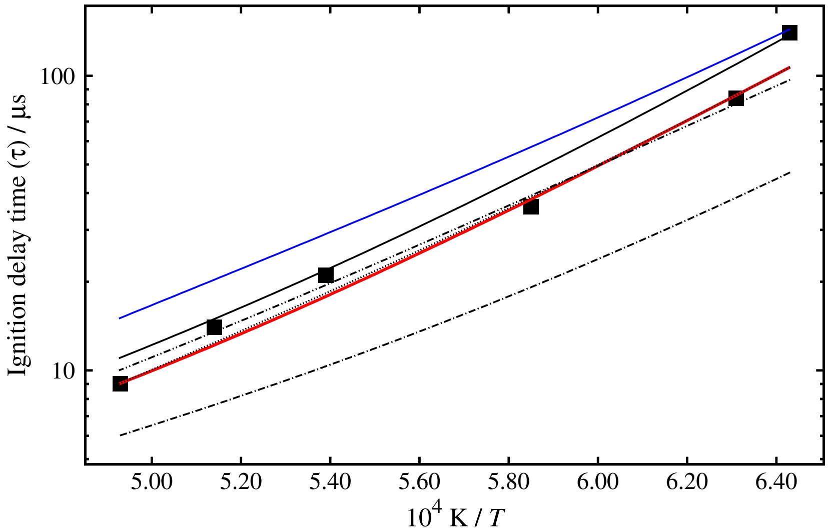

0.75% CH3OH, 1.25% O2, 98.00% Ar, Φ = 0.90, pav = 4.21 atm
Ignition delay time (τ) / µs
10
100
5.00
5.20
5.40
5.60
5.80
6.00
6.20
6.40
10^4 K / T

(c)


1.00% CH3OH, 1.00% O2, 98.00% Ar, Φ = 1.50, pav = 3.01 atm
Ignition delay time (τ) / µs
10
100
4.80
5.00
5.20
5.40
5.60
5.80
6.00
6.20
6.40
10^4 K / T

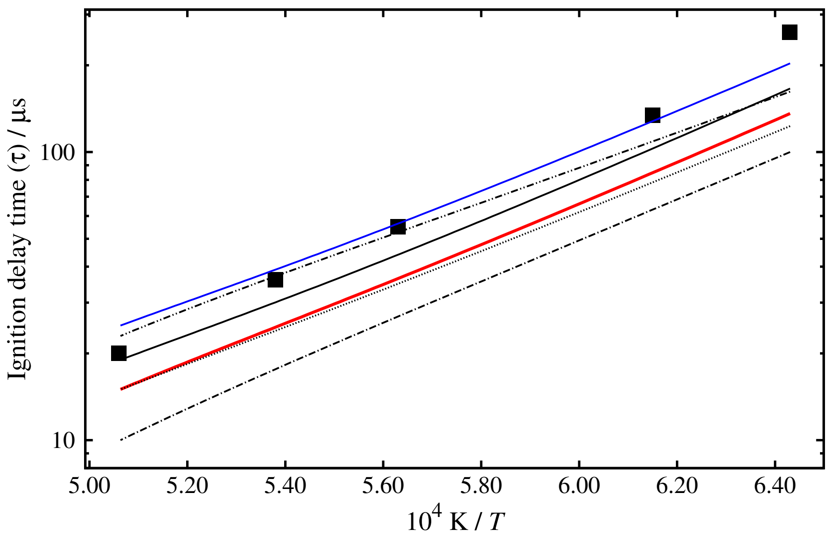
(d)

1.00% CH_3OH, 4.00% O_2, 95.00% Ar, Φ = 0.38, p_{av} = 3.02 atm

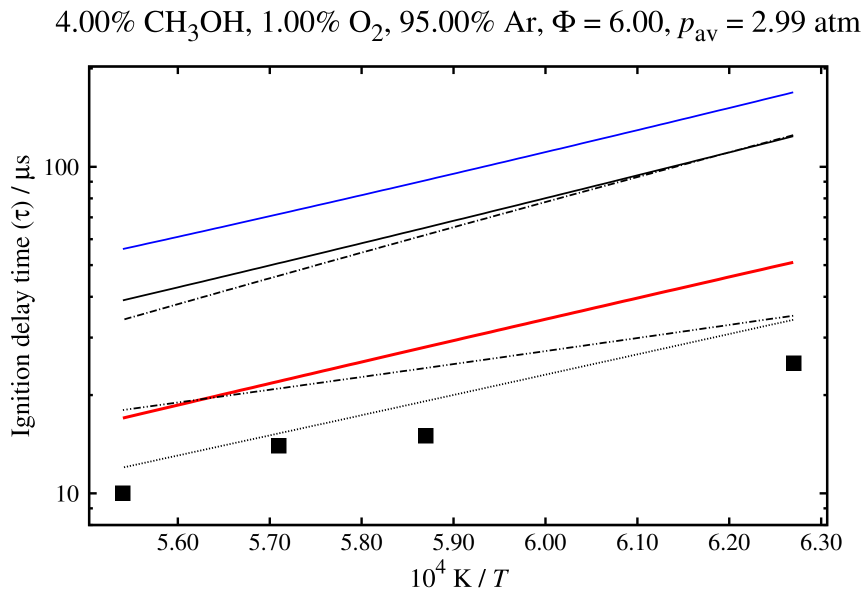


(e)

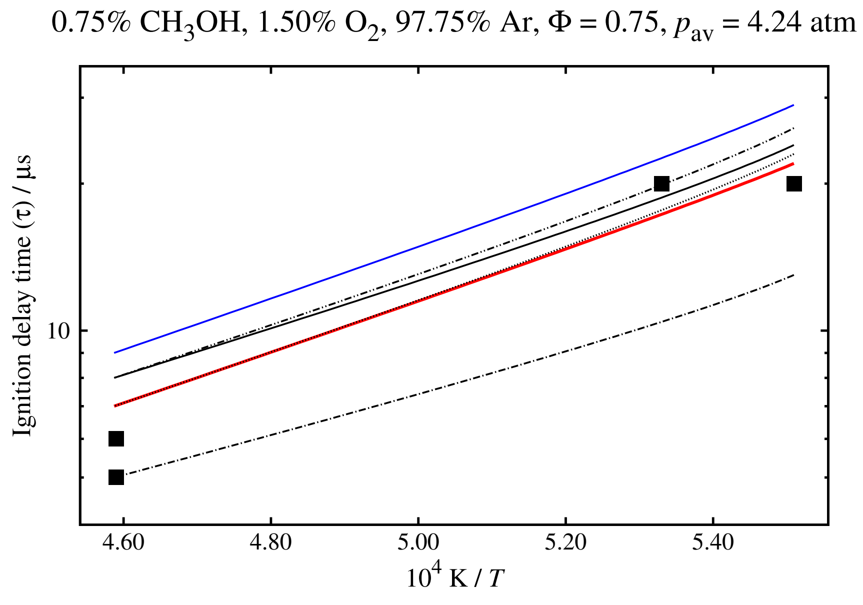
2.00% CH_3OH, 1.00% O_2, 97.00% Ar, Φ = 3.00, p_{av} = 2.94 atm



(f)



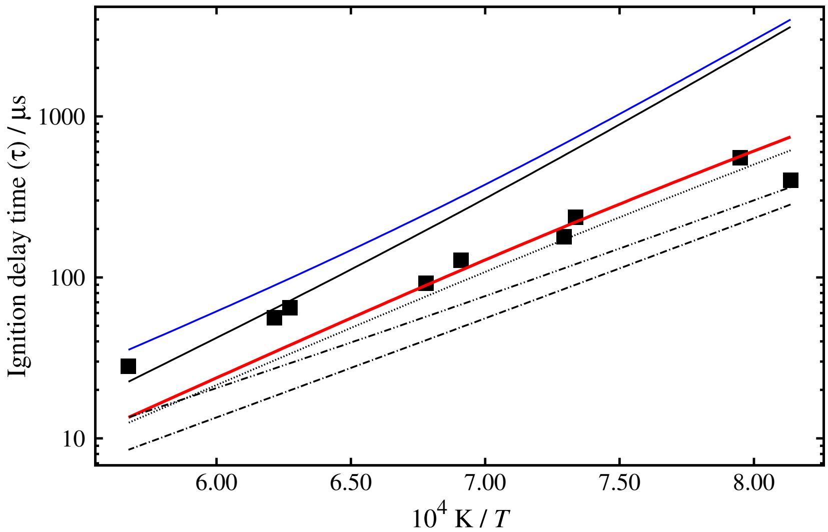
(g)



(h)

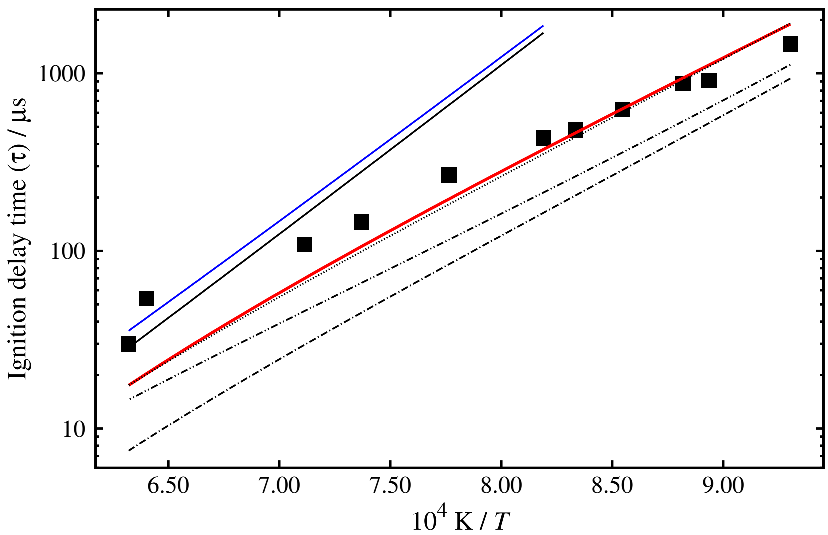
S62 Shock tube ignition delay times of methanol/oxygen/argon mixtures. Symbols are experimental data [48] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

5.70% CH_3OH, 8.60% O_2, 85.70% Ar, $\Phi = 1.00$, $p_{av} = 2.13$ atm

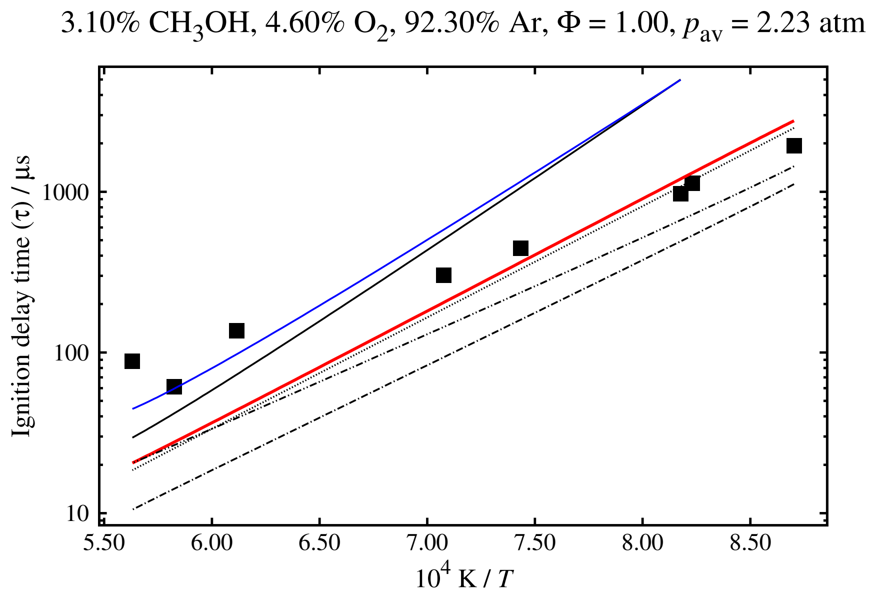


(a)

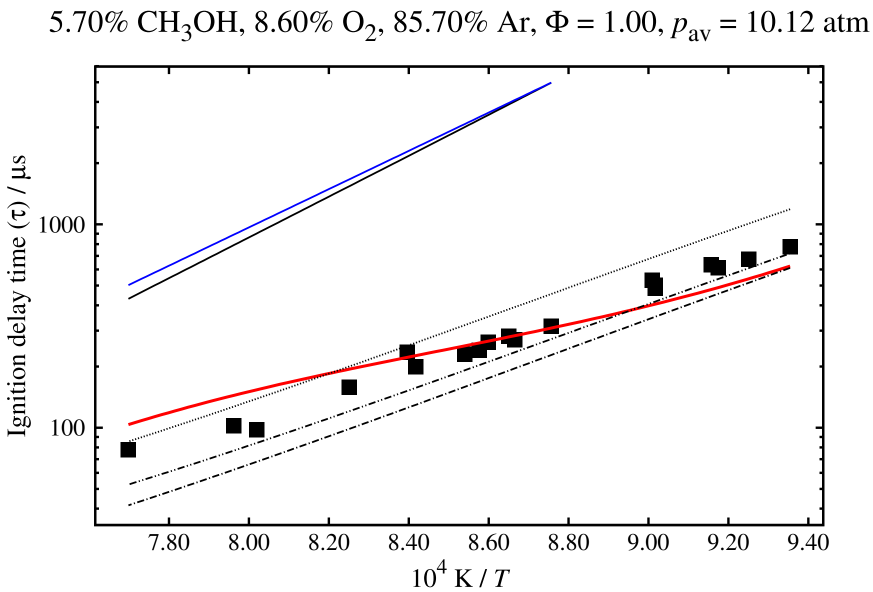
2.00% CH_3OH, 6.10% O_2, 91.90% Ar, $\Phi = 0.50$, $p_{av} = 11.63$ atm



(b)

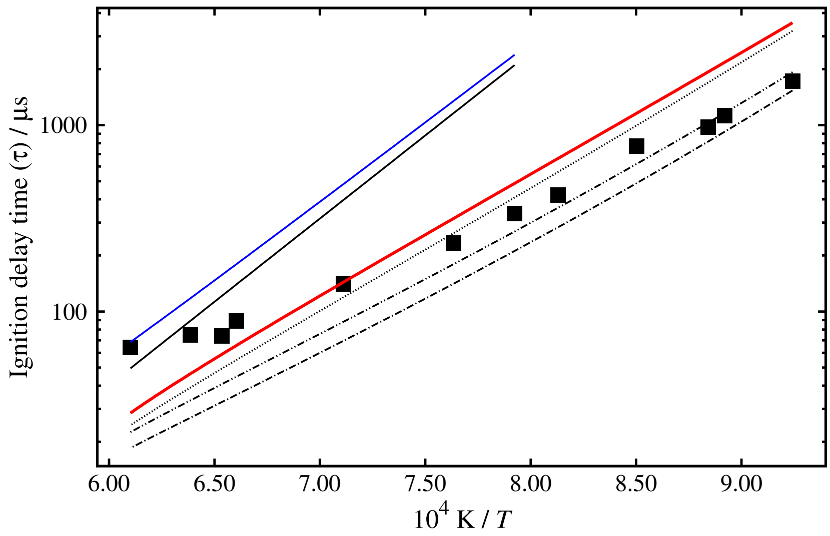

3.10% CH3OH, 4.60% O2, 92.30% Ar, Φ = 1.00, pav = 2.23 atm
Ignition delay time (τ) / µs
10
100
1000
5.50
6.00
6.50
7.00
7.50
8.00
8.50
10^4 K / T

(c)


5.70% CH3OH, 8.60% O2, 85.70% Ar, Φ = 1.00, pav = 10.12 atm
Ignition delay time (τ) / µs
100
1000
7.80
8.00
8.20
8.40
8.60
8.80
9.00
9.20
9.40
10^4 K / T

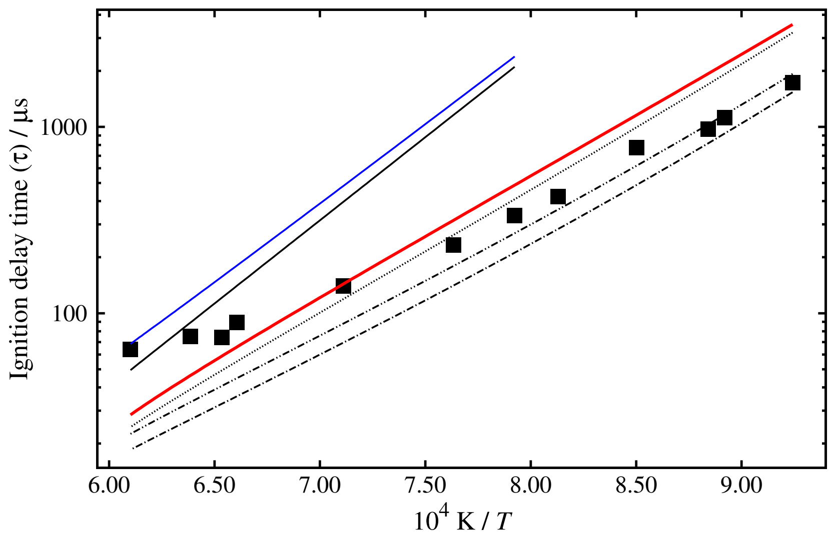
(d)

7.70% CH_3OH, 5.80% O_2, 86.50% Ar, Φ = 2.00, p_{av} = 2.18 atm



(e)

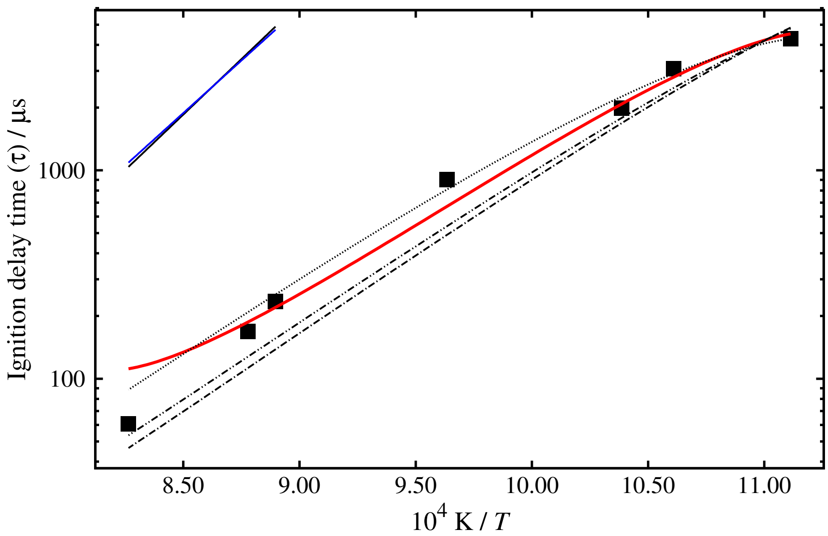
7.70% CH_3OH, 5.80% O_2, 86.50% Ar, Φ = 2.00, p_{av} = 2.18 atm



(f)

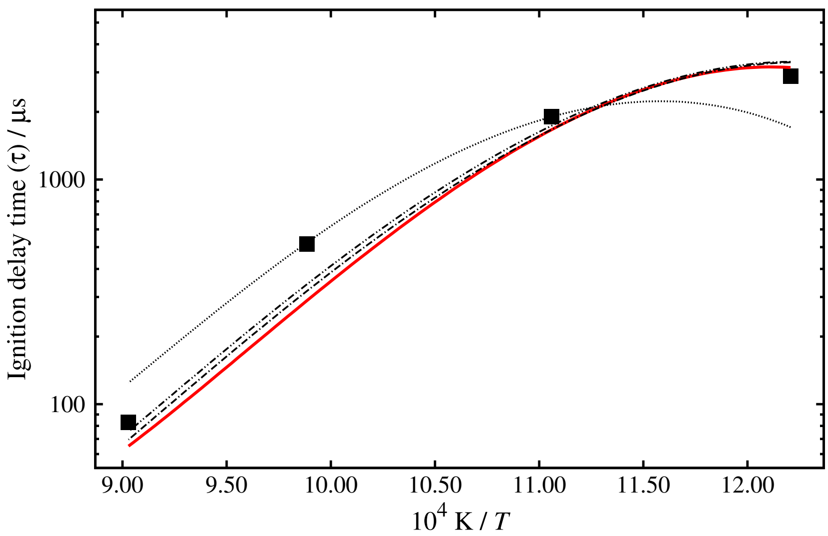
S63 Shock tube ignition delay times of methanol/oxygen/argon mixtures. Symbols are experimental data [49] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

12.39% CH_3OH, 18.58% O_2, 69.03% N_2, Φ = 1.00, p_{av} = 13.00 atm



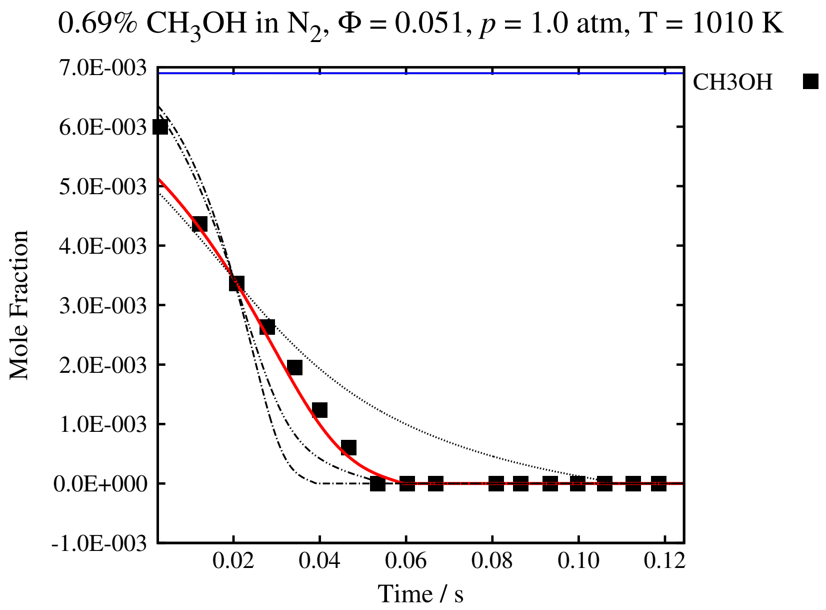
(a)

12.39% CH_3OH, 18.58% O_2, 69.03% N_2, Φ = 1.00, p_{av} = 40.00 atm



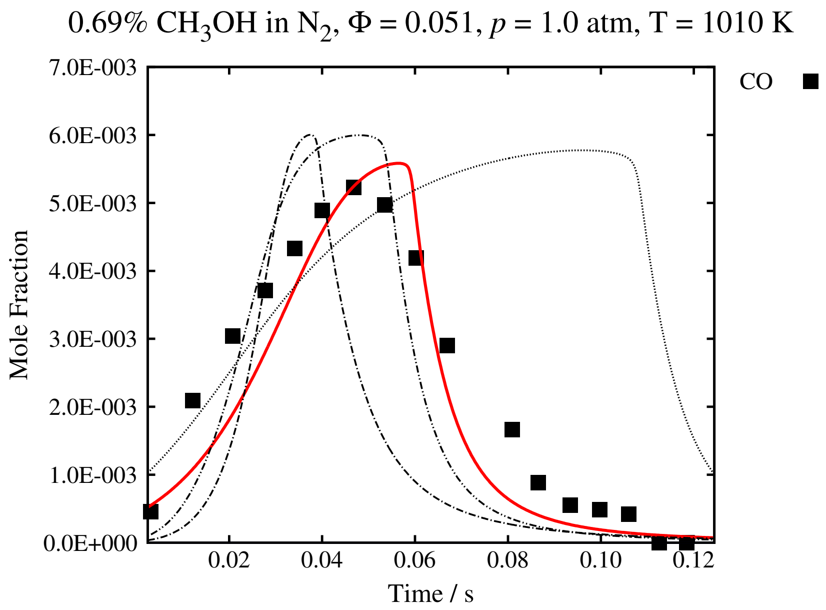
(b)

S64 Shock tube ignition delay times of methanol/air mixtures. Symbols are experimental data [50] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



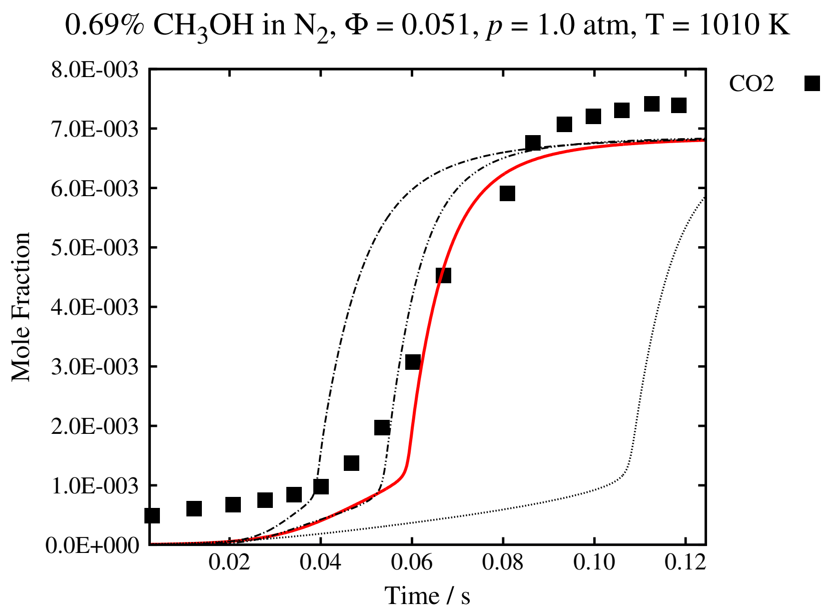
0.69% CH_3OH in N_2, Φ = 0.051, p = 1.0 atm, T = 1010 K
CH3OH
Mole Fraction
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
-1.0E-003
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

(a)



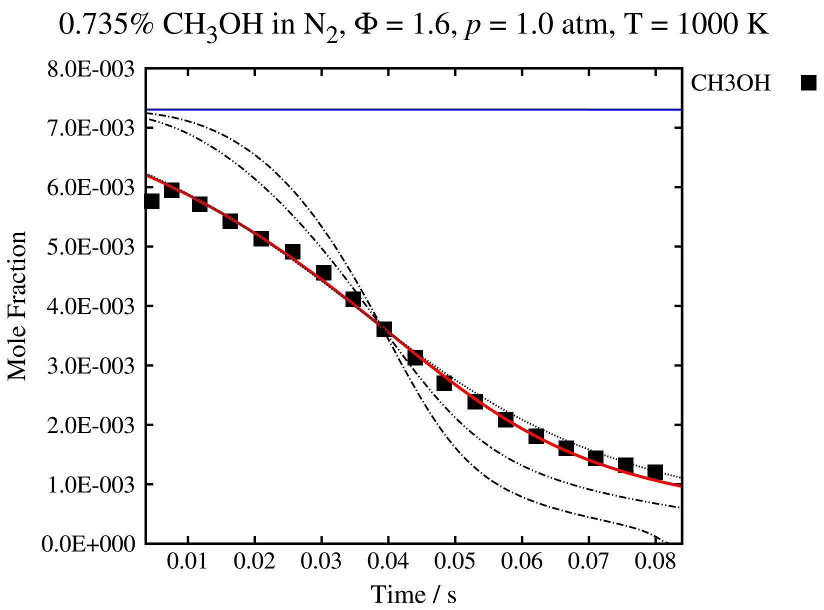
0.69% CH_3OH in N_2, Φ = 0.051, p = 1.0 atm, T = 1010 K
CO
Mole Fraction
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

(b)

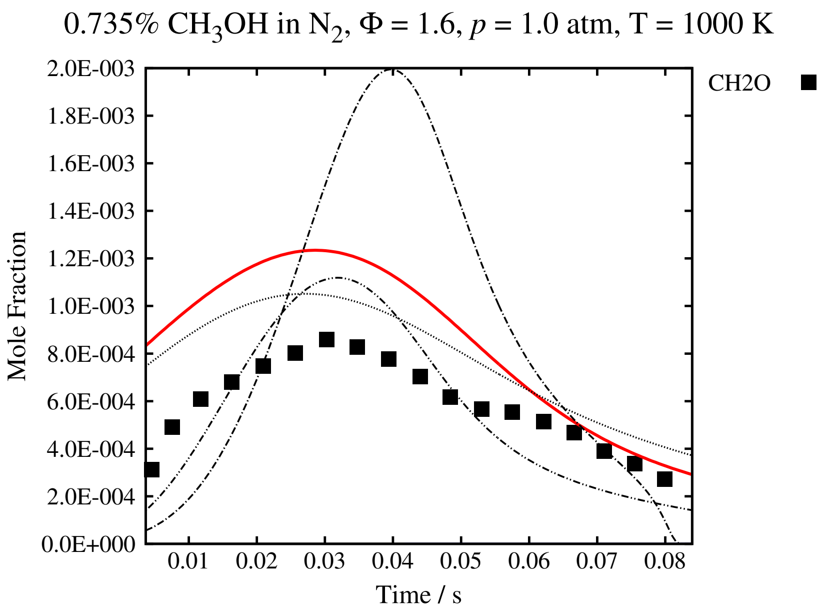


(c)

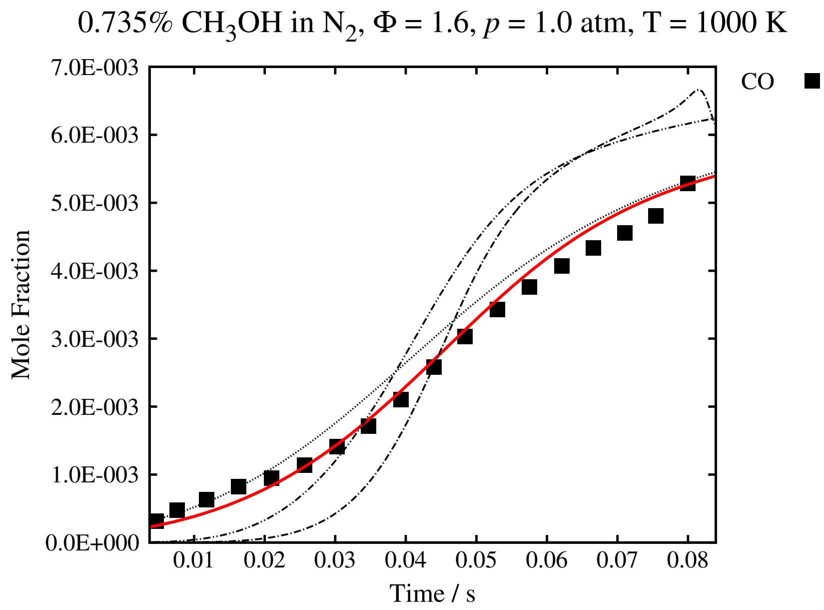
S65 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.735% CH_3OH in N_2, Φ = 1.6, p = 1.0 atm, T = 1000 K
CH3OH
Mole Fraction
Time / s
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

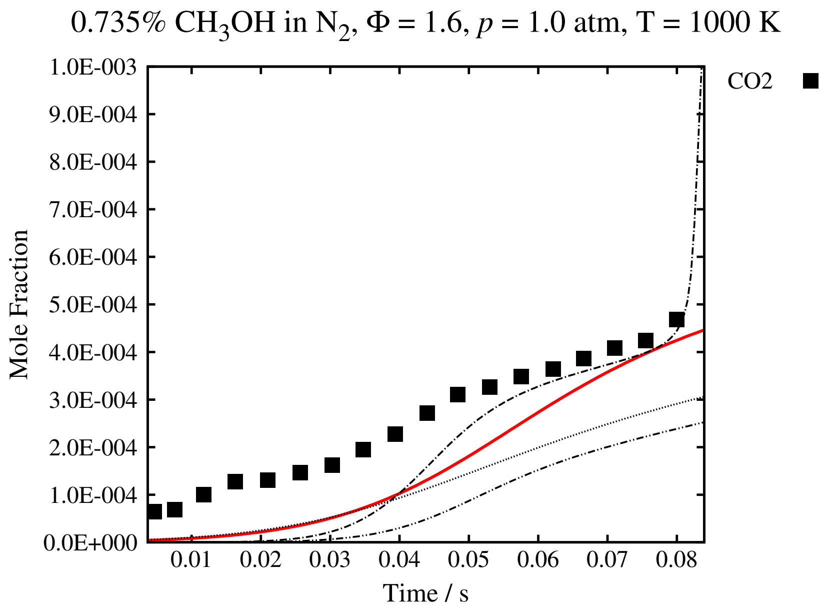
(a)


0.735% CH_3OH in N_2, Φ = 1.6, p = 1.0 atm, T = 1000 K
CH2O
Mole Fraction
Time / s
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

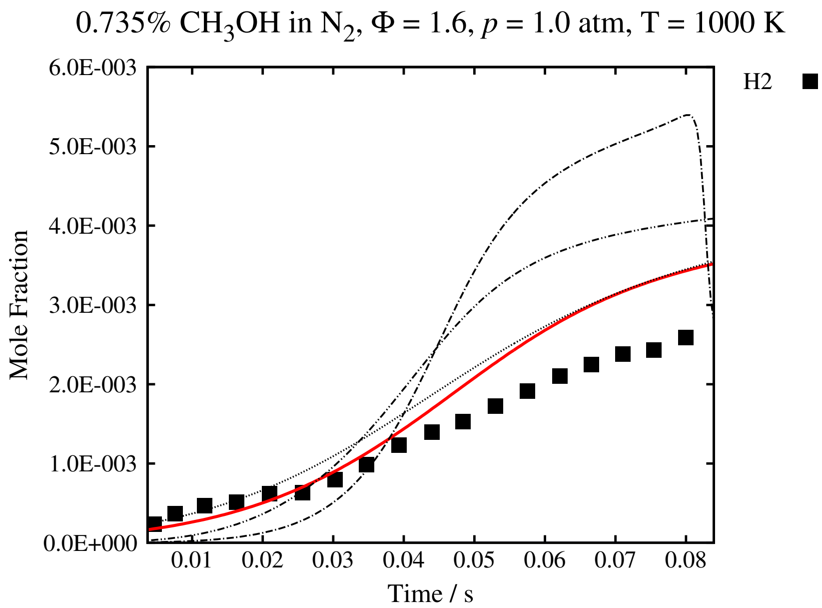
(b)


0.735% CH_3OH in N_2, Φ = 1.6, p = 1.0 atm, T = 1000 K
CO
Mole Fraction
Time / s
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

(c)

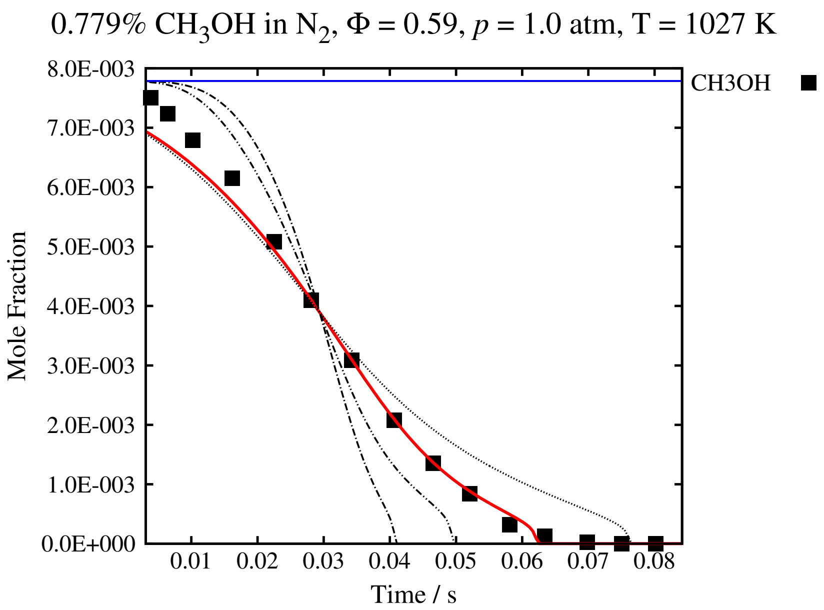

0.735% CH_3OH in N_2, Φ = 1.6, p = 1.0 atm, T = 1000 K
CO2
Mole Fraction
Time / s
1.0E-003
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

(d)

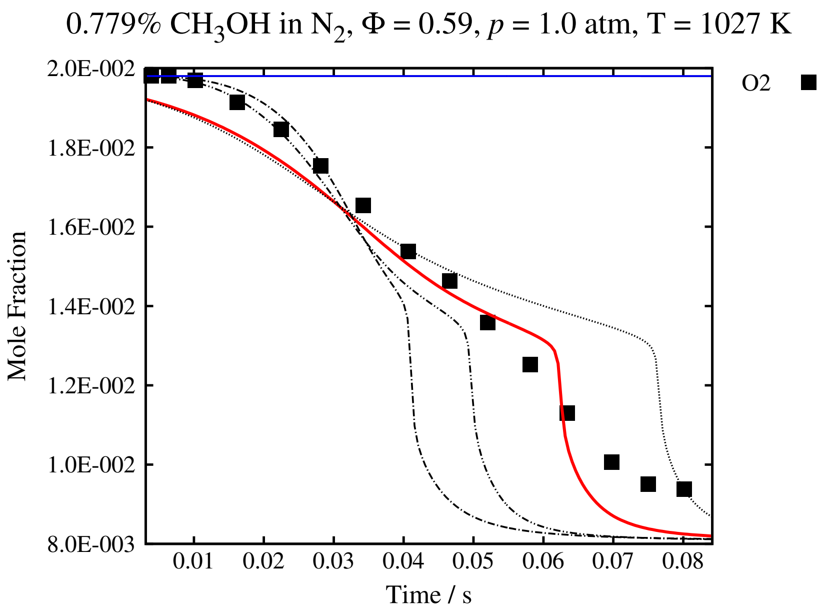


(e)

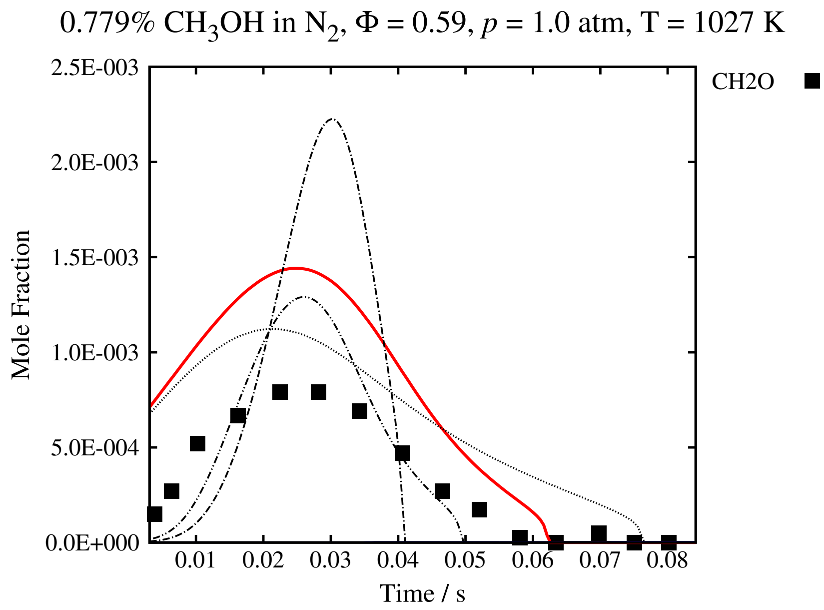
S66 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.779% CH3OH in N2, Φ = 0.59, p = 1.0 atm, T = 1027 K
CH3OH
Mole Fraction
Time / s
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

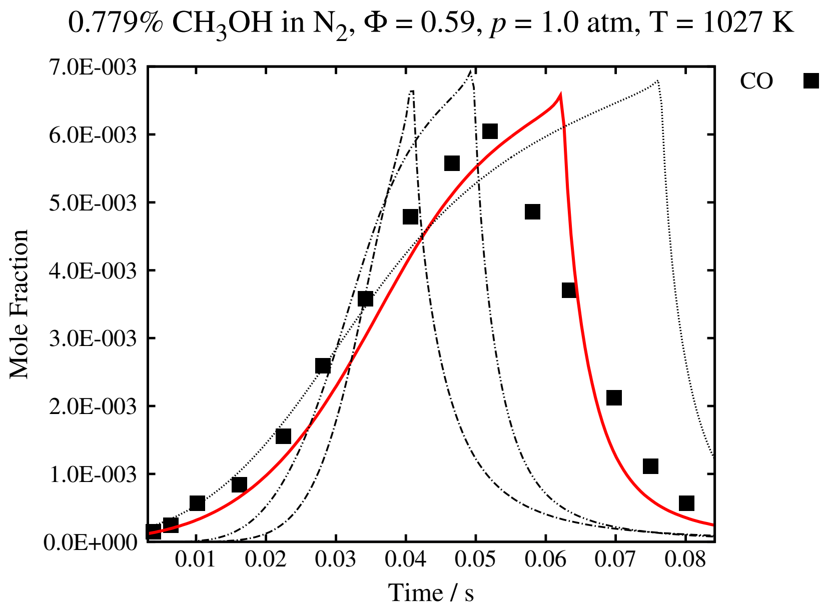
(a)


0.779% CH3OH in N2, Φ = 0.59, p = 1.0 atm, T = 1027 K
O2
Mole Fraction
Time / s
2.0E-002
1.8E-002
1.6E-002
1.4E-002
1.2E-002
1.0E-002
8.0E-003
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

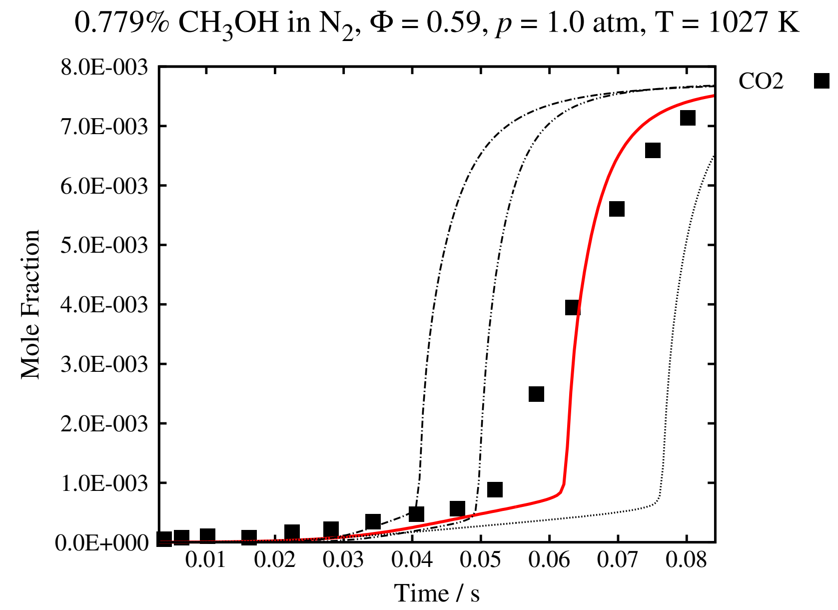
(b)


0.779% CH3OH in N2, Φ = 0.59, p = 1.0 atm, T = 1027 K
Mole Fraction
Time / s
CH2O
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

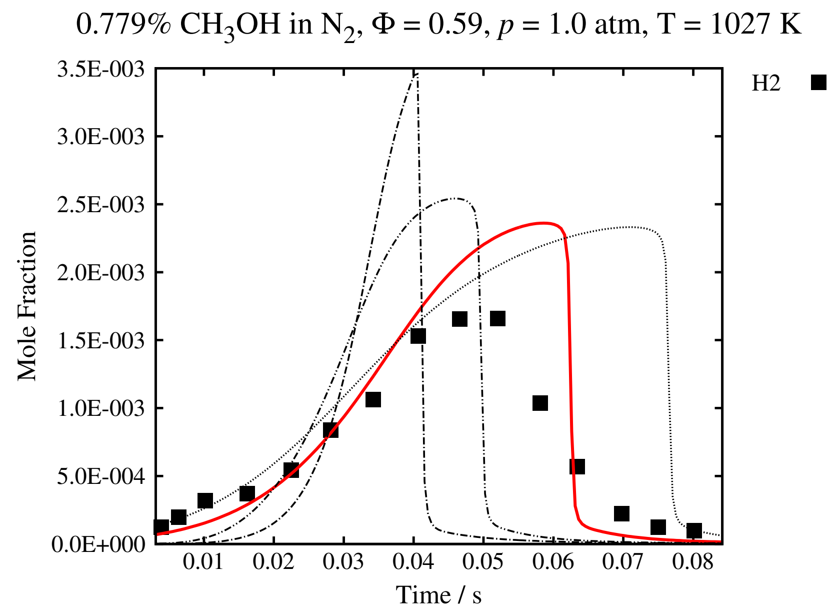
(c)


0.779% CH3OH in N2, Φ = 0.59, p = 1.0 atm, T = 1027 K
Mole Fraction
Time / s
CO
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08

(d)

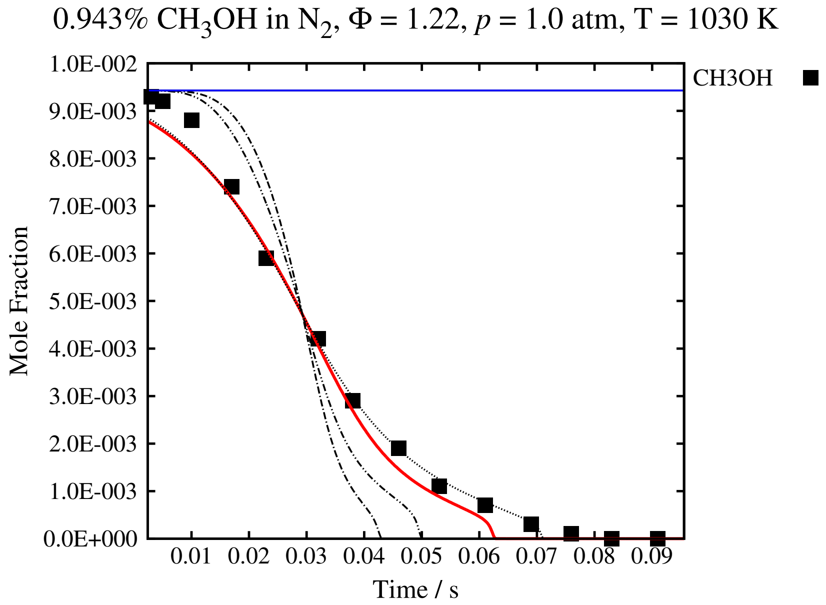


(e)

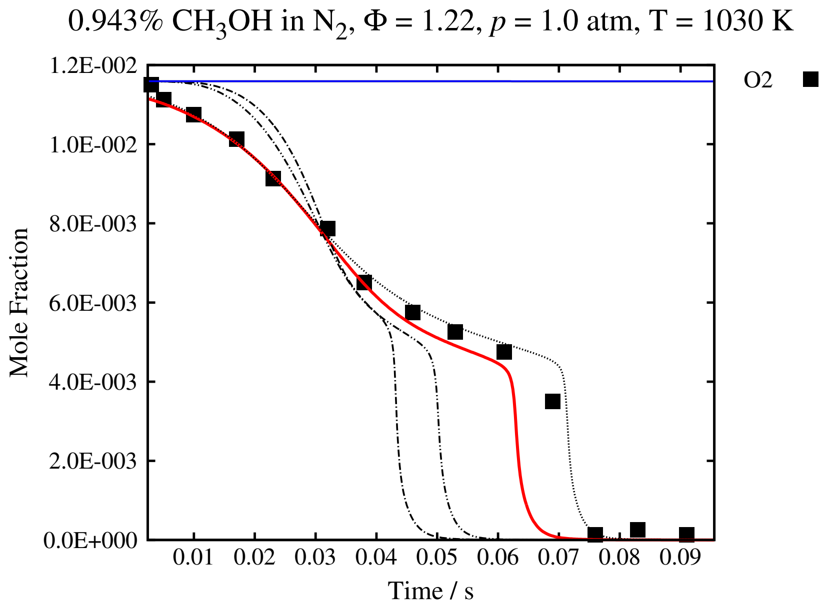


(f)

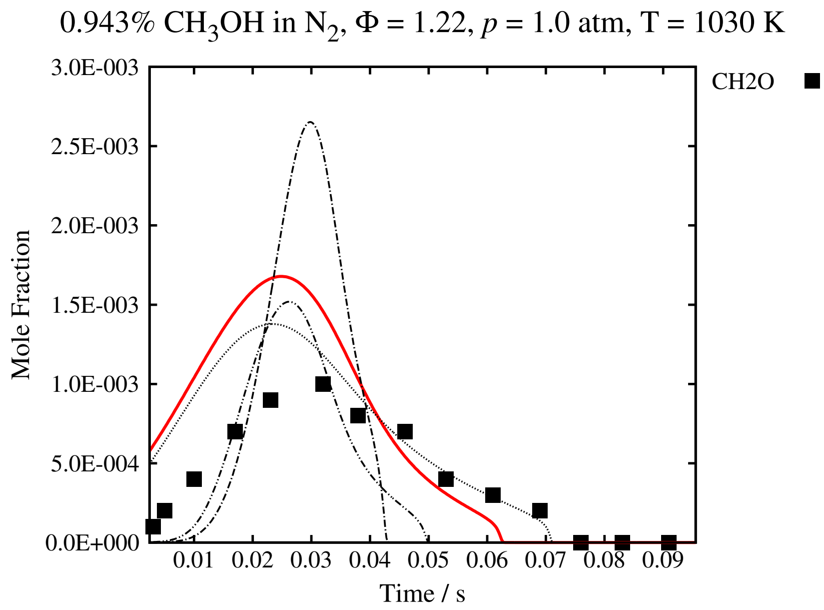
S67 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.943% CH_3OH in N_2, Φ = 1.22, p = 1.0 atm, T = 1030 K
CH3OH
Mole Fraction
Time / s
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09

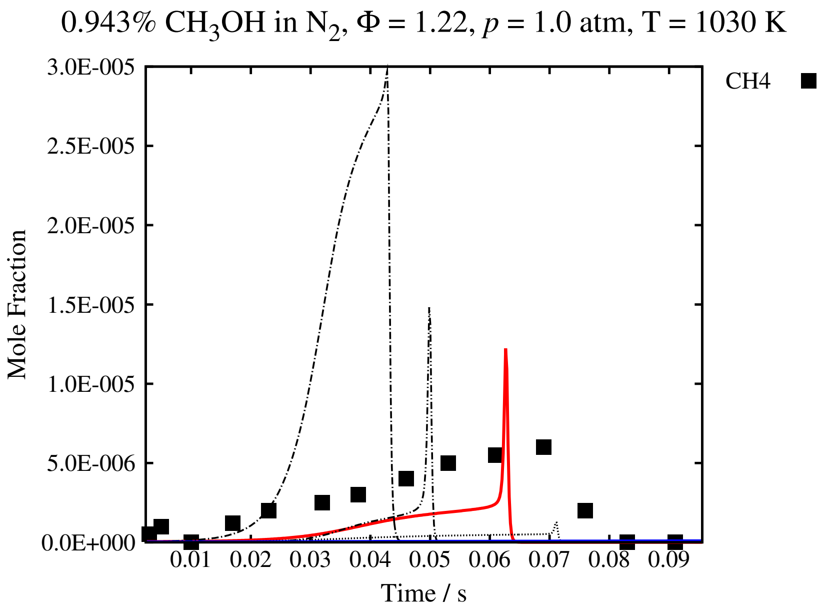
(a)


0.943% CH_3OH in N_2, Φ = 1.22, p = 1.0 atm, T = 1030 K
O2
Mole Fraction
Time / s
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09

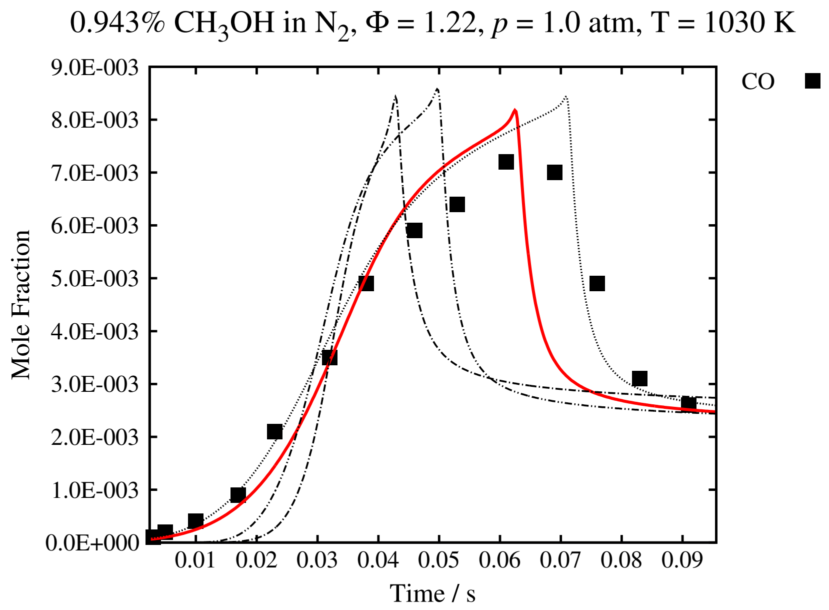
(b)


0.943% CH_3OH in N_2, Φ = 1.22, p = 1.0 atm, T = 1030 K
CH2O
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09
Time / s

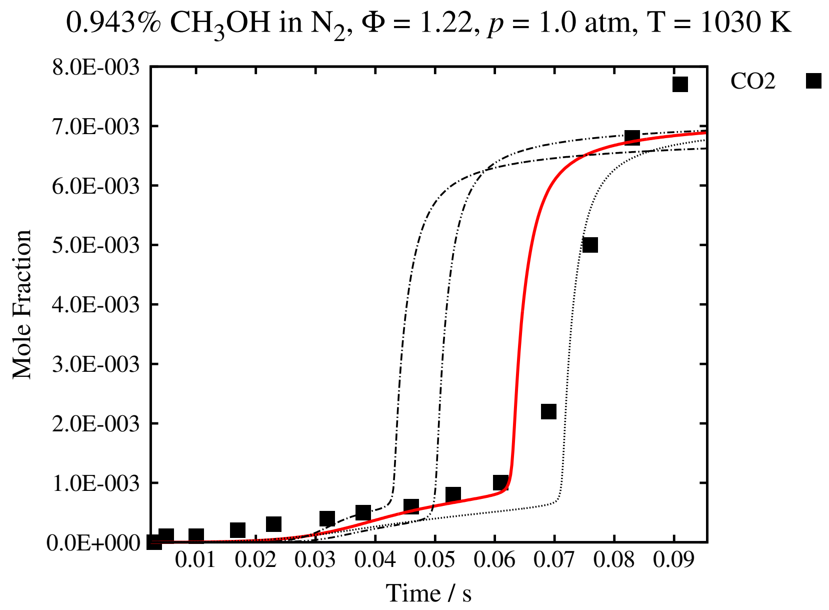
(c)


0.943% CH_3OH in N_2, Φ = 1.22, p = 1.0 atm, T = 1030 K
CH4
Mole Fraction
3.0E-005
2.5E-005
2.0E-005
1.5E-005
1.0E-005
5.0E-006
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09
Time / s

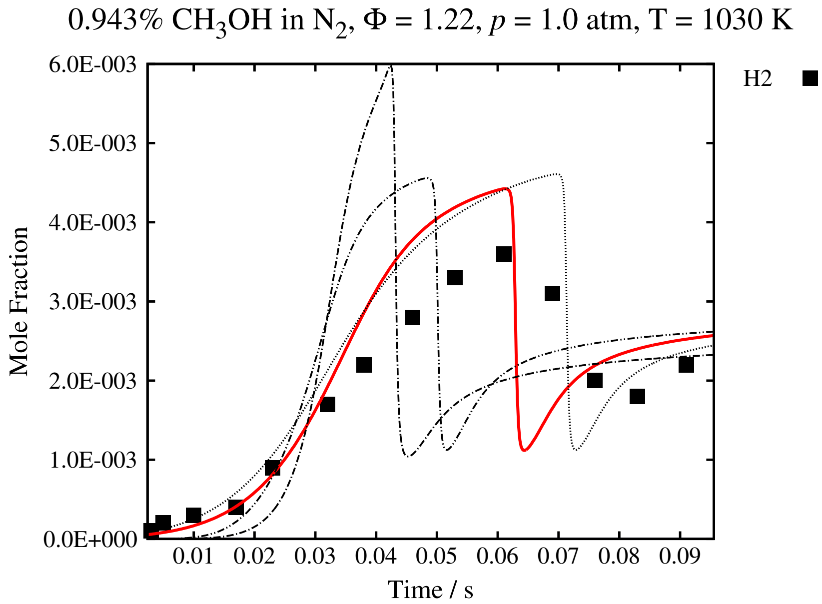
(d)


0.943% CH3OH in N2, Φ = 1.22, p = 1.0 atm, T = 1030 K
CO
Mole Fraction
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09
Time / s

(e)

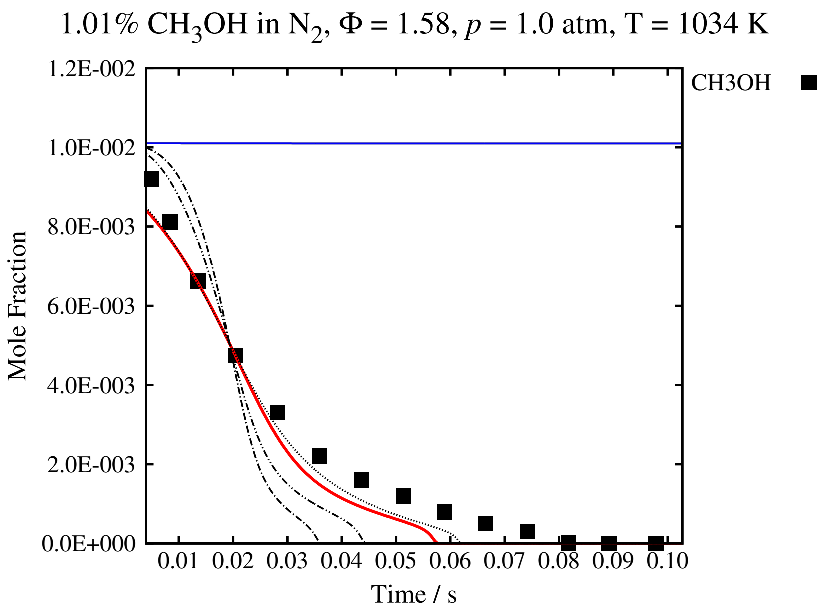

0.943% CH3OH in N2, Φ = 1.22, p = 1.0 atm, T = 1030 K
CO2
Mole Fraction
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09
Time / s

(f)

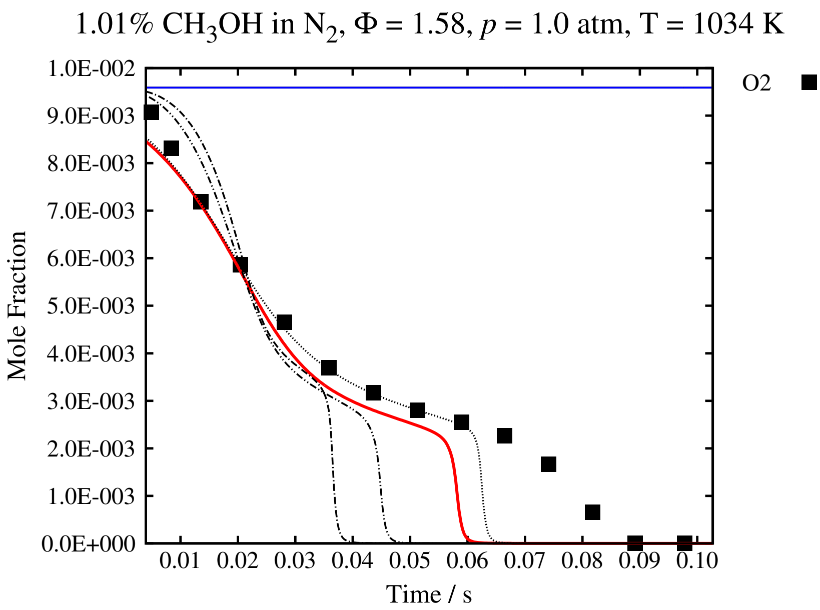


(g)

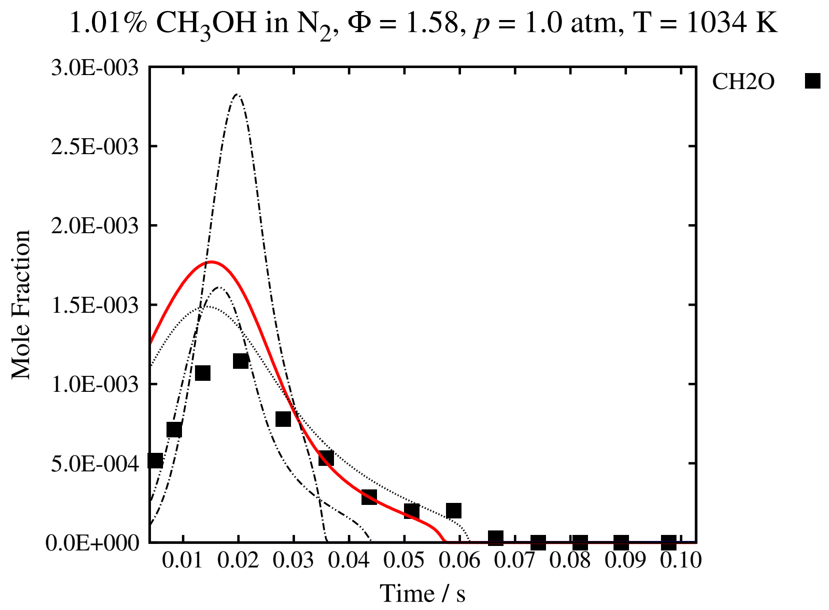
S68 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


1.01% CH3OH in N2, Φ = 1.58, p = 1.0 atm, T = 1034 K
CH3OH
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
Mole Fraction
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10
Time / s

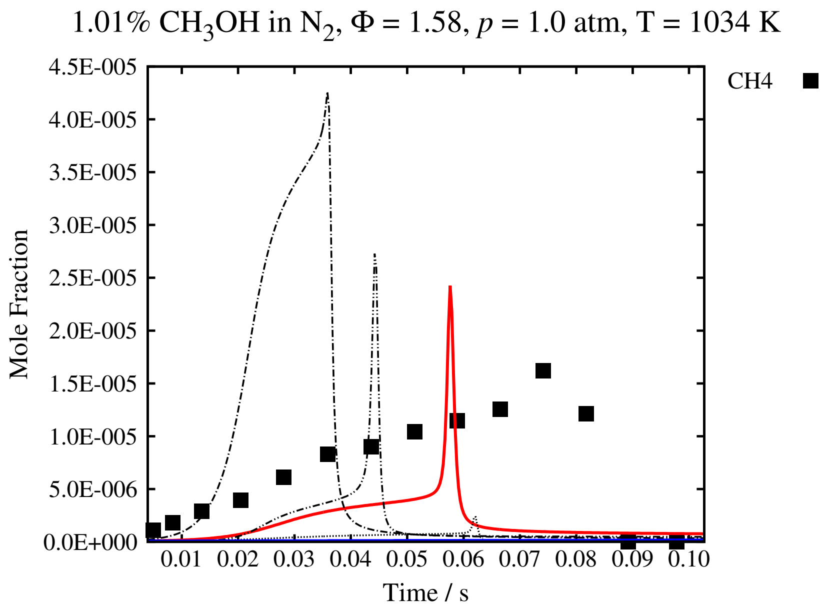
(a)


1.01% CH3OH in N2, Φ = 1.58, p = 1.0 atm, T = 1034 K
O2
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
Mole Fraction
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10
Time / s

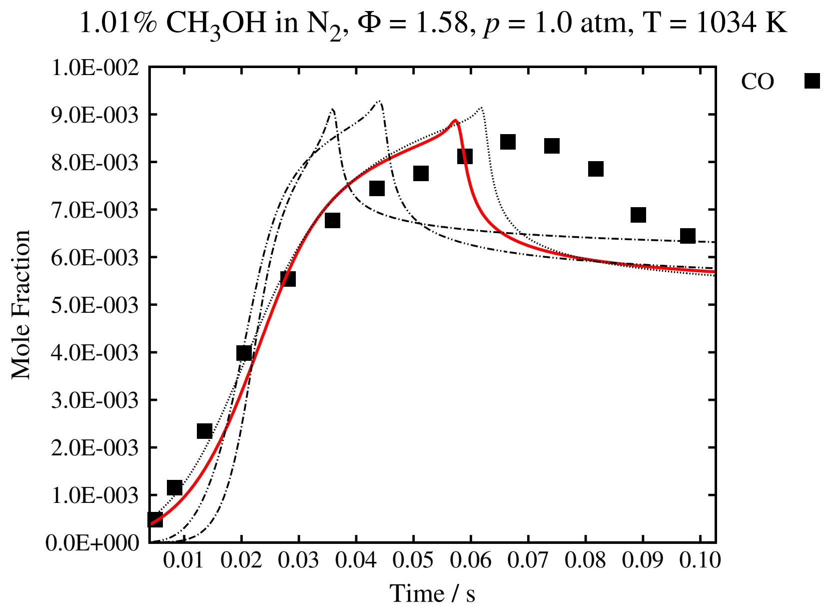
(b)


1.01% CH3OH in N2, Φ = 1.58, p = 1.0 atm, T = 1034 K
Mole Fraction
Time / s
CH2O
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10

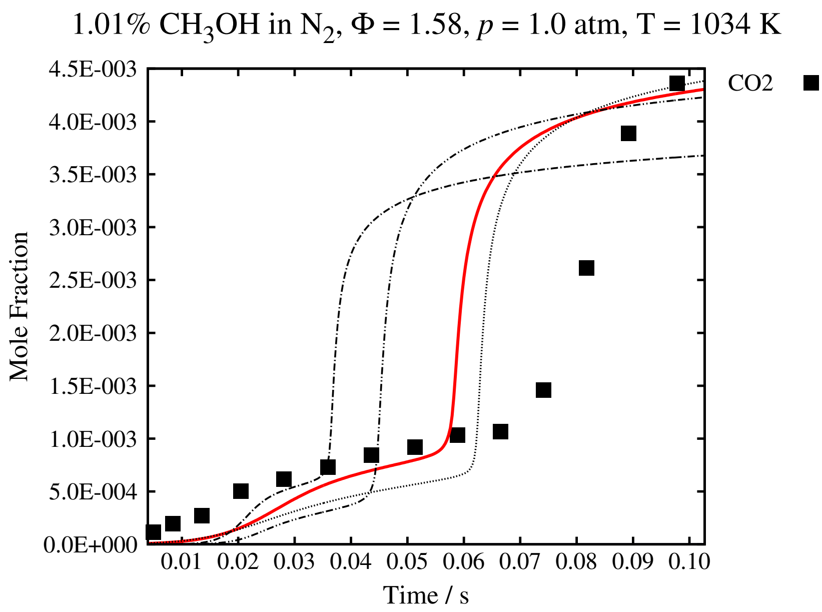
(c)


1.01% CH3OH in N2, Φ = 1.58, p = 1.0 atm, T = 1034 K
Mole Fraction
Time / s
CH4
4.5E-005
4.0E-005
3.5E-005
3.0E-005
2.5E-005
2.0E-005
1.5E-005
1.0E-005
5.0E-006
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10

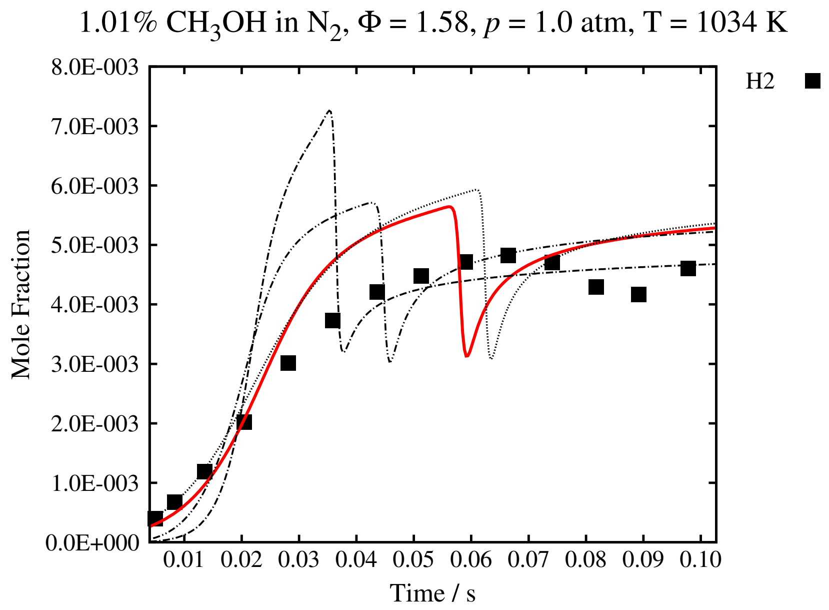
(d)


1.01% CH3OH in N2, Φ = 1.58, p = 1.0 atm, T = 1034 K
CO
Mole Fraction
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10
Time / s

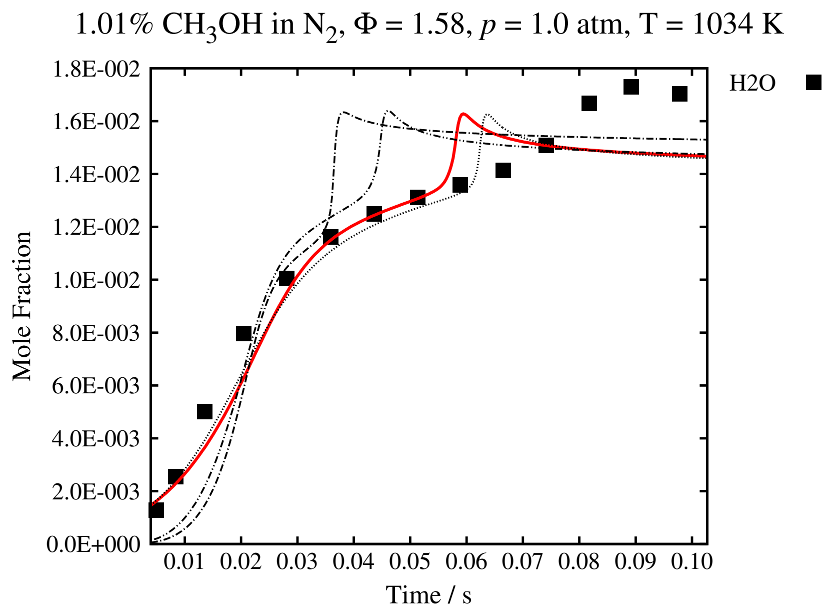
(e)


1.01% CH3OH in N2, Φ = 1.58, p = 1.0 atm, T = 1034 K
CO2
Mole Fraction
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10
Time / s

(f)

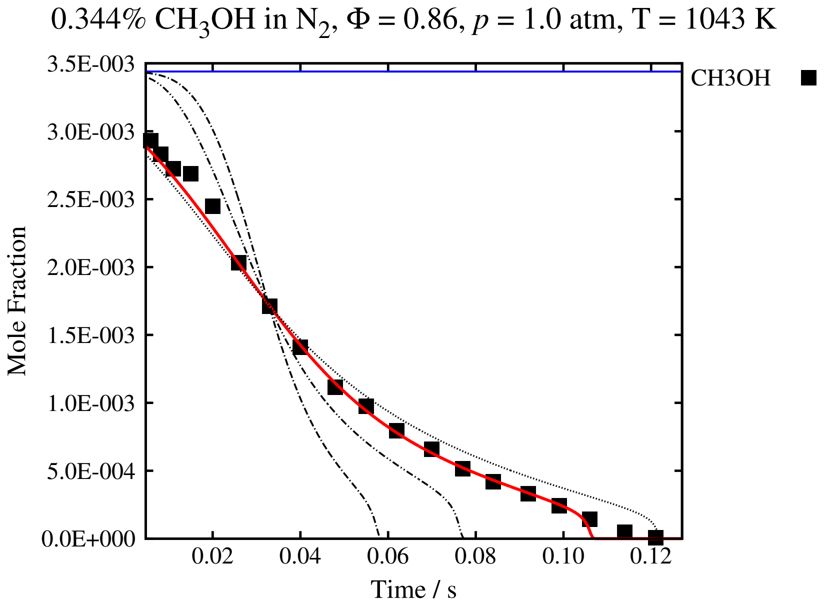


(g)

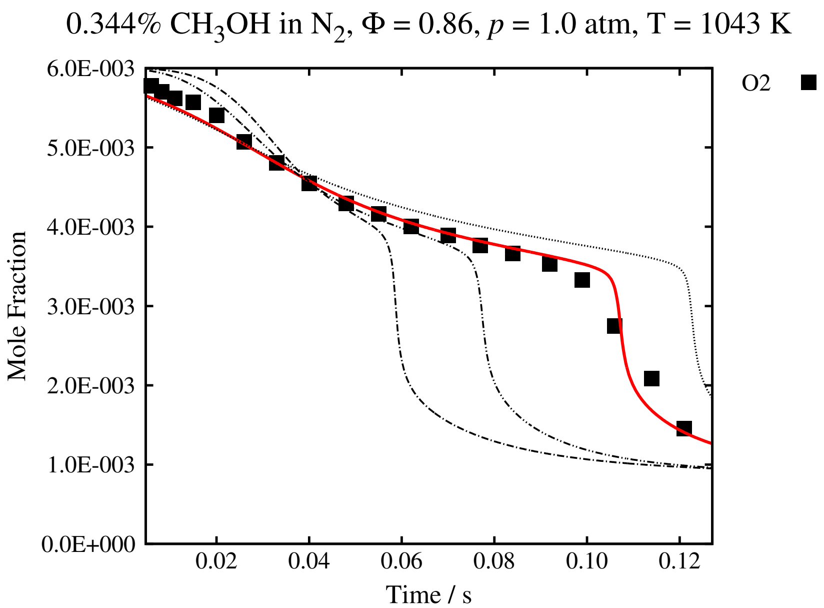


(h)

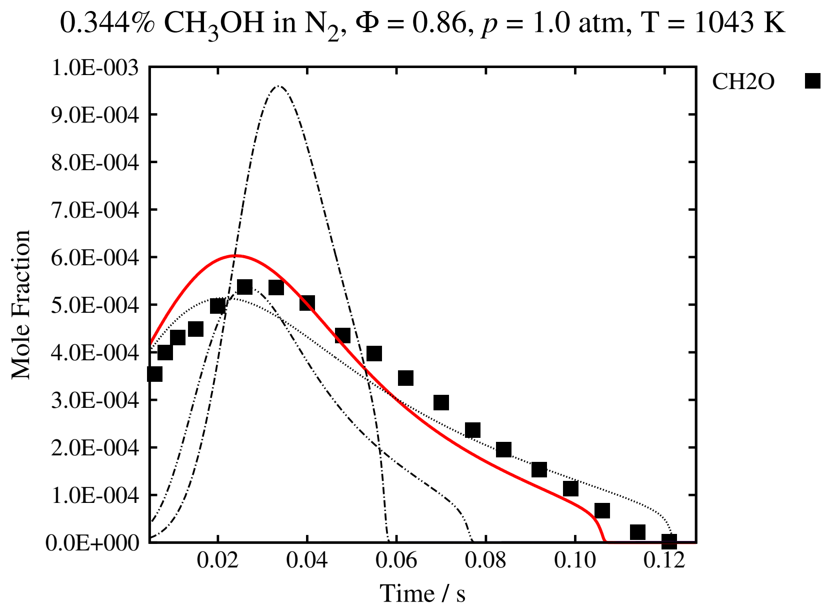
S69 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.344% CH3OH in N2, Φ = 0.86, p = 1.0 atm, T = 1043 K
CH3OH
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

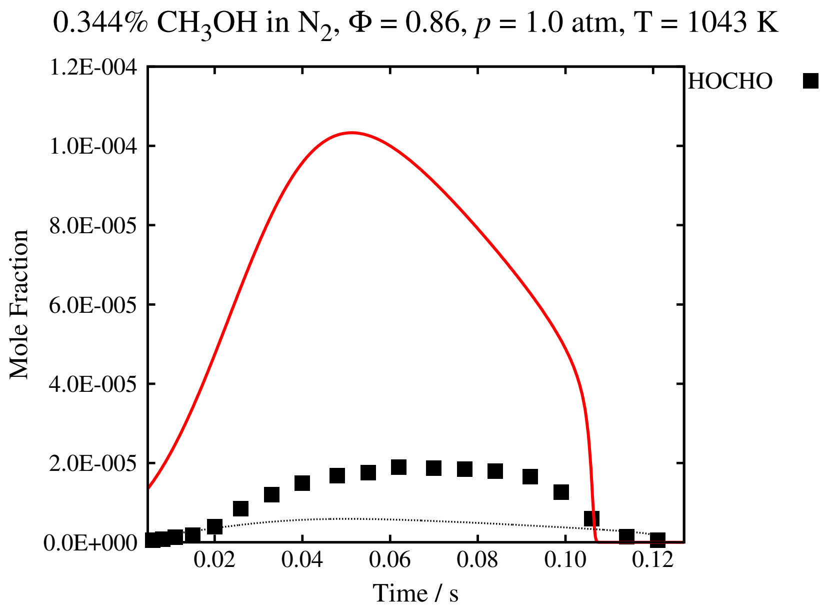
(a)


0.344% CH3OH in N2, Φ = 0.86, p = 1.0 atm, T = 1043 K
O2
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

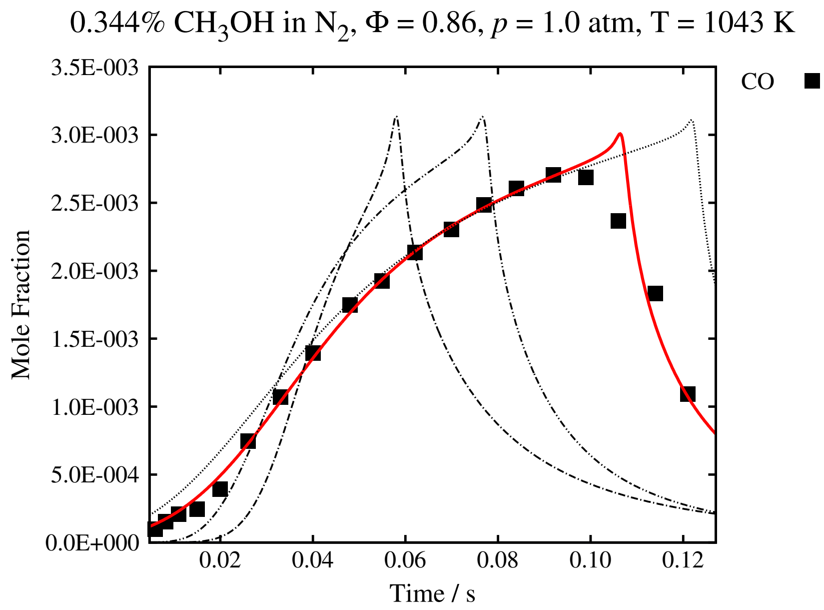
(b)


0.344% CH3OH in N2, Φ = 0.86, p = 1.0 atm, T = 1043 K
CH2O
Mole Fraction
1.0E-003
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

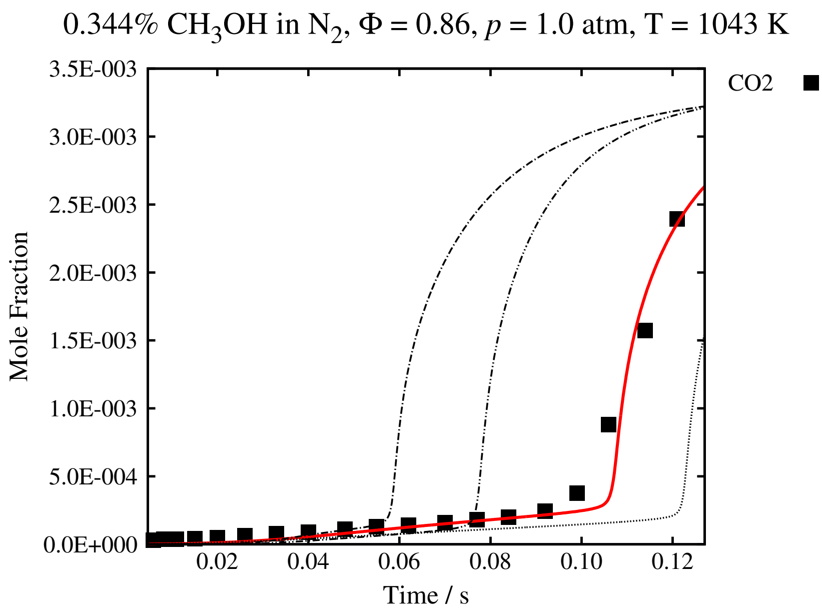
(c)


0.344% CH3OH in N2, Φ = 0.86, p = 1.0 atm, T = 1043 K
HOCHO
Mole Fraction
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

(d)

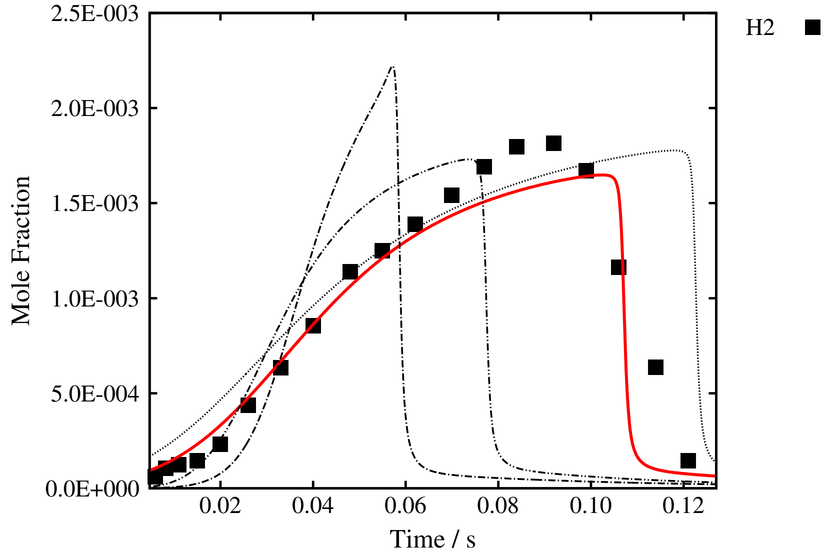

0.344% CH3OH in N2, Φ = 0.86, p = 1.0 atm, T = 1043 K
CO
Mole Fraction
Time / s
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12

(e)


0.344% CH3OH in N2, Φ = 0.86, p = 1.0 atm, T = 1043 K
CO2
Mole Fraction
Time / s
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12

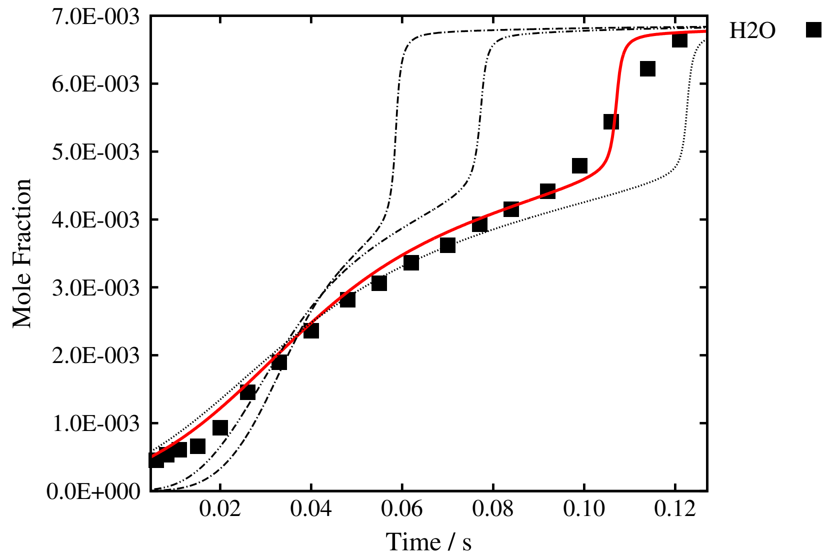
(f)

0.344% CH_3OH in N_2, Φ = 0.86, p = 1.0 atm, T = 1043 K



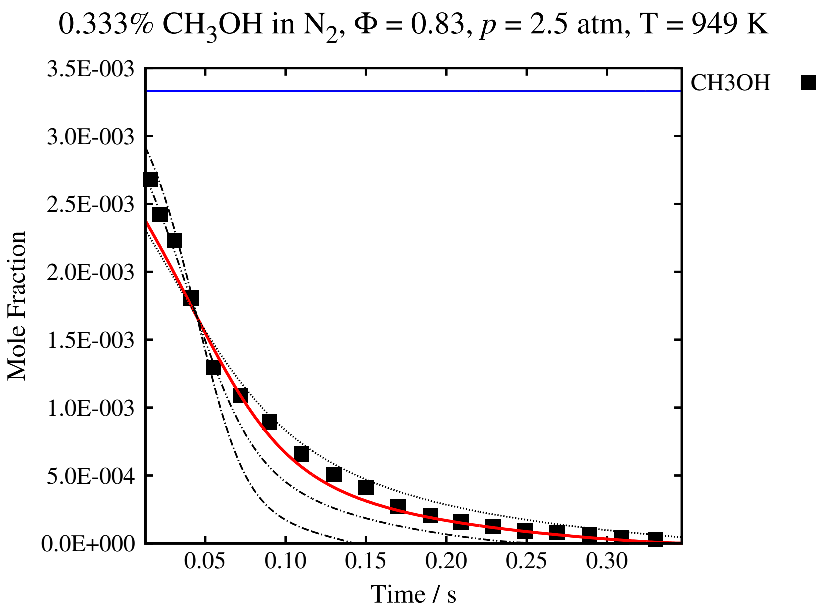
(g)

0.344% CH_3OH in N_2, Φ = 0.86, p = 1.0 atm, T = 1043 K

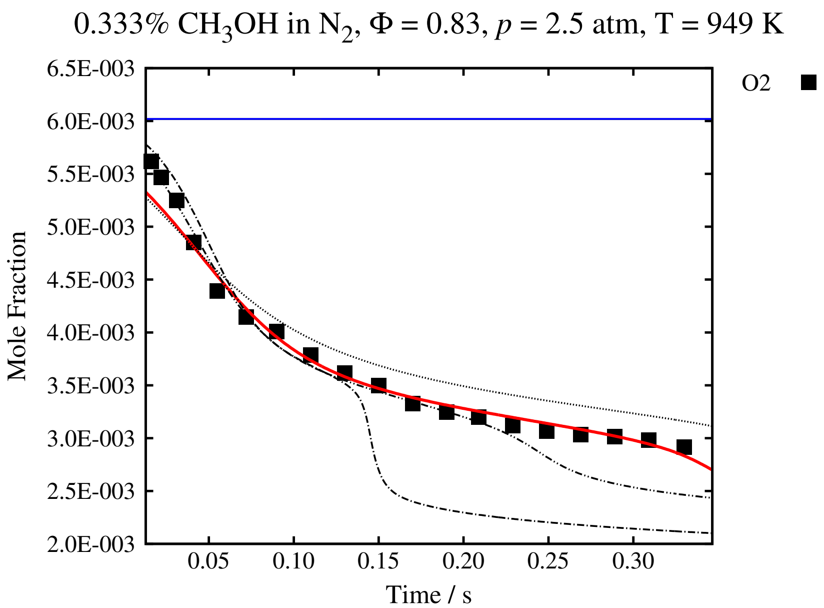


(h)

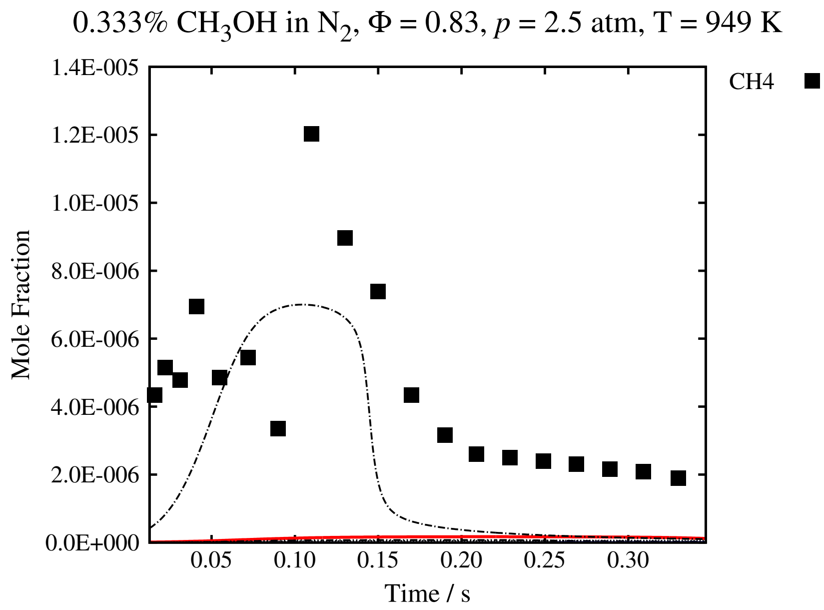
S70 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
CH3OH
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

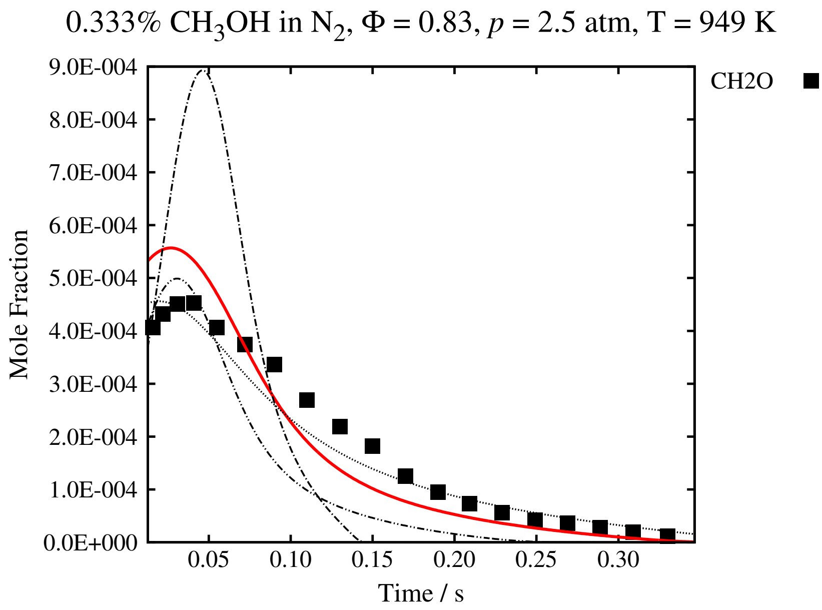
(a)


0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
O2
Mole Fraction
6.5E-003
6.0E-003
5.5E-003
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

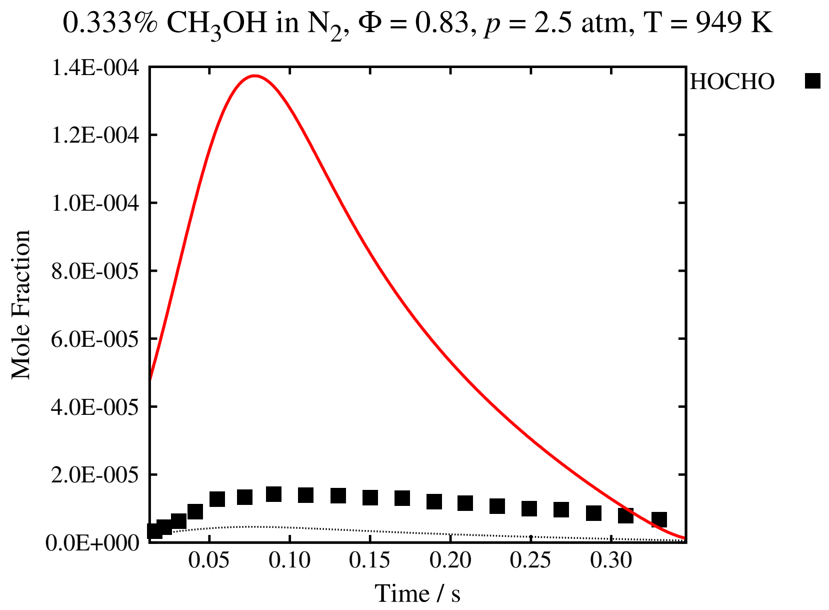
(b)


0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
CH4
Mole Fraction
1.4E-005
1.2E-005
1.0E-005
8.0E-006
6.0E-006
4.0E-006
2.0E-006
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

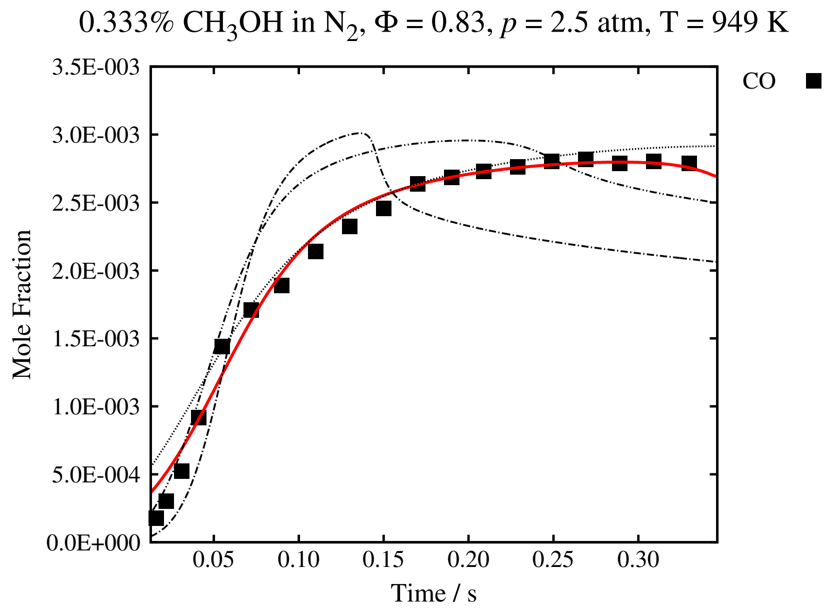
(c)


0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
CH2O
Mole Fraction
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

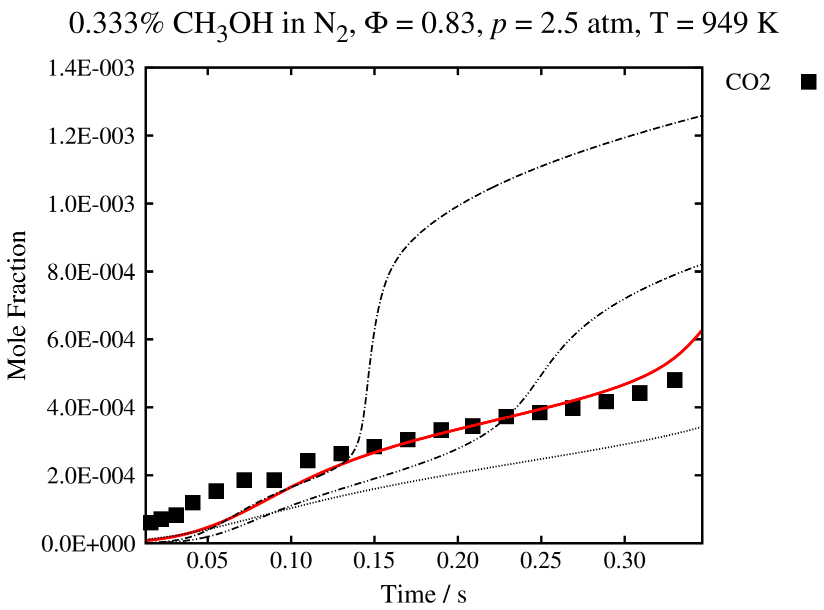
(d)


0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
HOCHO
Mole Fraction
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

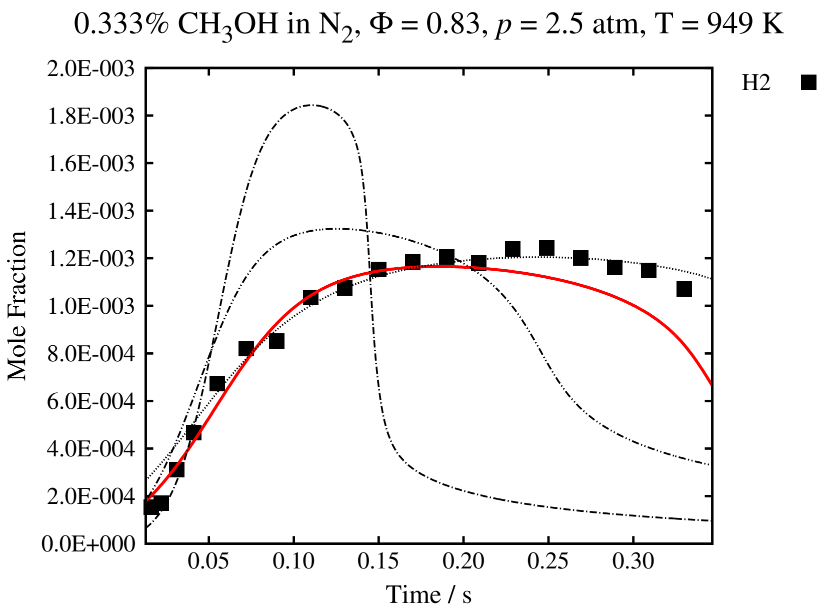
(e)


0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
CO
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

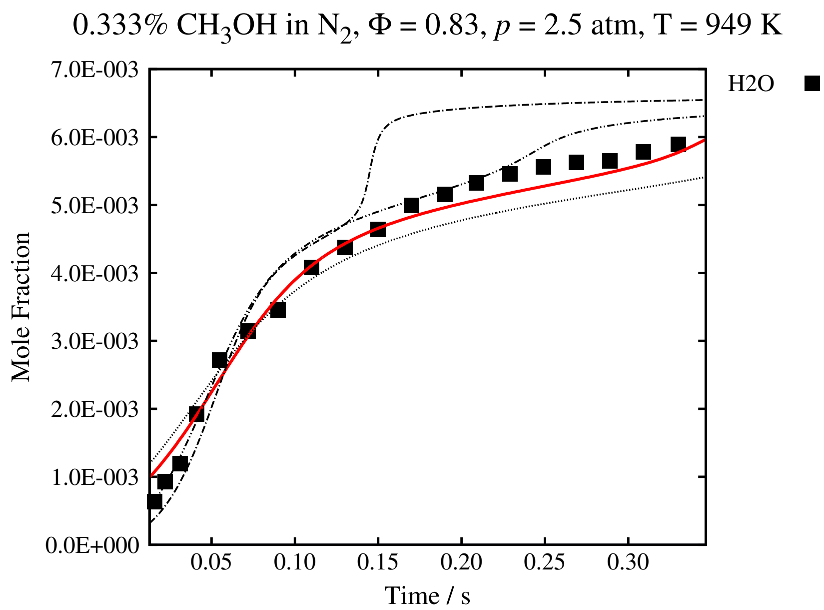
(f)


0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
CO2
Mole Fraction
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

(g)

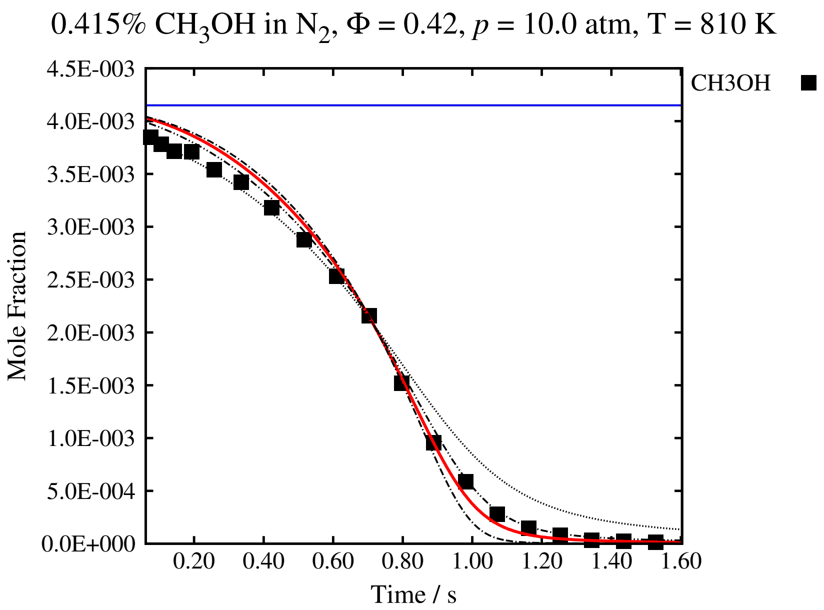

0.333% CH3OH in N2, Φ = 0.83, p = 2.5 atm, T = 949 K
H2
Mole Fraction
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

(h)

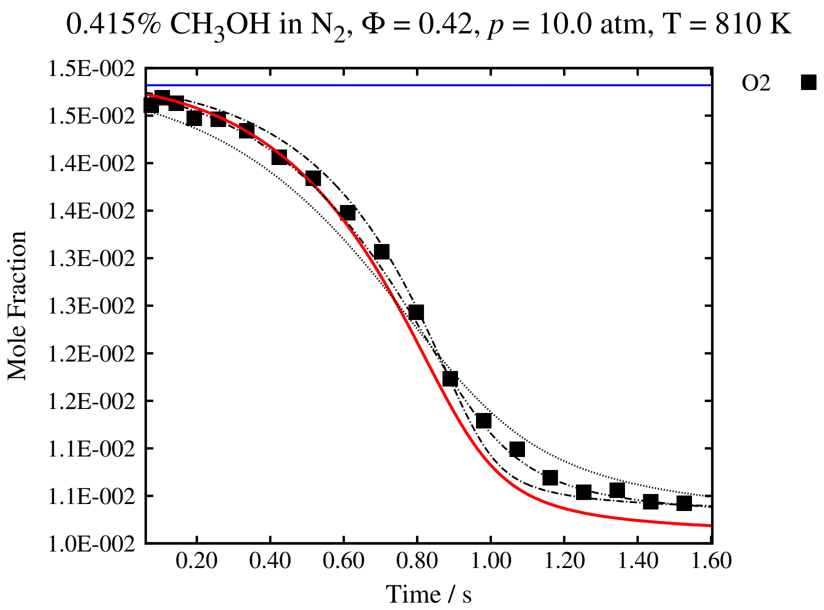


(i)

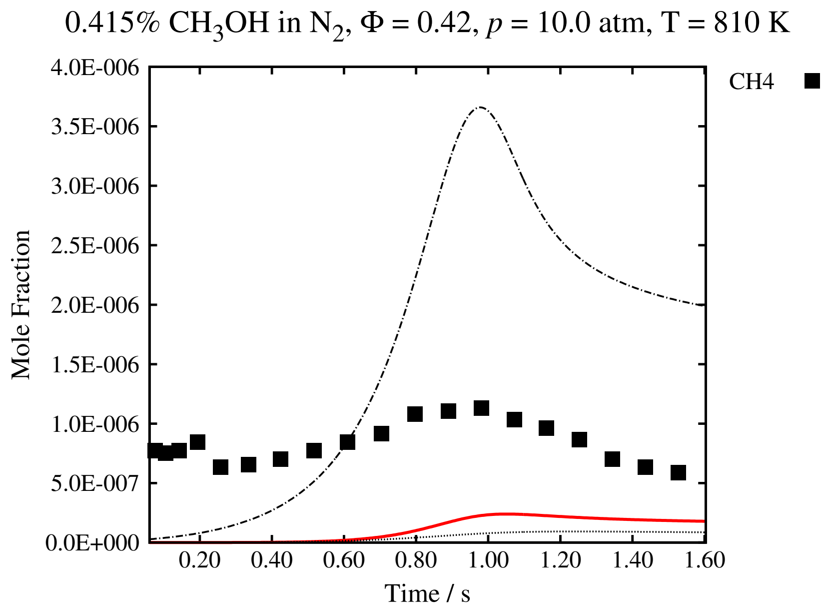
S71 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.415% CH_3OH in N_2, Φ = 0.42, *p* = 10.0 atm, T = 810 K
CH3OH
Mole Fraction
Time / s
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

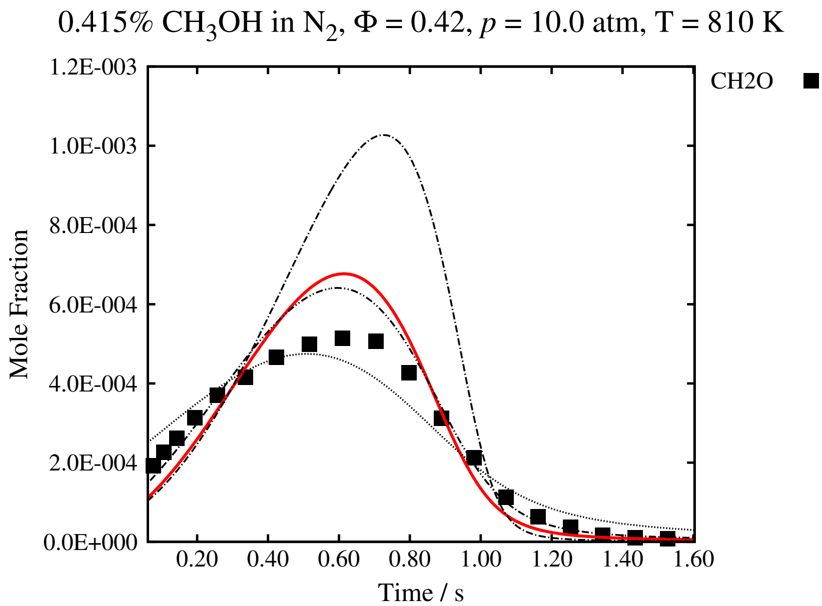
(a)


0.415% CH_3OH in N_2, Φ = 0.42, *p* = 10.0 atm, T = 810 K
O2
Mole Fraction
Time / s
1.5E-002
1.5E-002
1.4E-002
1.4E-002
1.3E-002
1.3E-002
1.2E-002
1.2E-002
1.1E-002
1.1E-002
1.0E-002
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

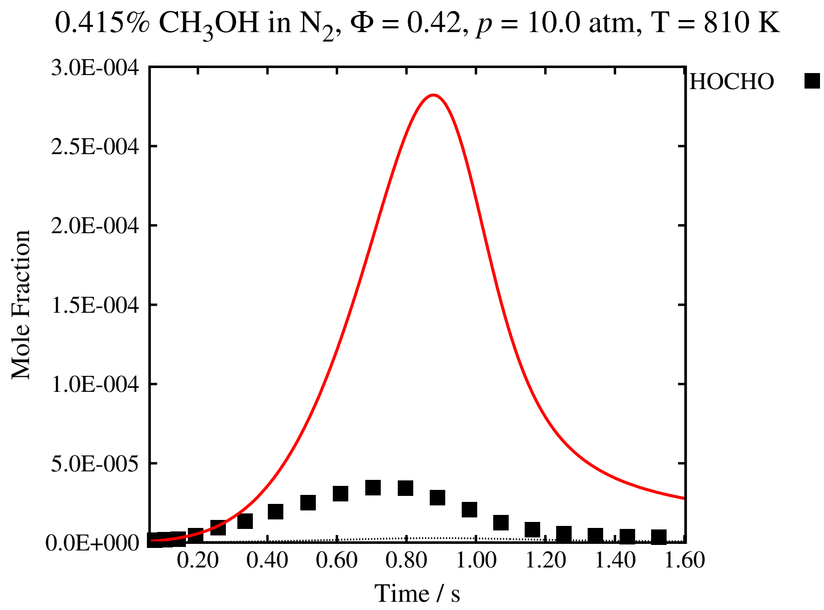
(b)


0.415% CH3OH in N2, Φ = 0.42, p = 10.0 atm, T = 810 K
CH4
Mole Fraction
Time / s
4.0E-006
3.5E-006
3.0E-006
2.5E-006
2.0E-006
1.5E-006
1.0E-006
5.0E-007
0.0E+000
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

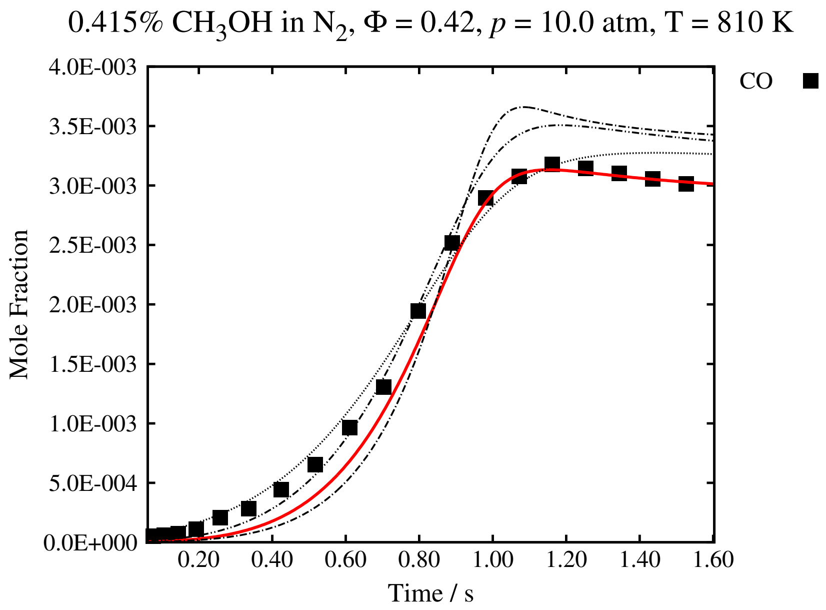
(c)


0.415% CH3OH in N2, Φ = 0.42, p = 10.0 atm, T = 810 K
CH2O
Mole Fraction
Time / s
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

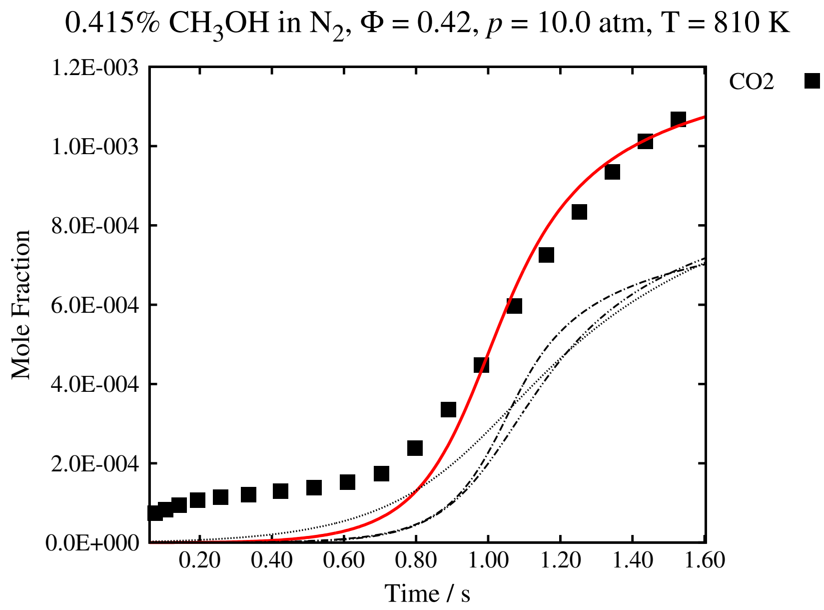
(d)


0.415% CH_3OH in N_2, Φ = 0.42, p = 10.0 atm, T = 810 K
HOCHO
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60
Time / s

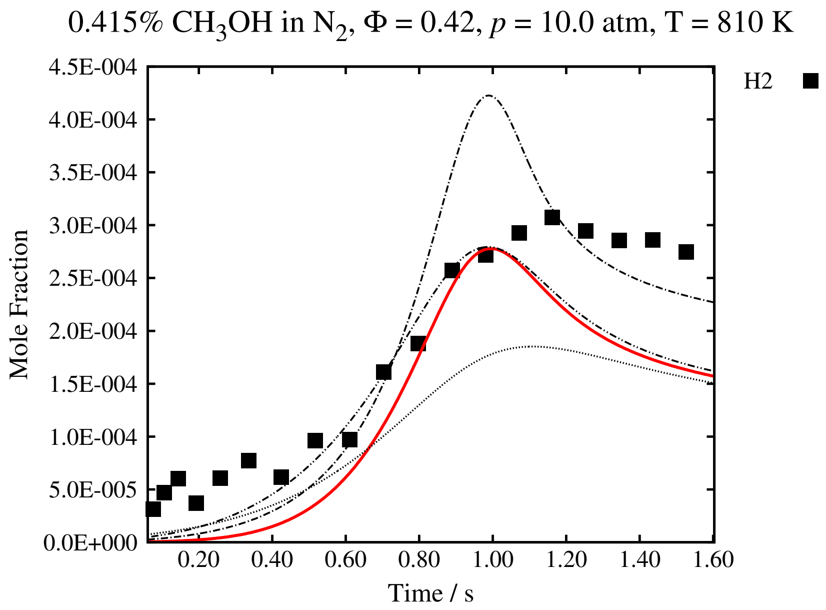
(e)


0.415% CH_3OH in N_2, Φ = 0.42, p = 10.0 atm, T = 810 K
CO
Mole Fraction
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60
Time / s

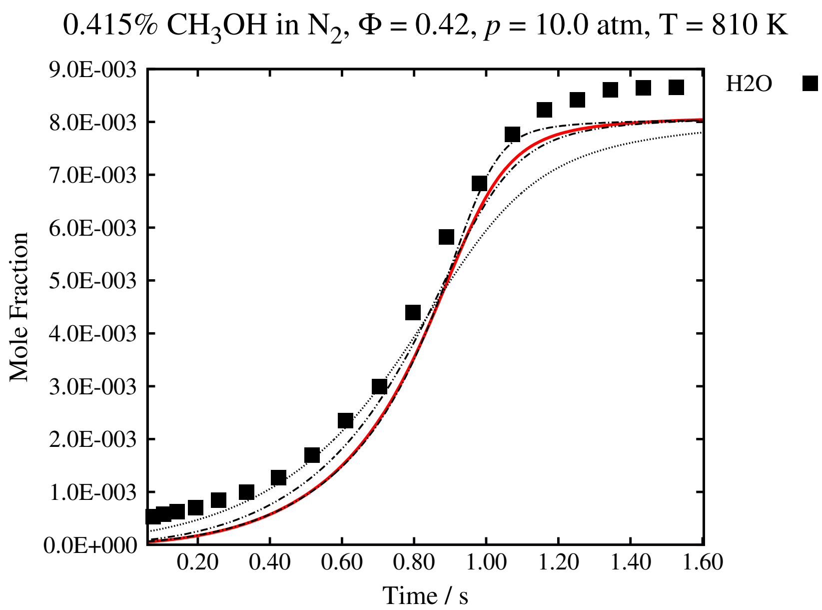
(f)


0.415% CH3OH in N2, Φ = 0.42, p = 10.0 atm, T = 810 K
CO2
Mole Fraction
Time / s
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

(g)


0.415% CH3OH in N2, Φ = 0.42, p = 10.0 atm, T = 810 K
H2
Mole Fraction
Time / s
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60

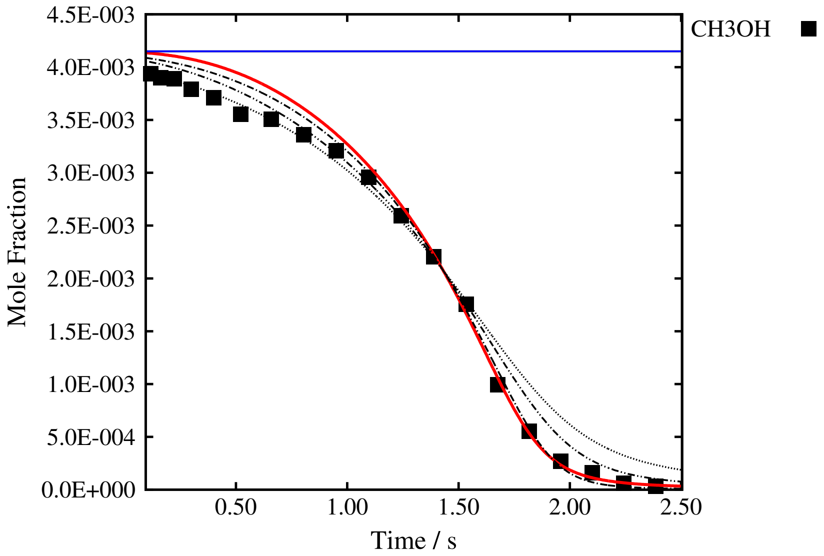
(h)



(i)

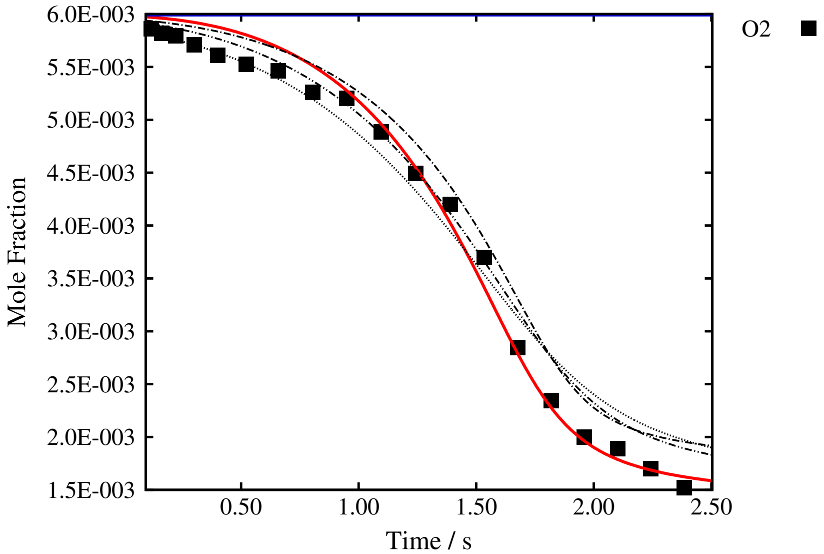
S72 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

0.415% CH_3OH in N_2, Φ = 1.04, p = 15.0 atm, T = 783 K



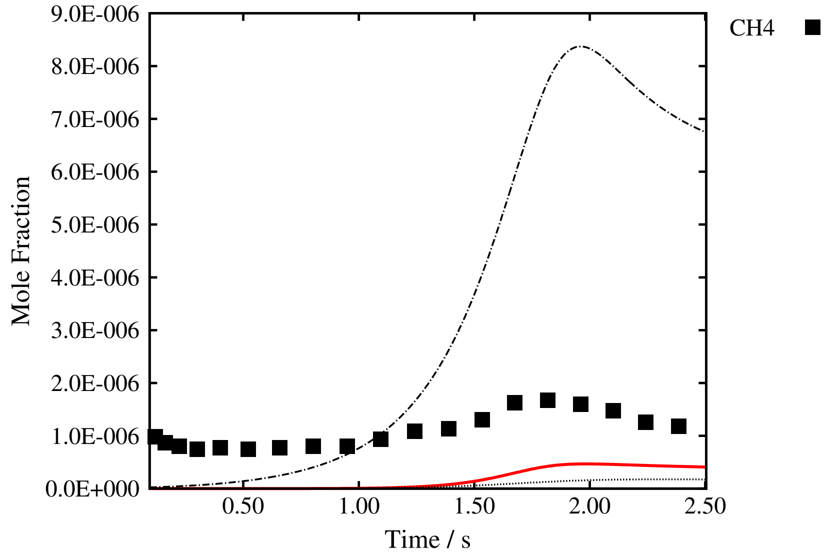
(a)

0.415% CH_3OH in N_2, Φ = 1.04, p = 15.0 atm, T = 783 K



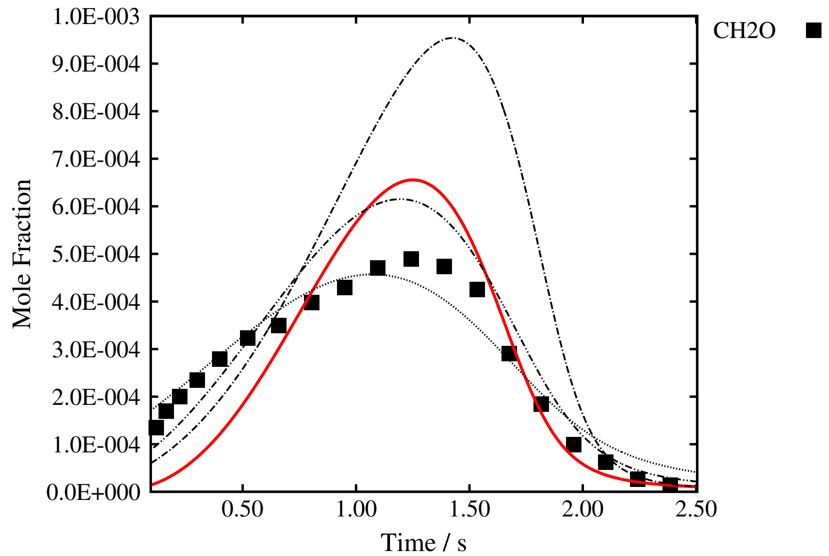
(b)

0.415% CH_3OH in N_2, Φ = 1.04, p = 15.0 atm, T = 783 K

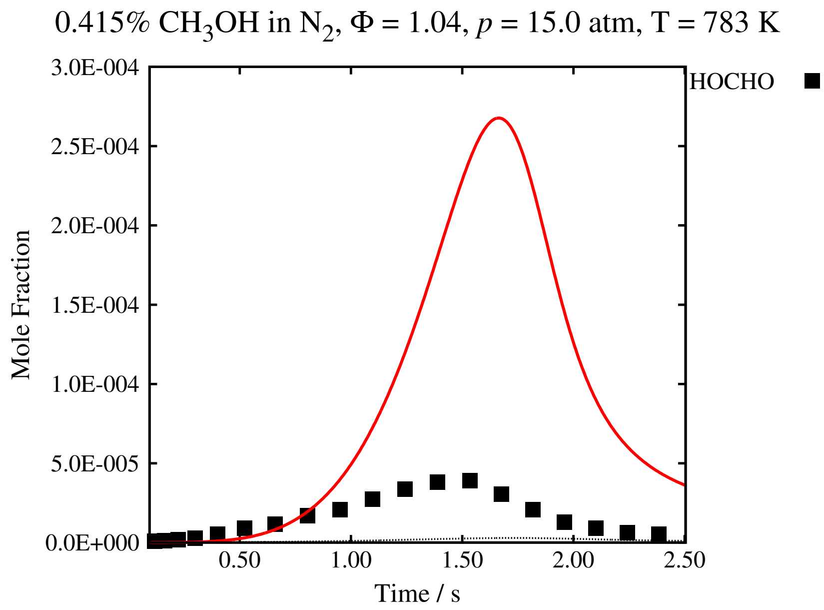


(c)

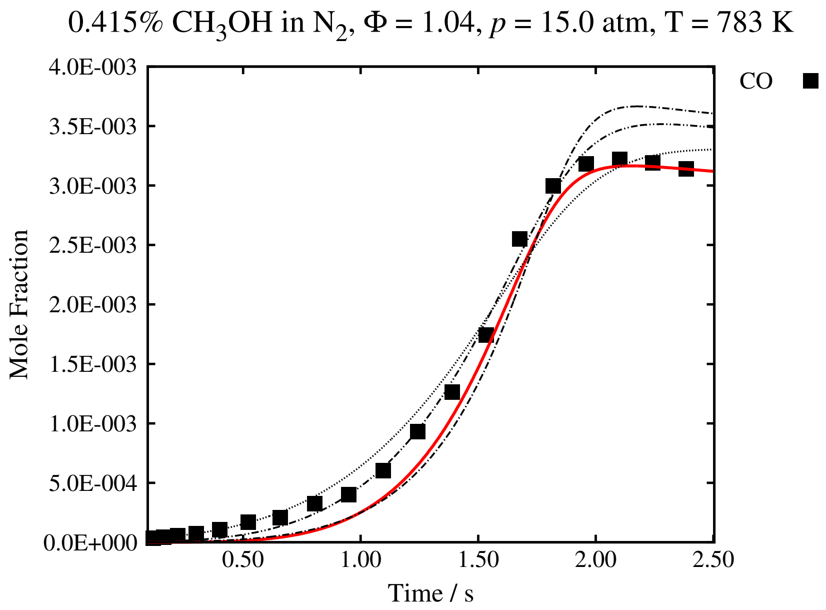
0.415% CH_3OH in N_2, Φ = 1.04, p = 15.0 atm, T = 783 K



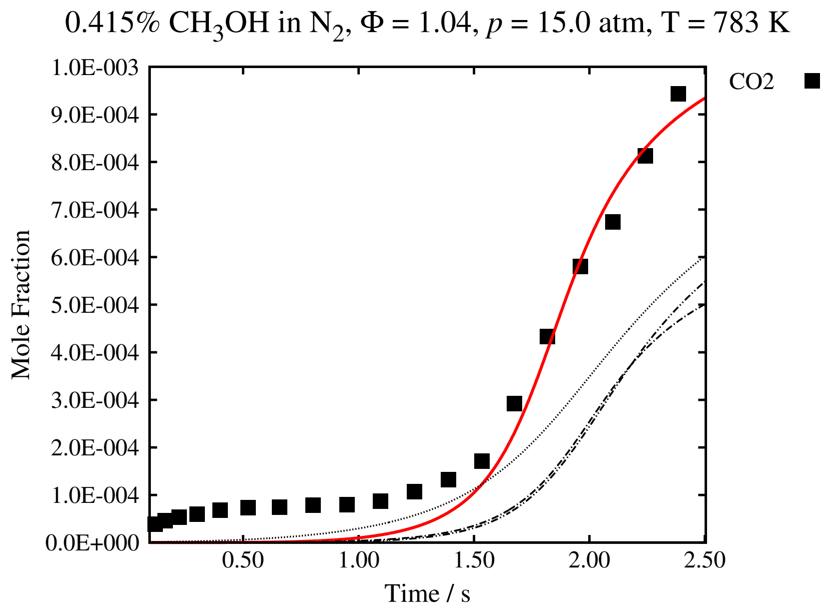
(d)


0.415% CH3OH in N2, Φ = 1.04, p = 15.0 atm, T = 783 K
HOCHO
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

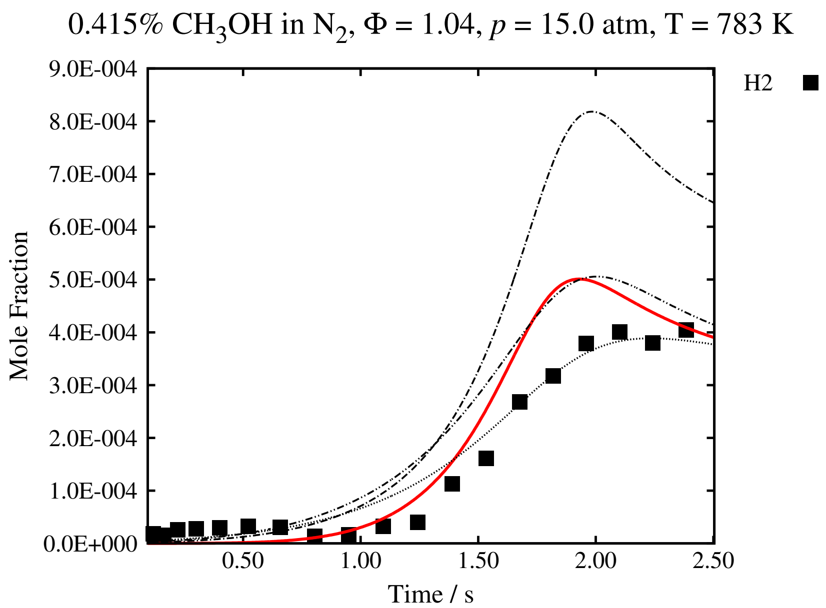
(e)


0.415% CH3OH in N2, Φ = 1.04, p = 15.0 atm, T = 783 K
CO
Mole Fraction
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

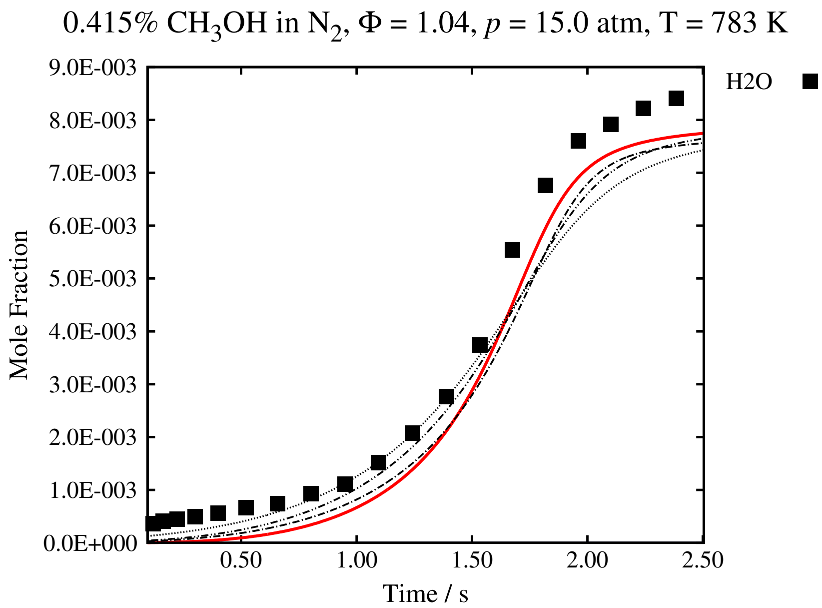
(f)


0.415% CH_3OH in N_2, Φ = 1.04, p = 15.0 atm, T = 783 K
CO2
Mole Fraction
1.0E-003
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

(g)

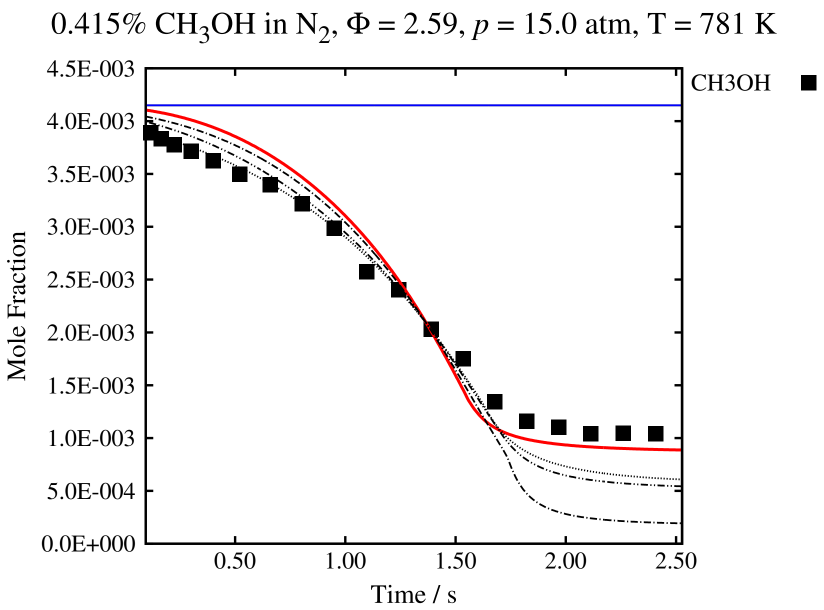

0.415% CH_3OH in N_2, Φ = 1.04, p = 15.0 atm, T = 783 K
H2
Mole Fraction
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

(h)

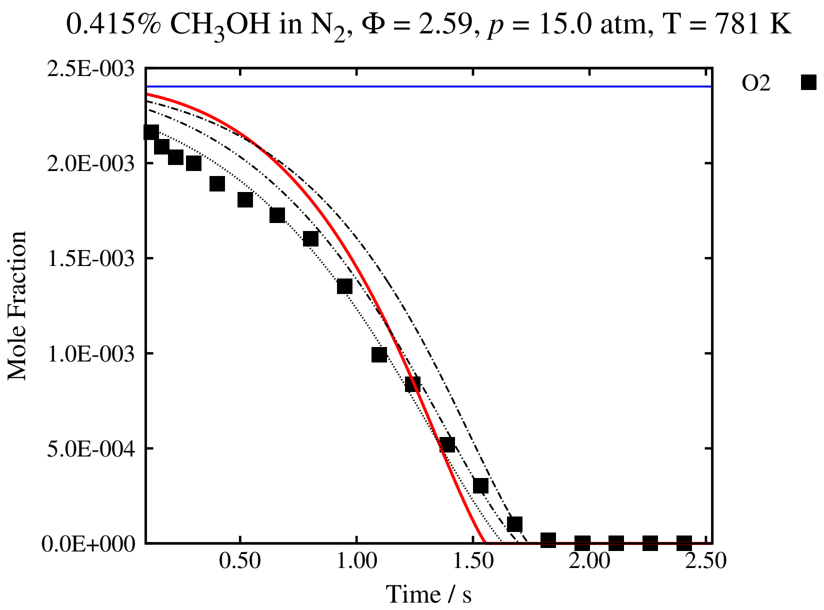


(i)

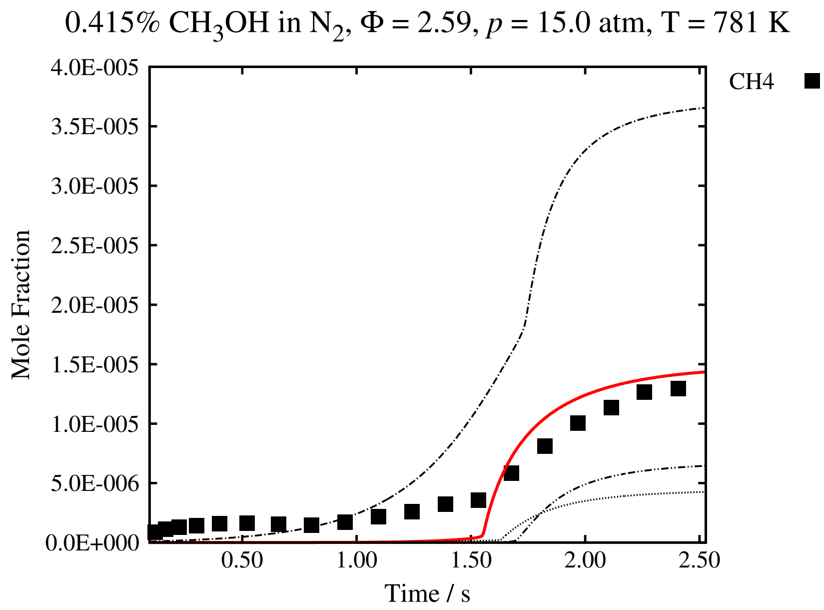
S73 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.415% CH_3OH in N_2, Φ = 2.59, *p* = 15.0 atm, T = 781 K
CH3OH
Mole Fraction
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

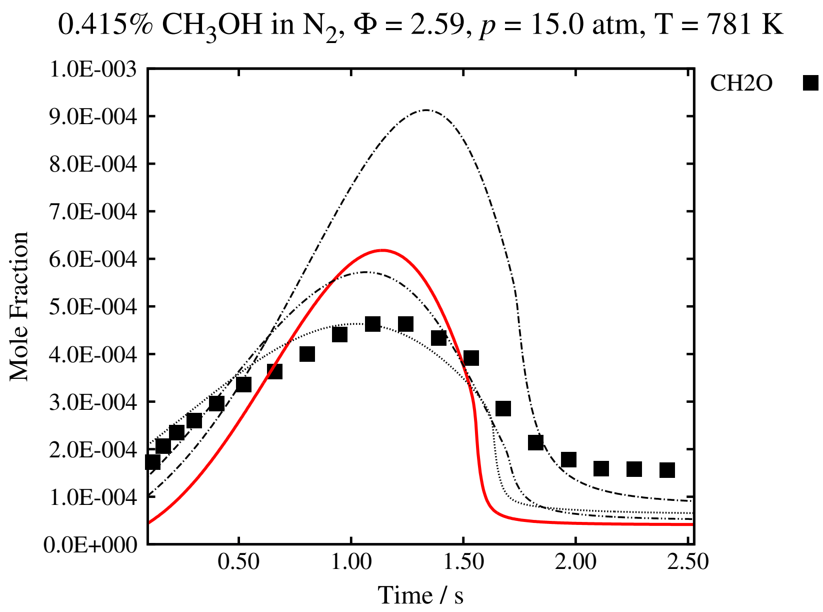
(a)


0.415% CH_3OH in N_2, Φ = 2.59, *p* = 15.0 atm, T = 781 K
O2
Mole Fraction
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

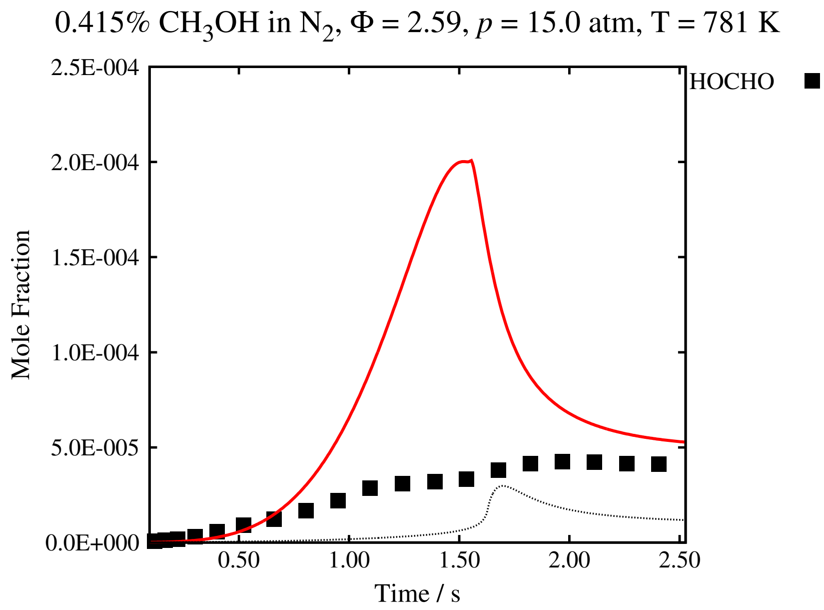
(b)


0.415% CH3OH in N2, Φ = 2.59, p = 15.0 atm, T = 781 K
CH4
Mole Fraction
Time / s
4.0E-005
3.5E-005
3.0E-005
2.5E-005
2.0E-005
1.5E-005
1.0E-005
5.0E-006
0.0E+000
0.50
1.00
1.50
2.00
2.50

(c)

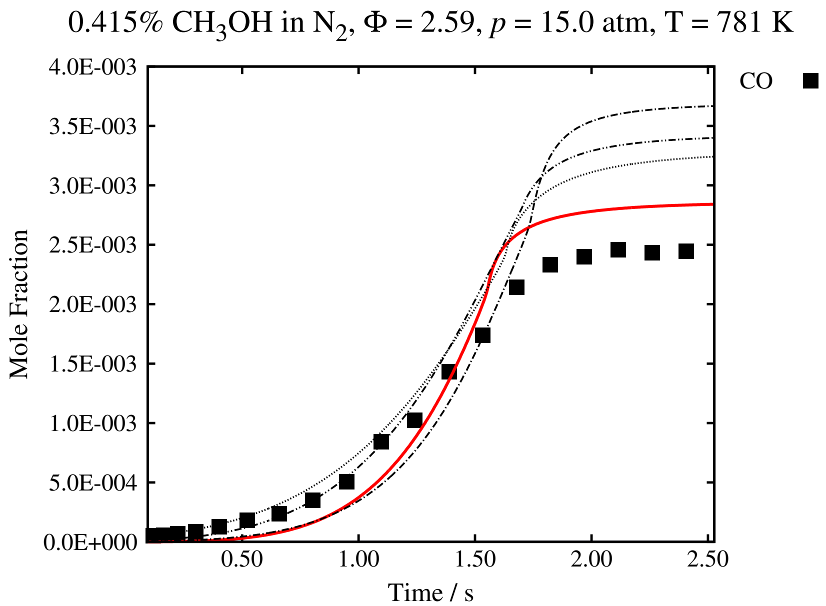

0.415% CH3OH in N2, Φ = 2.59, p = 15.0 atm, T = 781 K
CH2O
Mole Fraction
Time / s
1.0E-003
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50

(d)



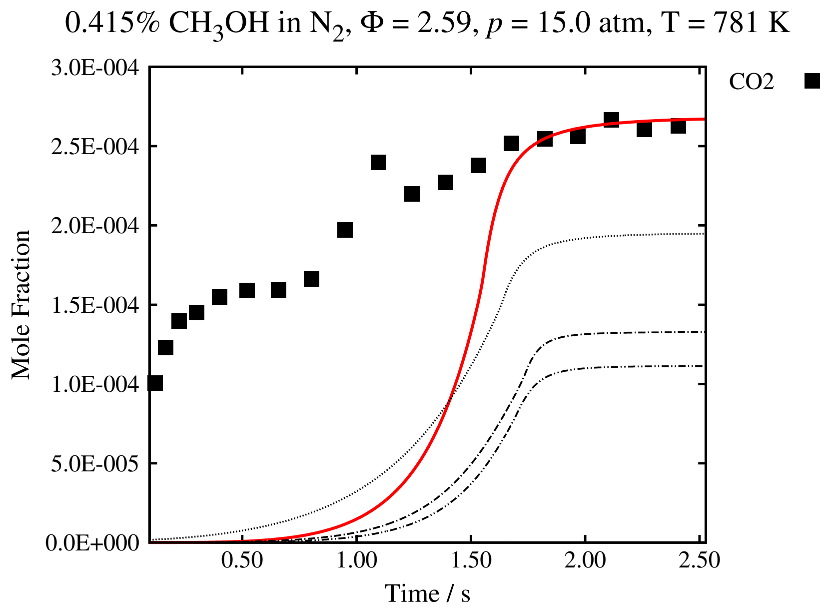
0.415% CH$_3$OH in N$_2$, Φ = 2.59, p = 15.0 atm, T = 781 K
HOCHO
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

(e)

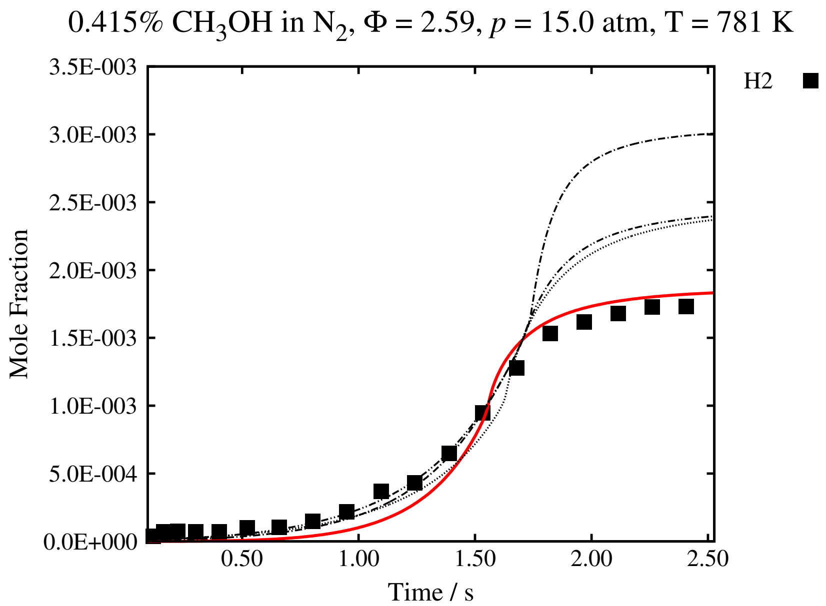


0.415% CH$_3$OH in N$_2$, Φ = 2.59, p = 15.0 atm, T = 781 K
CO
Mole Fraction
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

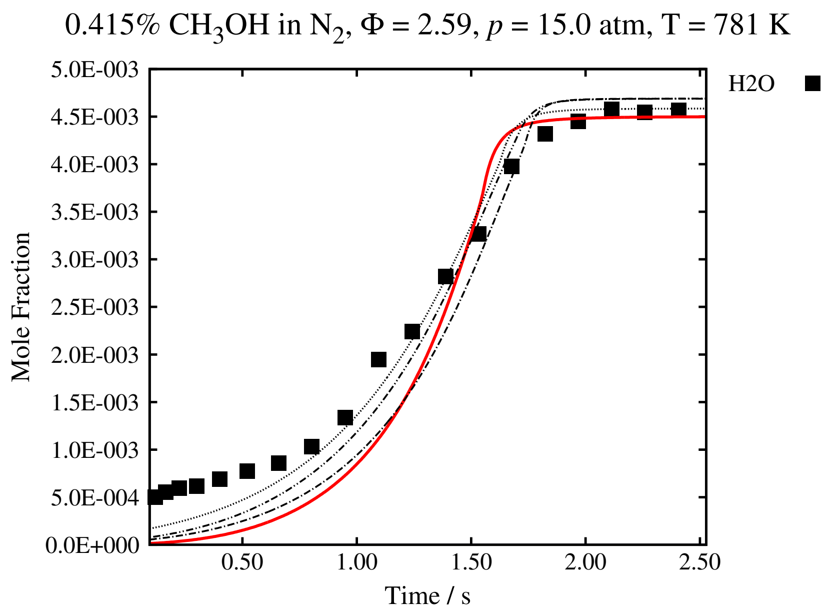
(f)


0.415% CH3OH in N2, Φ = 2.59, p = 15.0 atm, T = 781 K
CO2
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

(g)

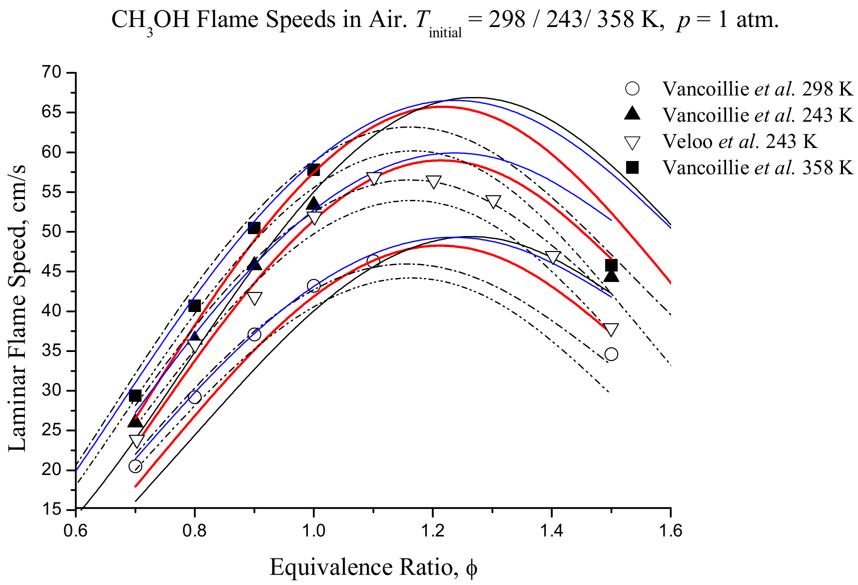

0.415% CH3OH in N2, Φ = 2.59, p = 15.0 atm, T = 781 K
H2
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.50
1.00
1.50
2.00
2.50
Time / s

(h)



(i)

S74 Flow reactor species profiles of methanol/oxygen/nitrogen mixtures. Symbols are experimental data [51] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

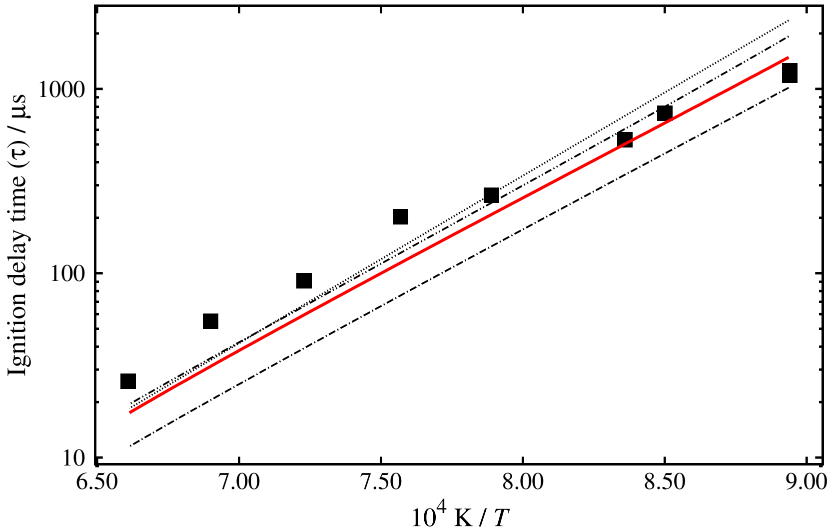


S75 Laminar flame speed measurements methanol/air mixtures. Symbols are experimental data [52, 53] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

2.8. Ethanol

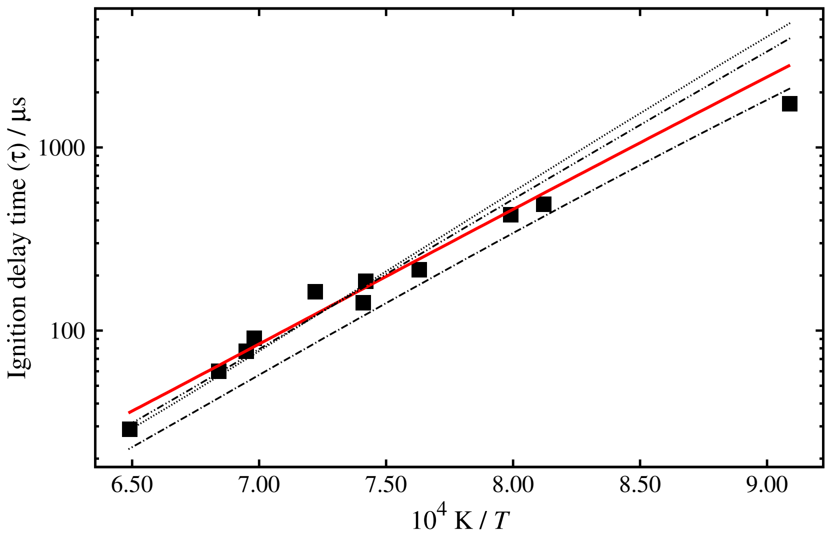
2.8.1. Shock Tube

1.00% C_2H_5OH, 6.20% O_2, 92.80% Ar, $\Phi = 0.50$, $p_{av} = 11.63$ atm

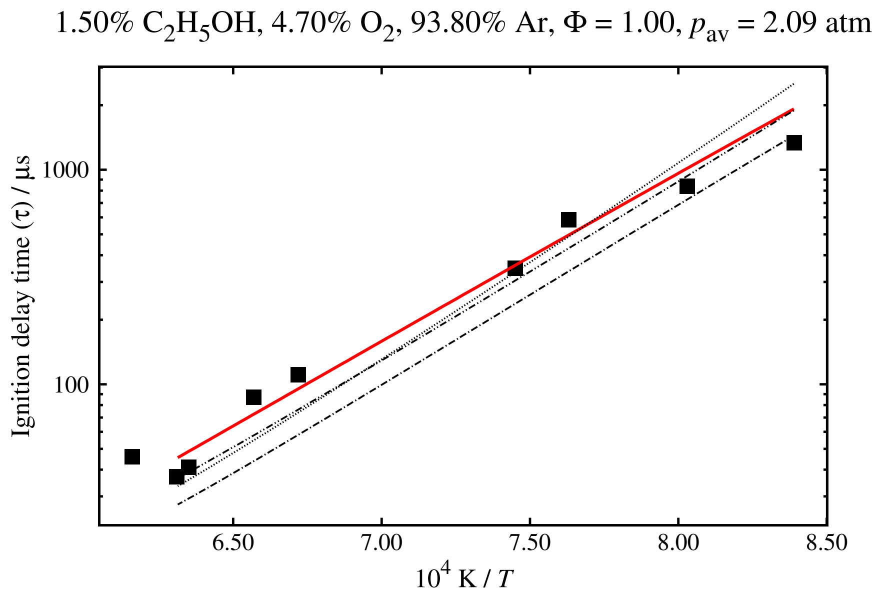


(a)

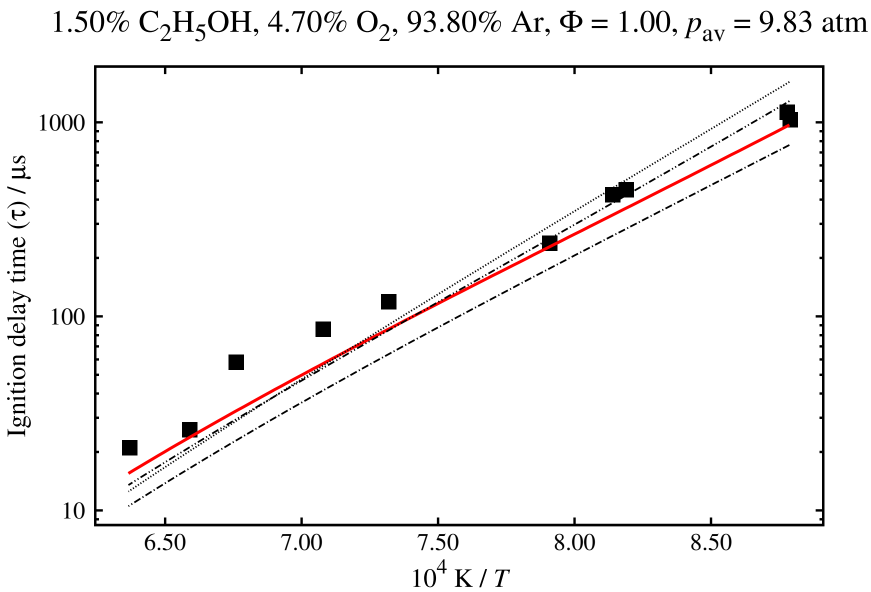
2.90% C_2H_5OH, 8.50% O_2, 88.30% Ar, $\Phi = 1.00$, $p_{av} = 2.32$ atm



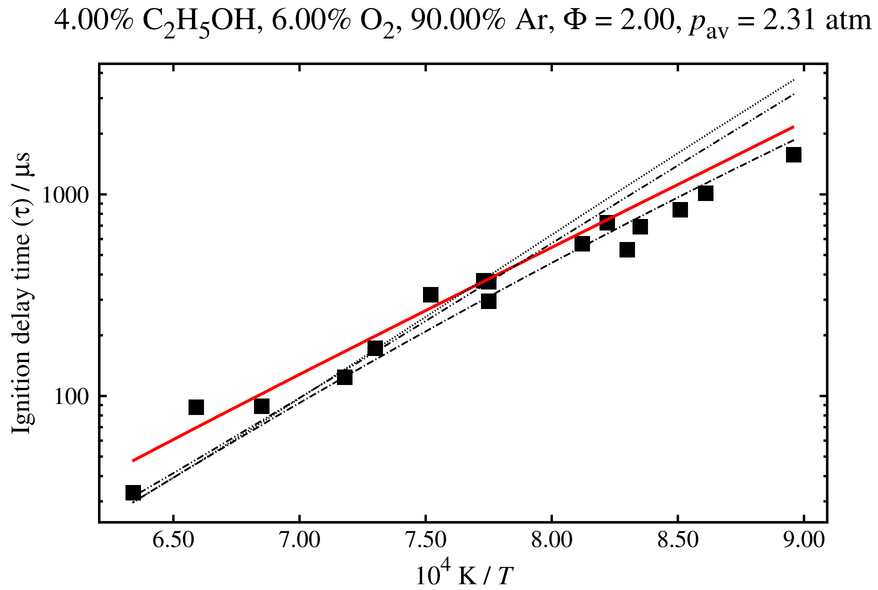
(b)


1.50% C2H5OH, 4.70% O2, 93.80% Ar, Φ = 1.00, pav = 2.09 atm
Ignition delay time (τ) / μs
1000
100
6.50
7.00
7.50
8.00
8.50
10^4 K / T

(c)

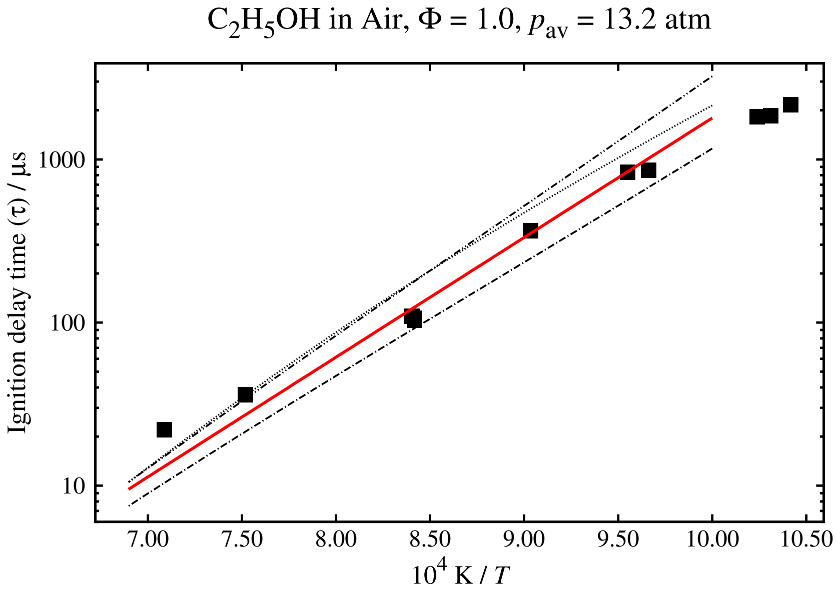

1.50% C2H5OH, 4.70% O2, 93.80% Ar, Φ = 1.00, pav = 9.83 atm
Ignition delay time (τ) / μs
1000
100
10
6.50
7.00
7.50
8.00
8.50
10^4 K / T

(d)



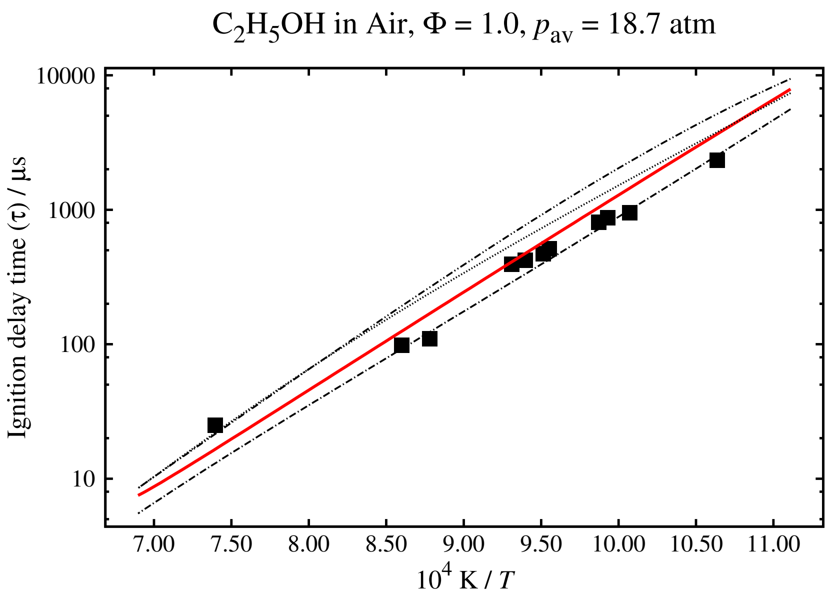
(e)

S76 Shock tube ignition delay times of ethanol/oxygen/argon mixtures. Symbols are experimental data [49] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



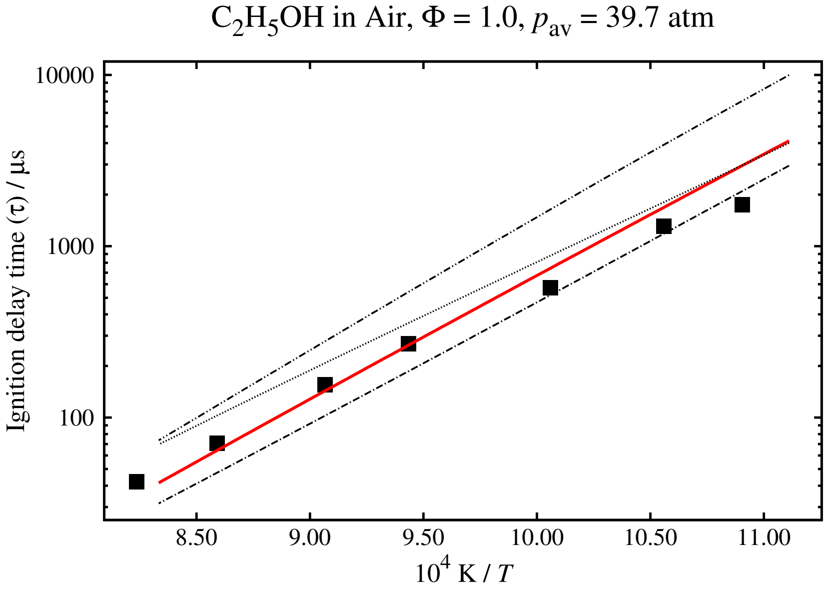
C_2H_5OH in Air, Φ = 1.0, p_{av} = 13.2 atm
Ignition delay time (τ) / µs
10
100
1000
7.00
7.50
8.00
8.50
9.00
9.50
10.00
10.50
10^4 K / T

(a)

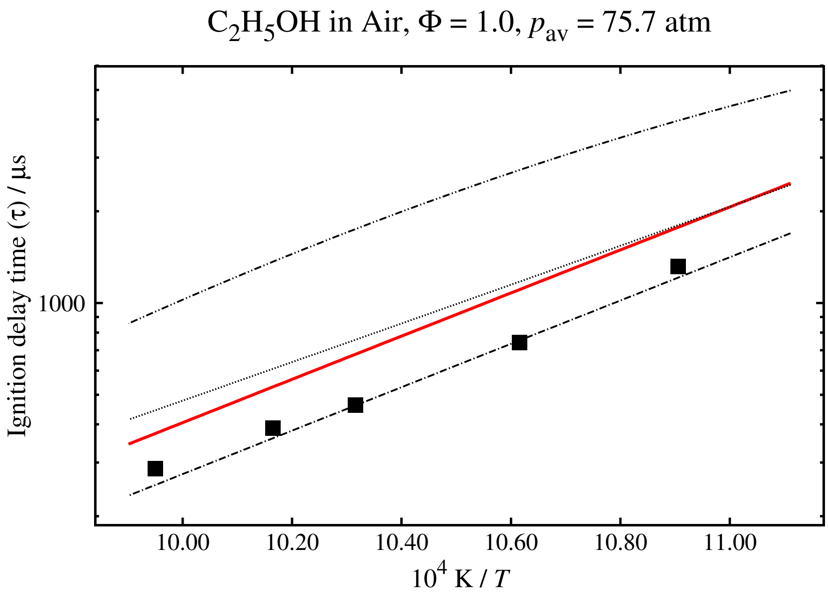


C_2H_5OH in Air, Φ = 1.0, p_{av} = 18.7 atm
Ignition delay time (τ) / µs
10
100
1000
10000
7.00
7.50
8.00
8.50
9.00
9.50
10.00
10.50
11.00
10^4 K / T

(b)

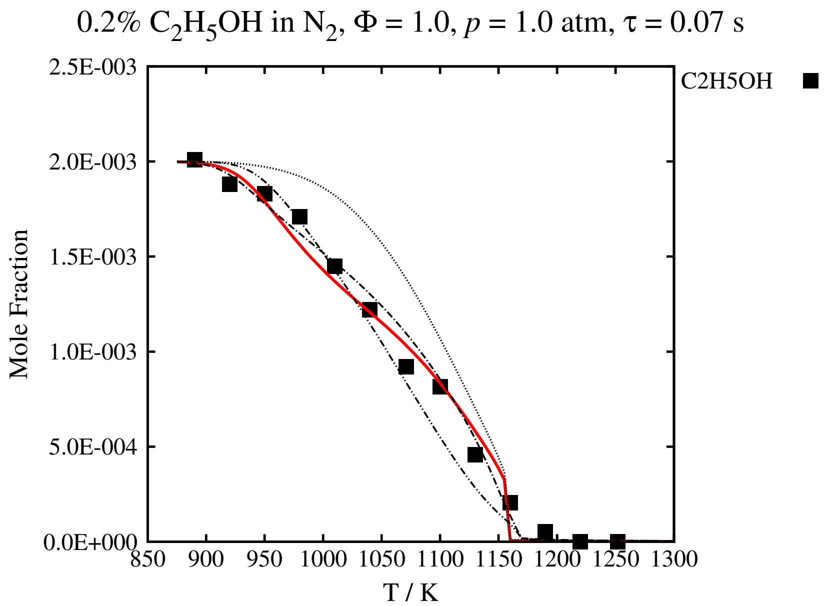


(c)

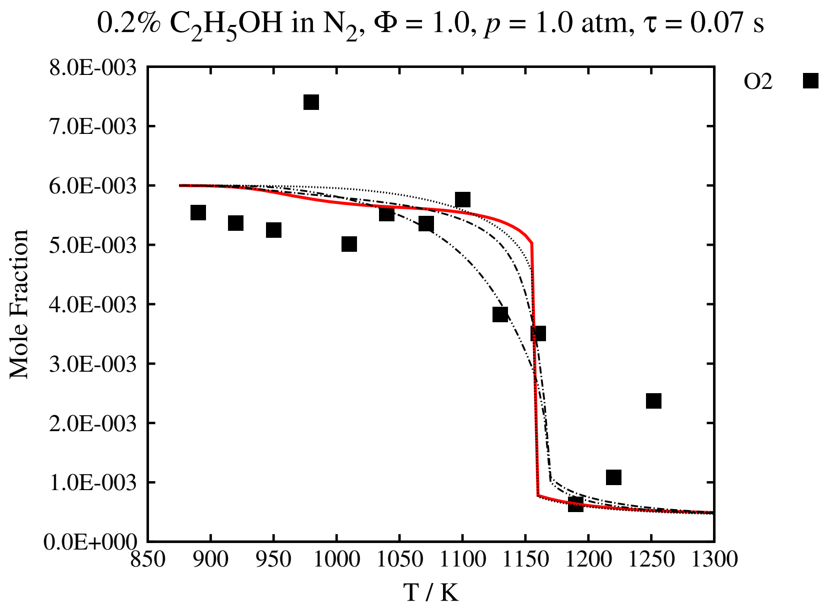


(d)

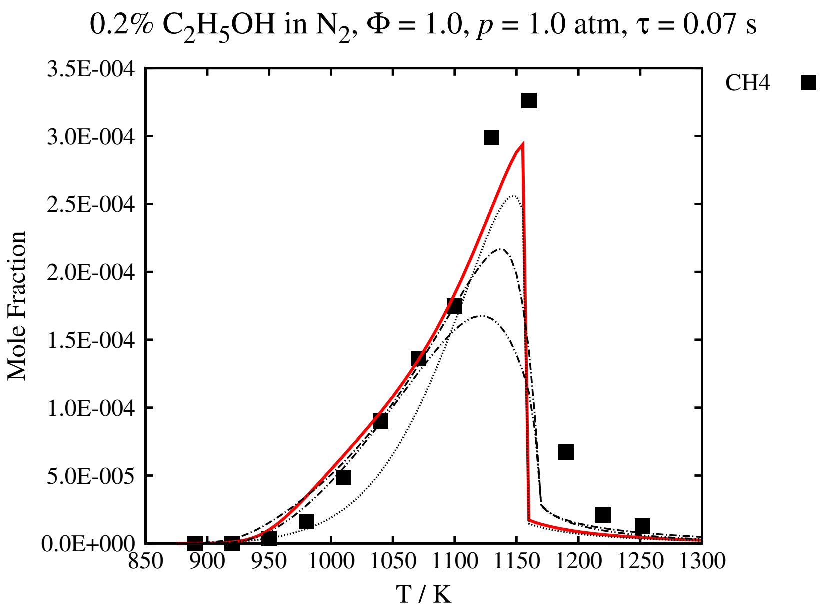
S77 Shock tube ignition delay times of ethanol/air. Symbols are experimental data [54] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, — USC II.


0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
C2H5OH
Mole Fraction
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

(a)

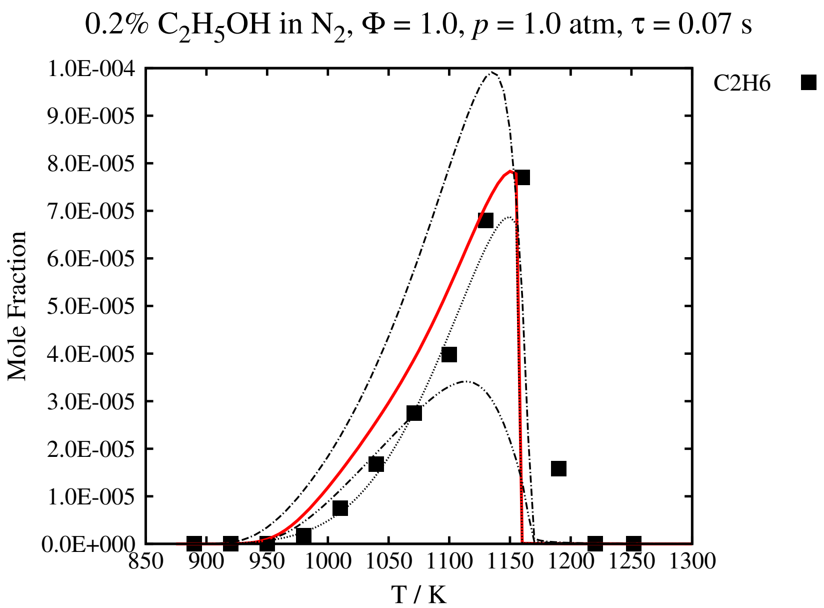

0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
O2
Mole Fraction
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

(b)



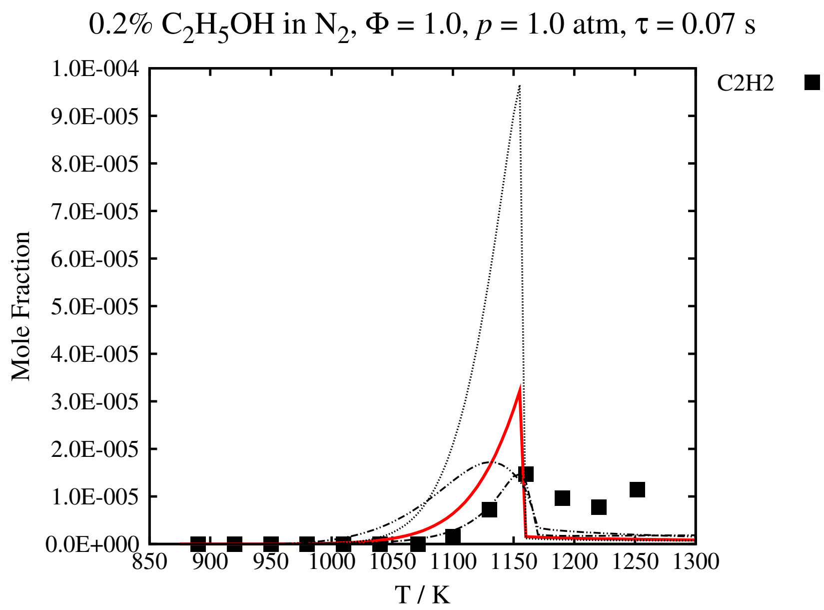
0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
CH4
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

(c)



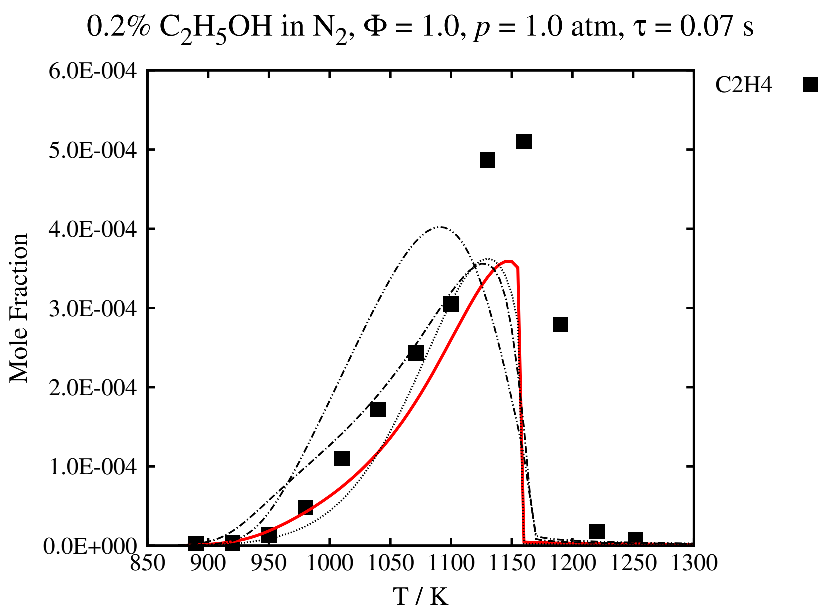
0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
C2H6
Mole Fraction
1.0E-004
9.0E-005
8.0E-005
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

(d)



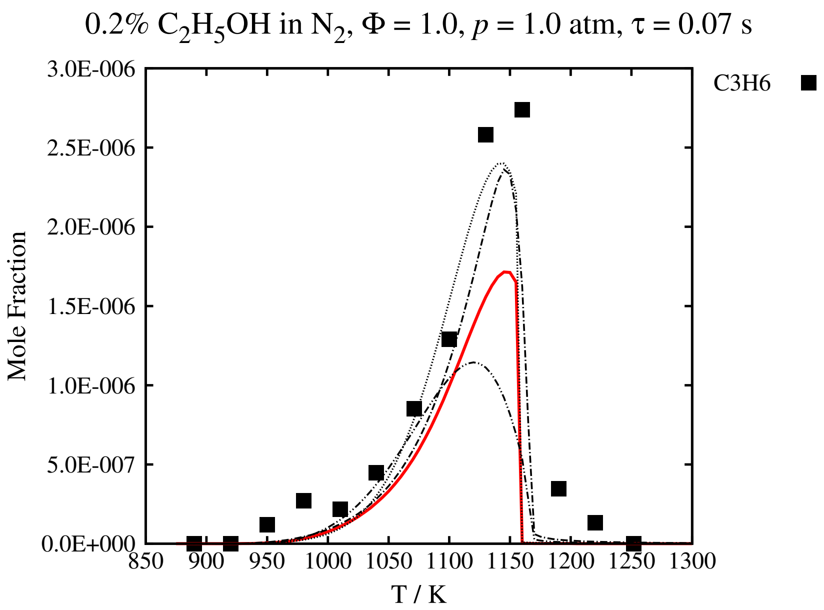
0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
C2H2
Mole Fraction
1.0E-004
9.0E-005
8.0E-005
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

(e)

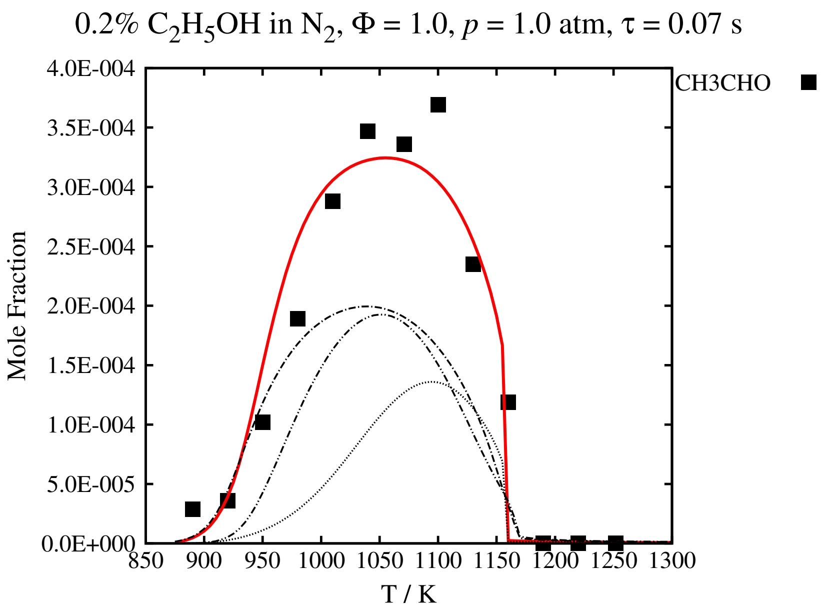


0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
C2H4
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

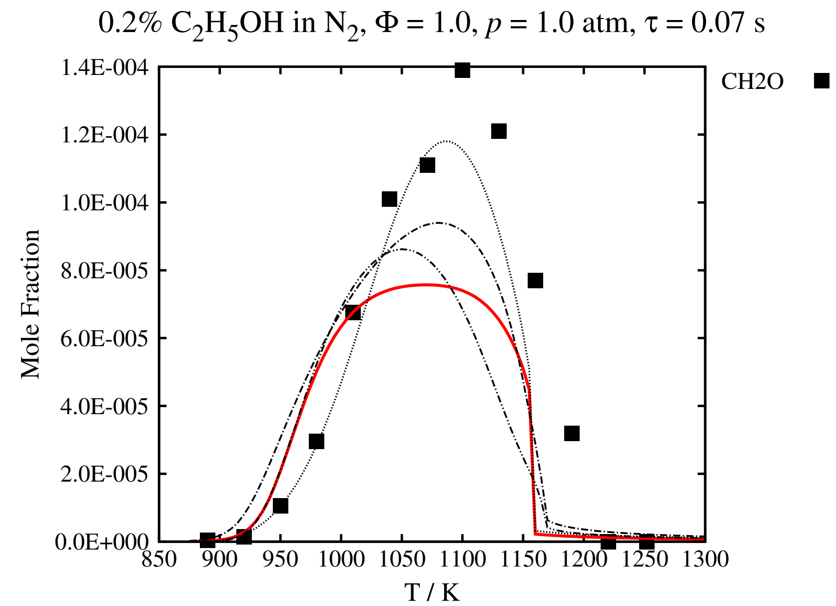
(f)


0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
C3H6
Mole Fraction
T / K
3.0E-006
2.5E-006
2.0E-006
1.5E-006
1.0E-006
5.0E-007
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
1300

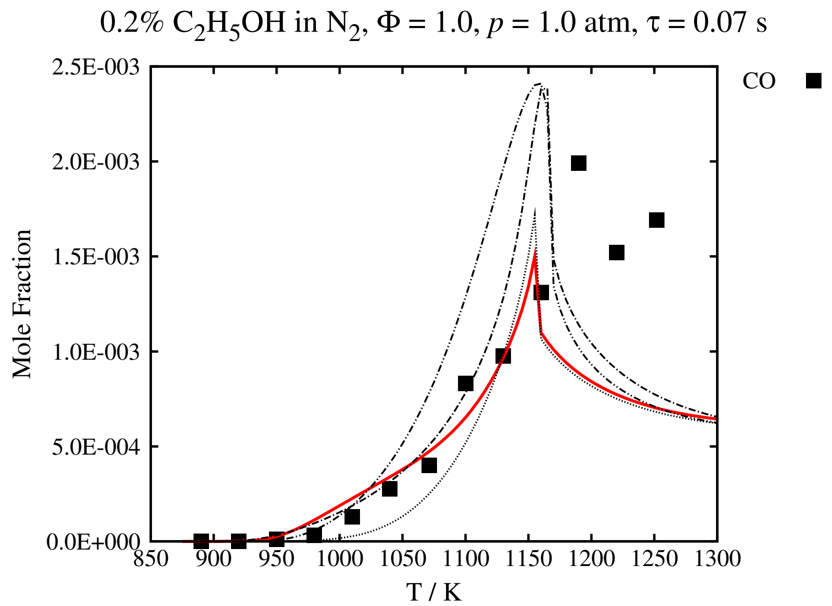
(g)


0.2% C2H5OH in N2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
CH3CHO
Mole Fraction
T / K
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
1300

(h)

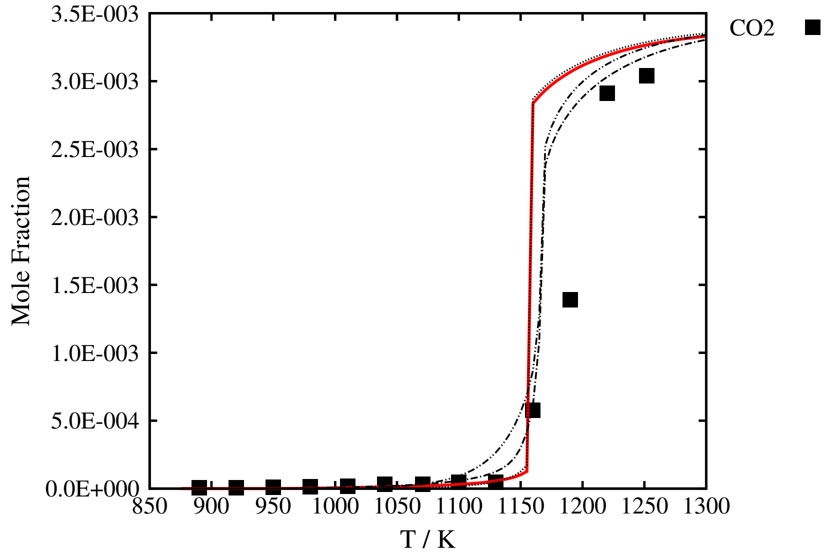

0.2% C_2H_5OH in N_2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
CH2O
Mole Fraction
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

(i)


0.2% C_2H_5OH in N_2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s
CO
Mole Fraction
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

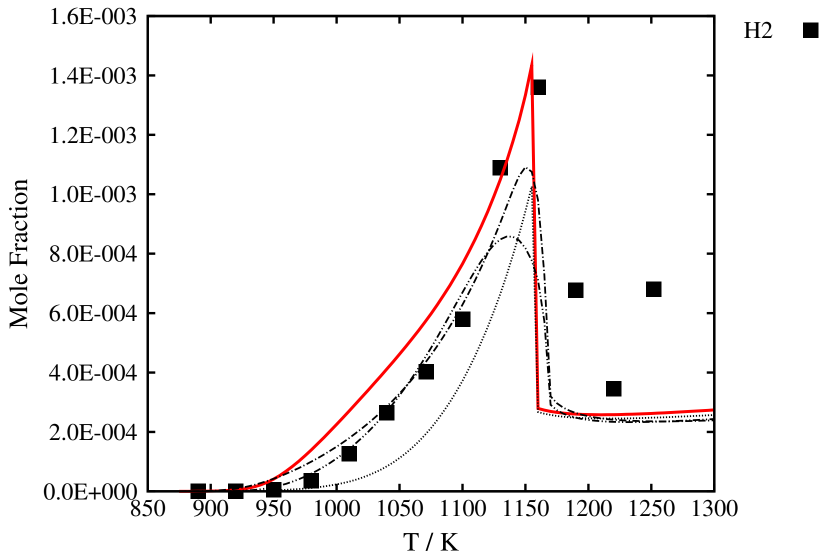
(j)

0.2% C_2H_5OH in N_2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s

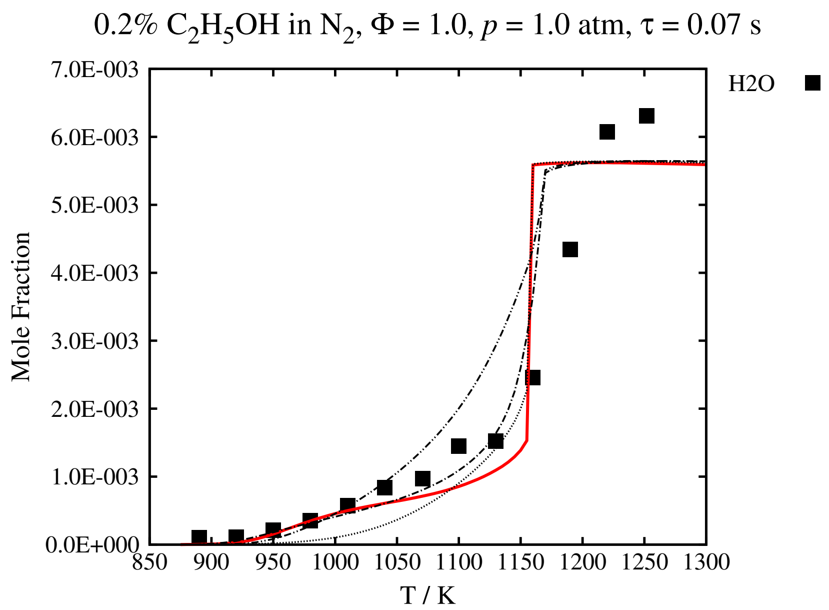


(k)

0.2% C_2H_5OH in N_2, Φ = 1.0, p = 1.0 atm, τ = 0.07 s

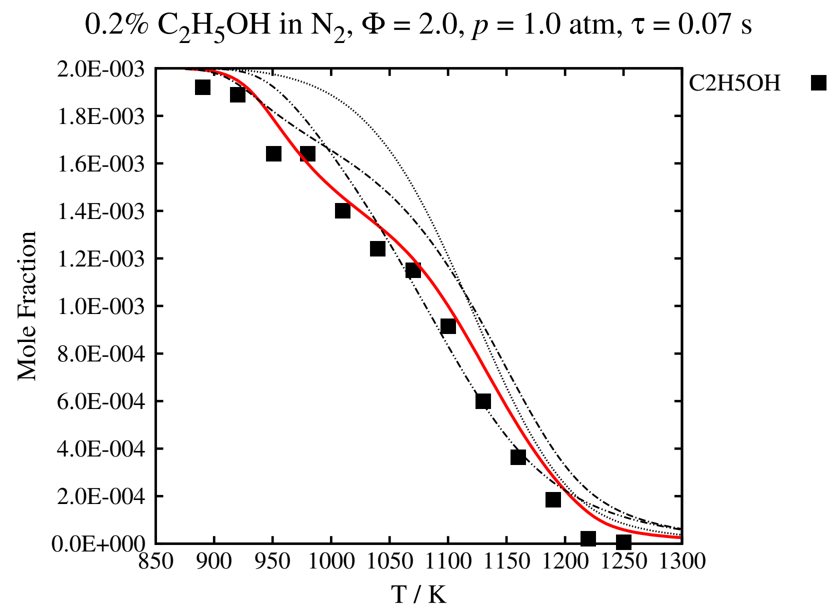


(l)

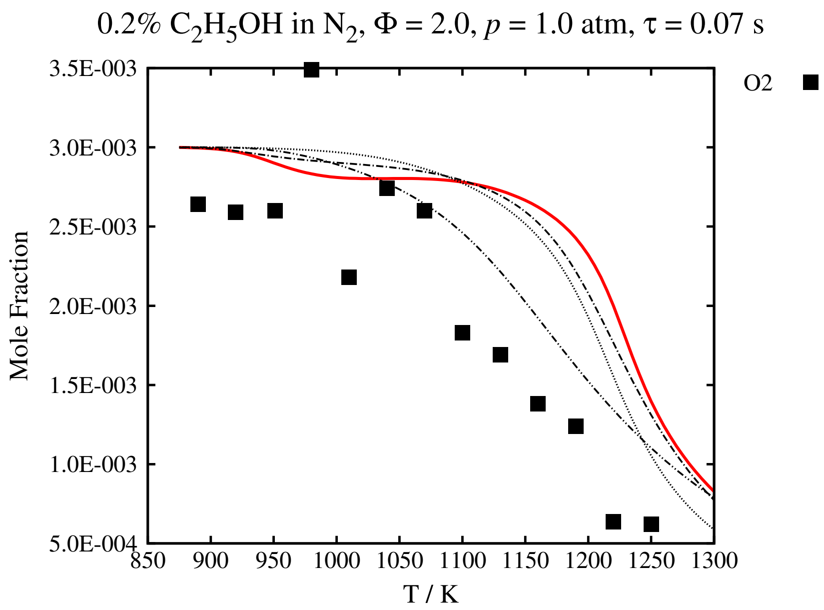


(m)

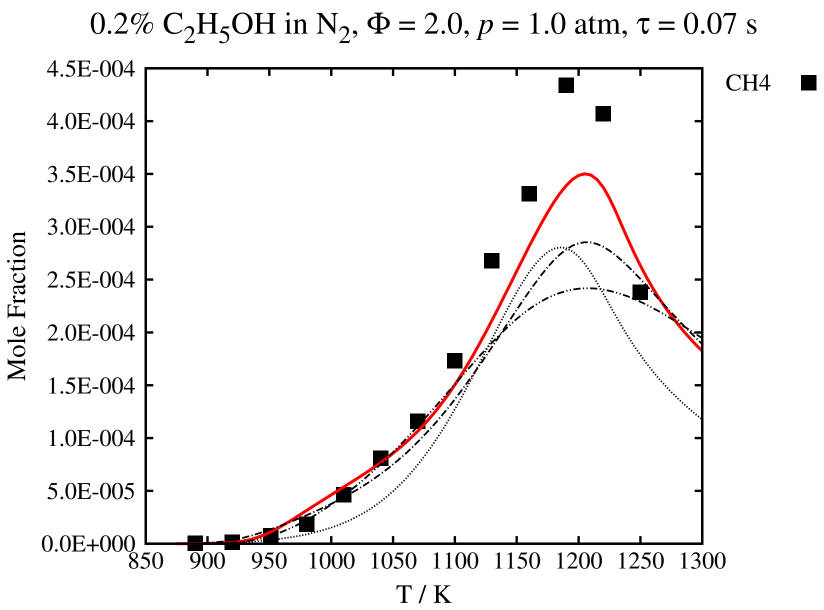
S78 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.2% C2H5OH in N2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s
C2H5OH
Mole Fraction
T / K
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
1300

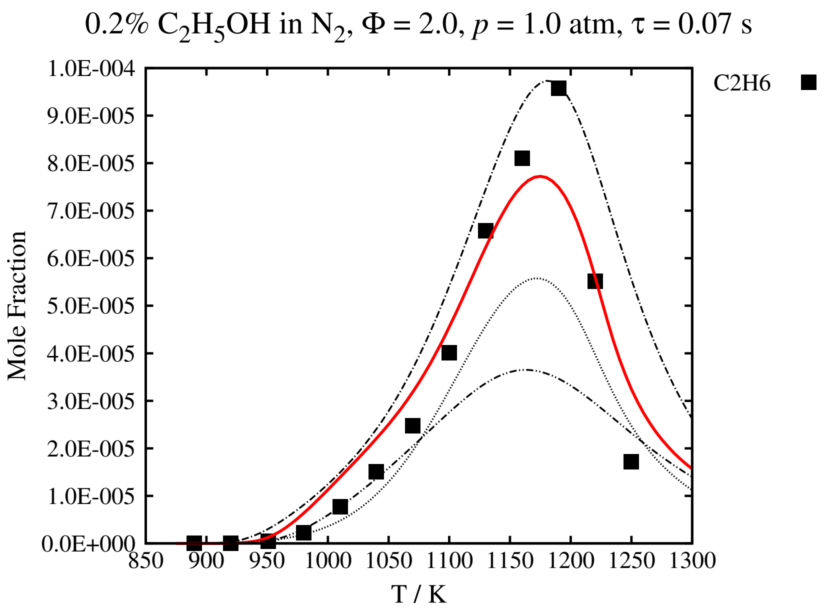
(a)


0.2% C2H5OH in N2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s
O2
Mole Fraction
T / K
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
850
900
950
1000
1050
1100
1150
1200
1250
1300

(b)

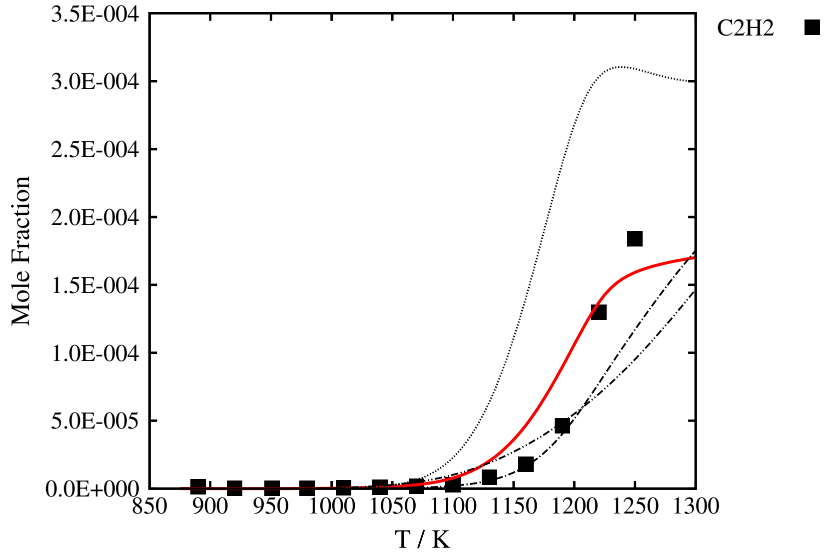

0.2% C2H5OH in N2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s
CH4
Mole Fraction
T / K
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
1300

(c)


0.2% C2H5OH in N2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s
C2H6
Mole Fraction
T / K
1.0E-004
9.0E-005
8.0E-005
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
1300

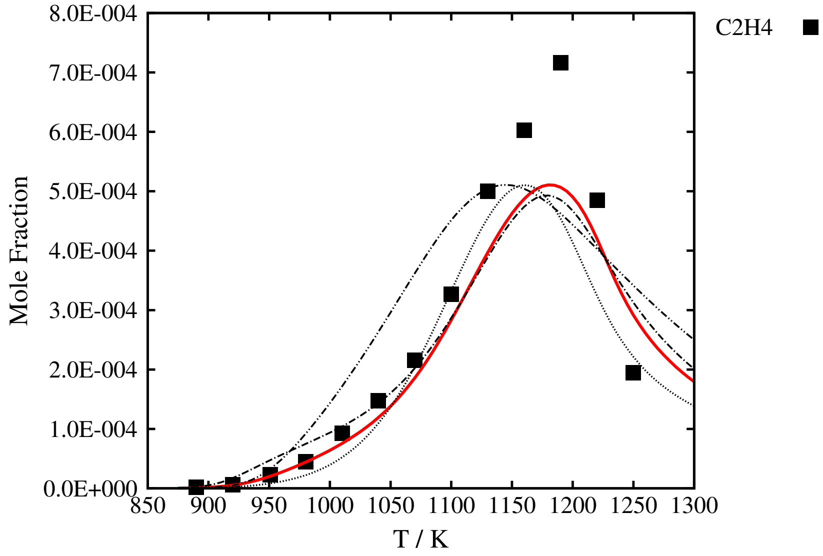
(d)

0.2% C_2H_5OH in N_2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s



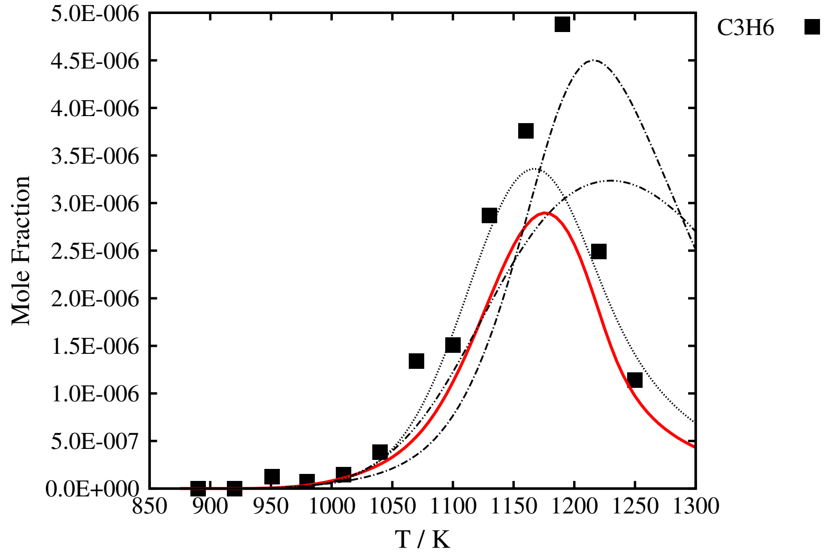
(e)

0.2% C_2H_5OH in N_2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s



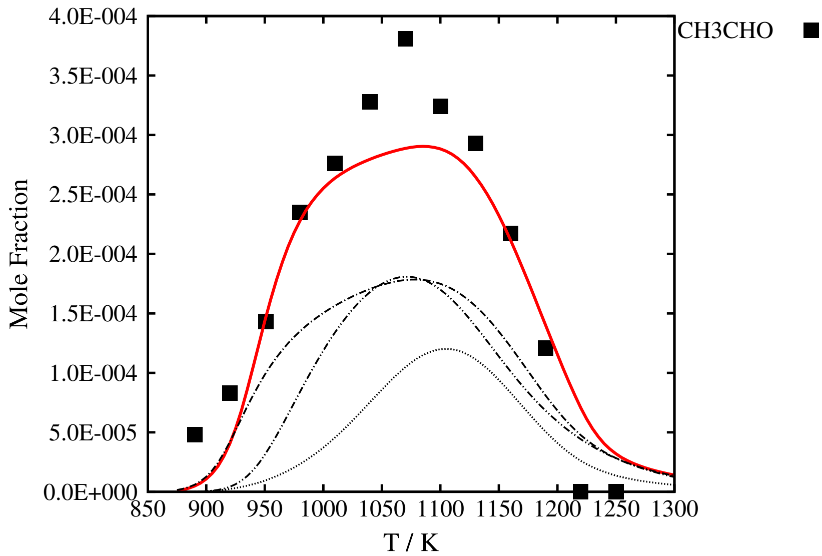
(f)

0.2% C_2H_5OH in N_2, $\Phi = 2.0$, $p = 1.0$ atm, $\tau = 0.07$ s

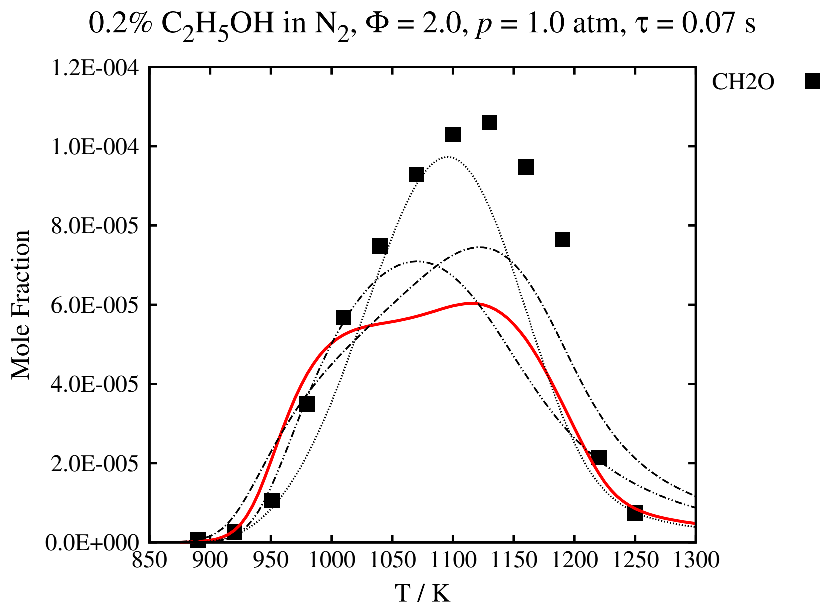


(g)

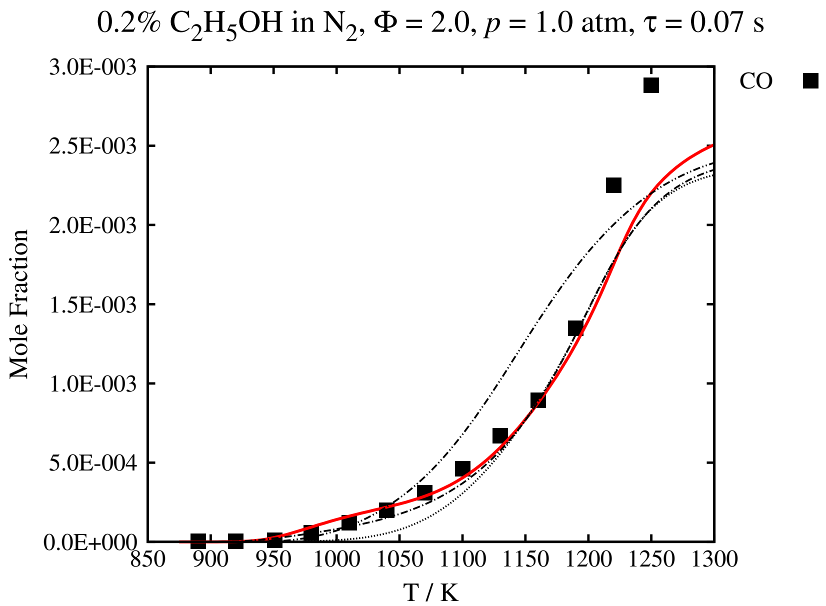
0.2% C_2H_5OH in N_2, $\Phi = 2.0$, $p = 1.0$ atm, $\tau = 0.07$ s



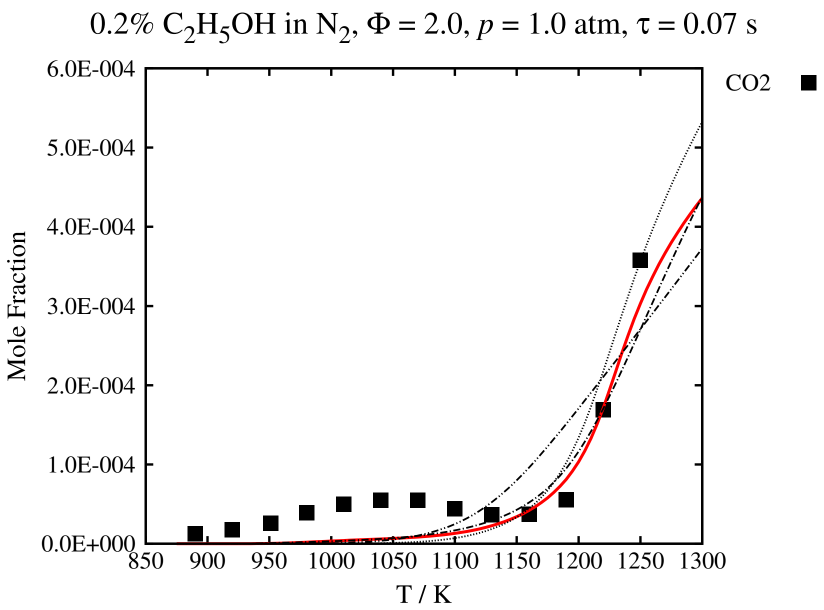
(h)


0.2% C_2H_5OH in N_2, $\Phi = 2.0$, $p = 1.0$ atm, $\tau = 0.07$ s
CH2O
Mole Fraction
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

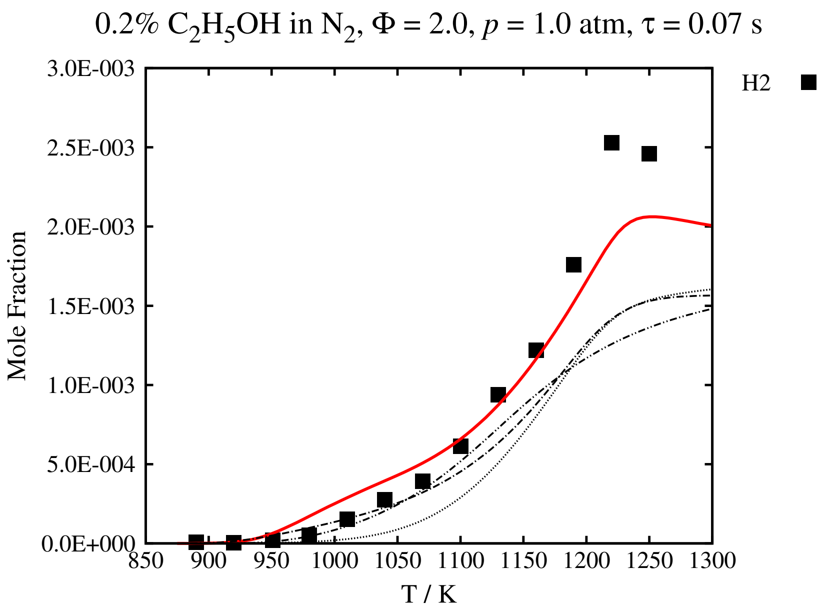
(i)


0.2% C_2H_5OH in N_2, $\Phi = 2.0$, $p = 1.0$ atm, $\tau = 0.07$ s
CO
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250 1300
T / K

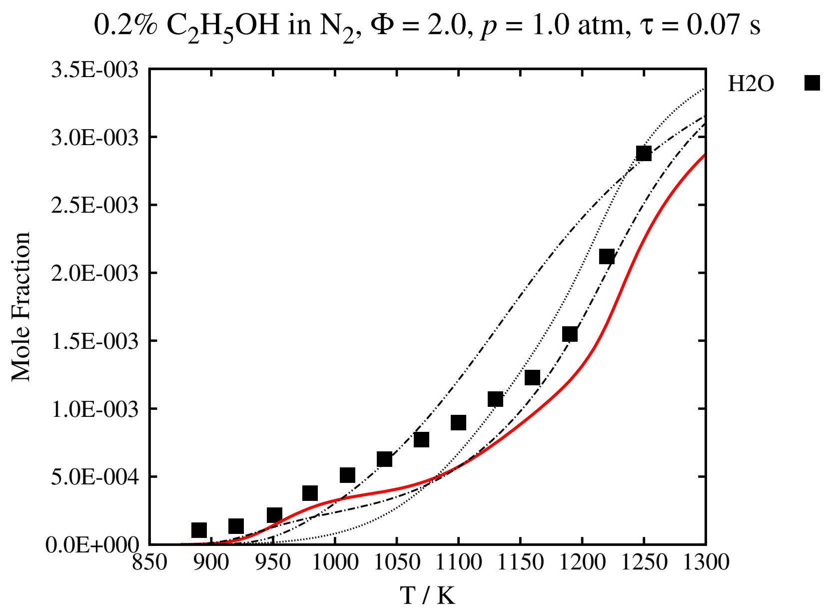
(j)


0.2% C_2H_5OH in N_2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s
CO2
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
1300
T / K

(k)

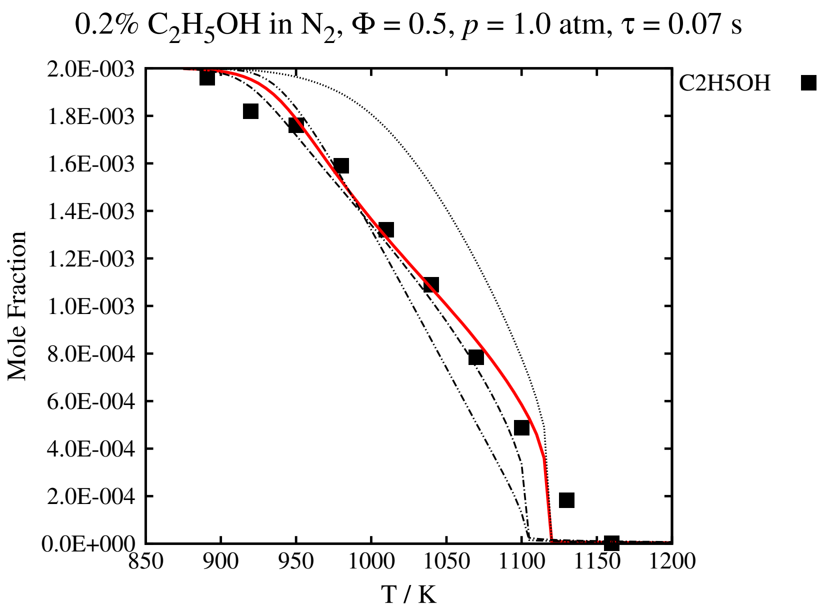

0.2% C_2H_5OH in N_2, Φ = 2.0, p = 1.0 atm, τ = 0.07 s
H2
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
1300
T / K

(l)

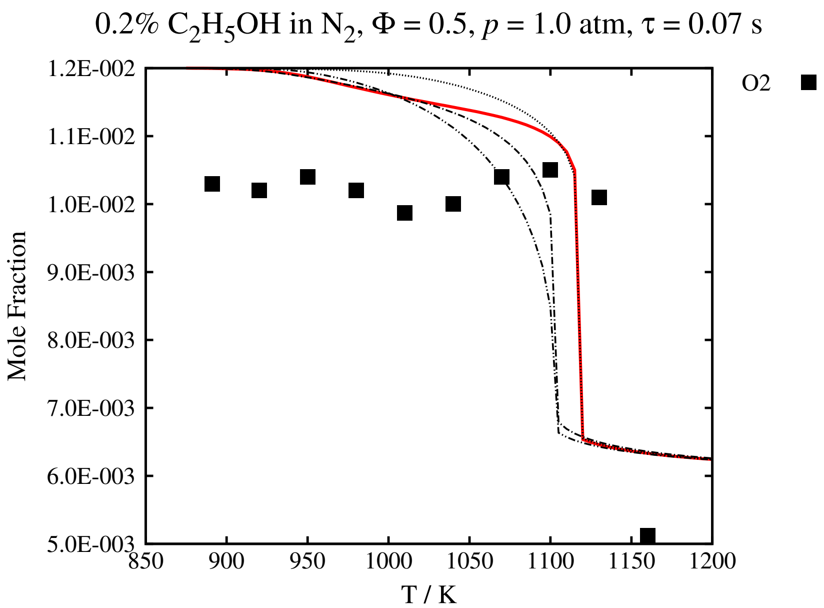


(m)

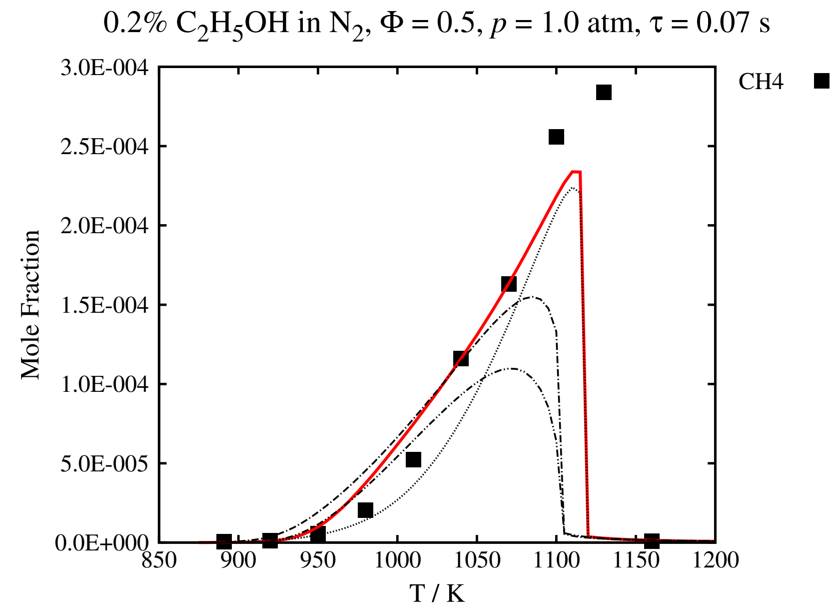
S79 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.2% C_2H_5OH in N_2, Φ = 0.5, p = 1.0 atm, τ = 0.07 s
C2H5OH
Mole Fraction
T / K
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200

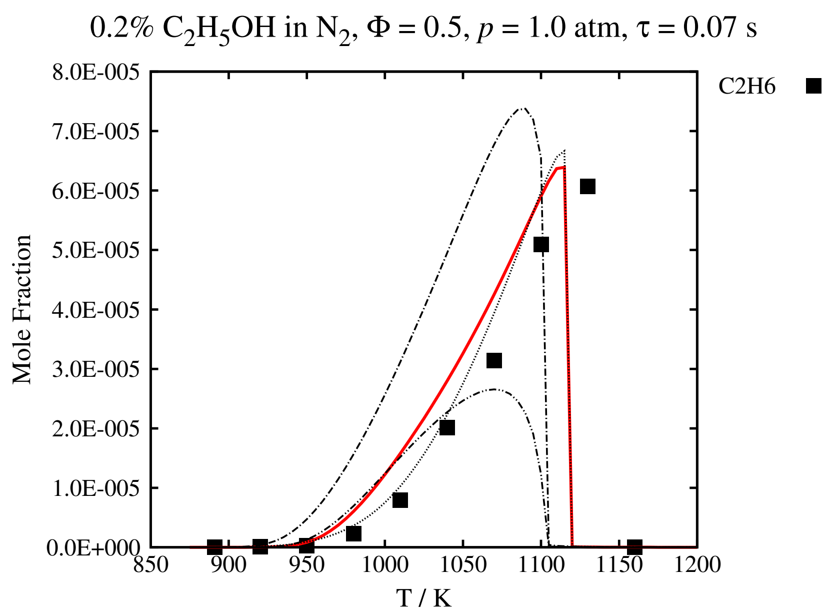
(a)


0.2% C_2H_5OH in N_2, Φ = 0.5, p = 1.0 atm, τ = 0.07 s
O2
Mole Fraction
T / K
1.2E-002
1.1E-002
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
850
900
950
1000
1050
1100
1150
1200

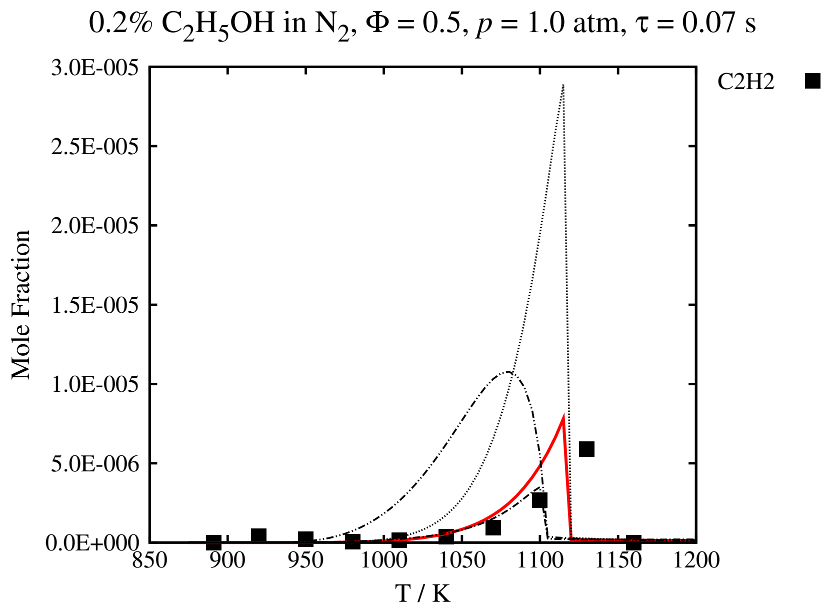
(b)


0.2% C2H5OH in N2, Φ = 0.5, p = 1.0 atm, τ = 0.07 s
CH4
Mole Fraction
T / K
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200

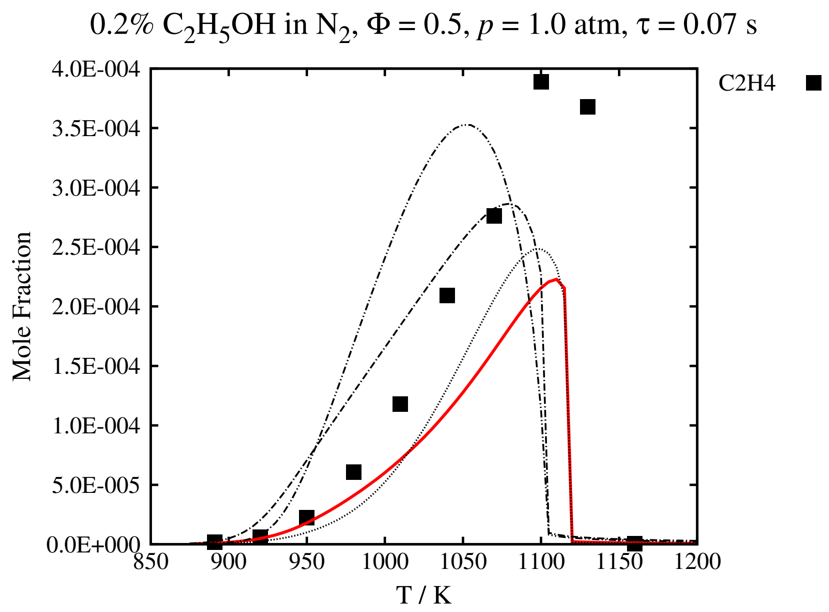
(c)


0.2% C2H5OH in N2, Φ = 0.5, p = 1.0 atm, τ = 0.07 s
C2H6
Mole Fraction
T / K
8.0E-005
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200

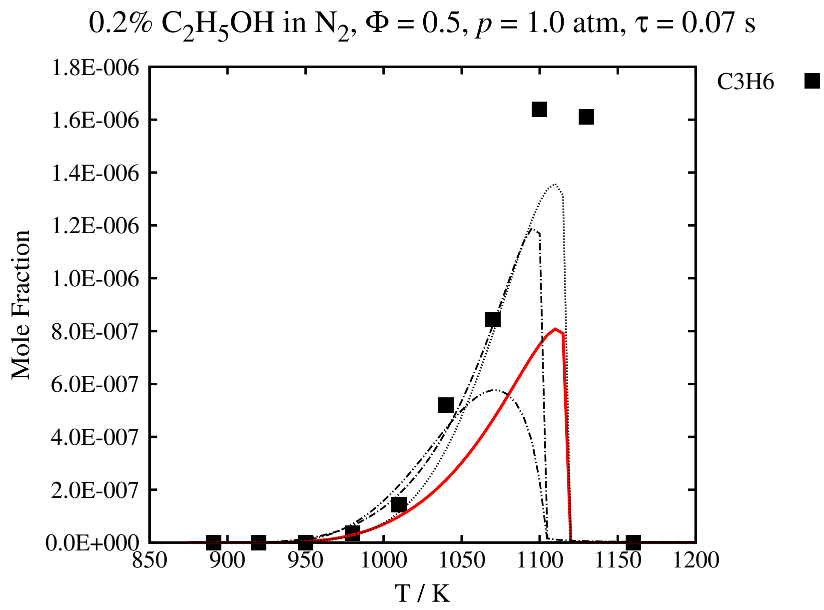
(d)


0.2% C_2H_5OH in N_2, $\Phi = 0.5$, $p = 1.0$ atm, $\tau = 0.07$ s
C2H2
Mole Fraction
3.0E-005
2.5E-005
2.0E-005
1.5E-005
1.0E-005
5.0E-006
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

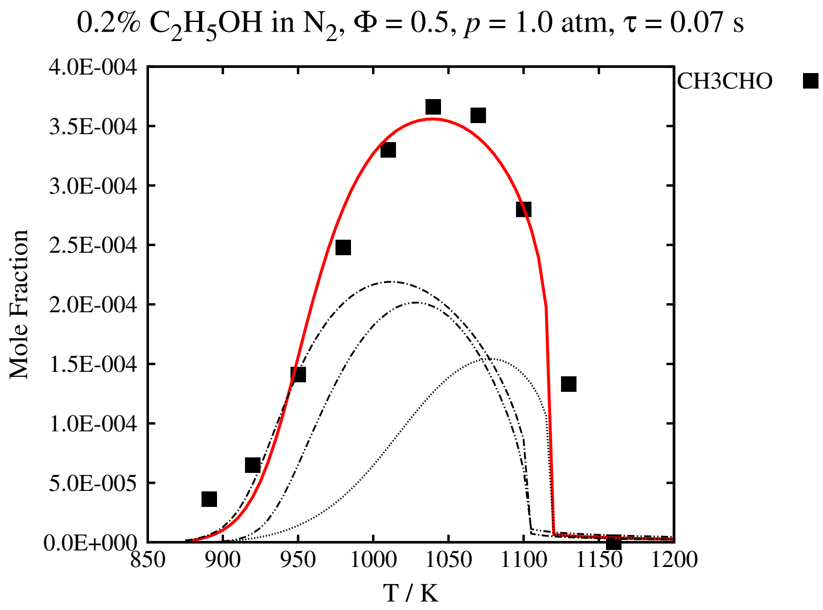
(e)


0.2% C_2H_5OH in N_2, $\Phi = 0.5$, $p = 1.0$ atm, $\tau = 0.07$ s
C2H4
Mole Fraction
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

(f)

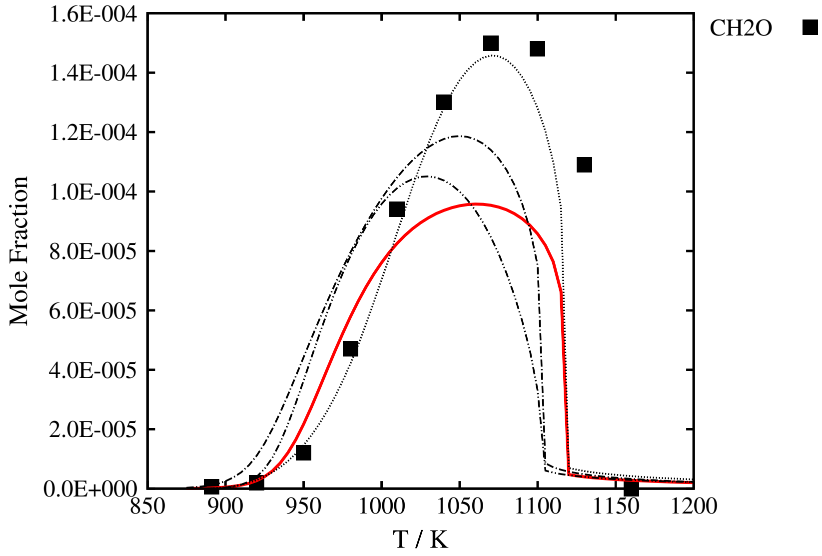

0.2% C2H5OH in N2, Φ = 0.5, p = 1.0 atm, τ = 0.07 s
C3H6
Mole Fraction
T / K
1.8E-006
1.6E-006
1.4E-006
1.2E-006
1.0E-006
8.0E-007
6.0E-007
4.0E-007
2.0E-007
0.0E+000
850
900
950
1000
1050
1100
1150
1200

(g)


0.2% C2H5OH in N2, Φ = 0.5, p = 1.0 atm, τ = 0.07 s
CH3CHO
Mole Fraction
T / K
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200

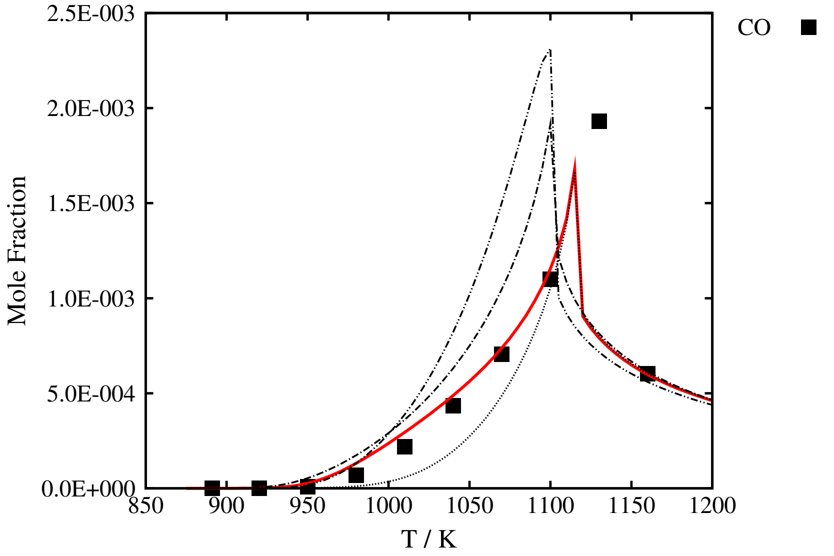
(h)

0.2% C_2H_5OH in N_2, $\Phi = 0.5$, $p = 1.0$ atm, $\tau = 0.07$ s



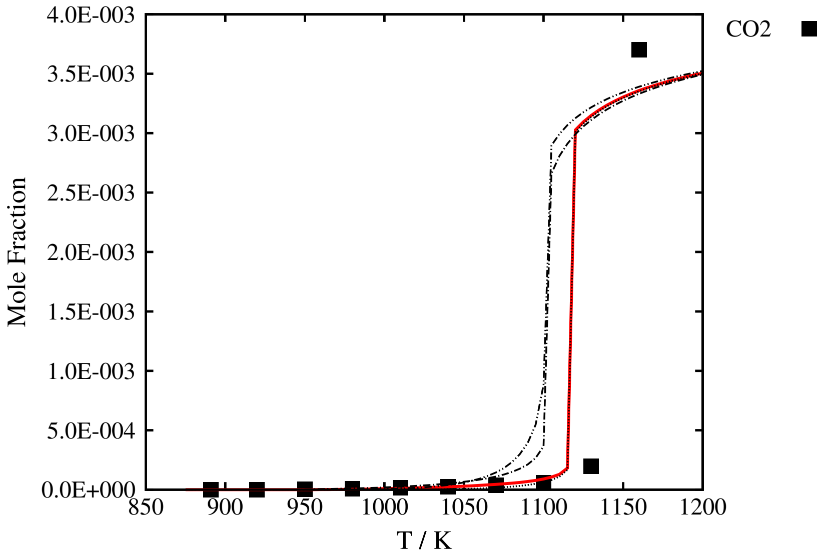
(i)

0.2% C_2H_5OH in N_2, $\Phi = 0.5$, $p = 1.0$ atm, $\tau = 0.07$ s



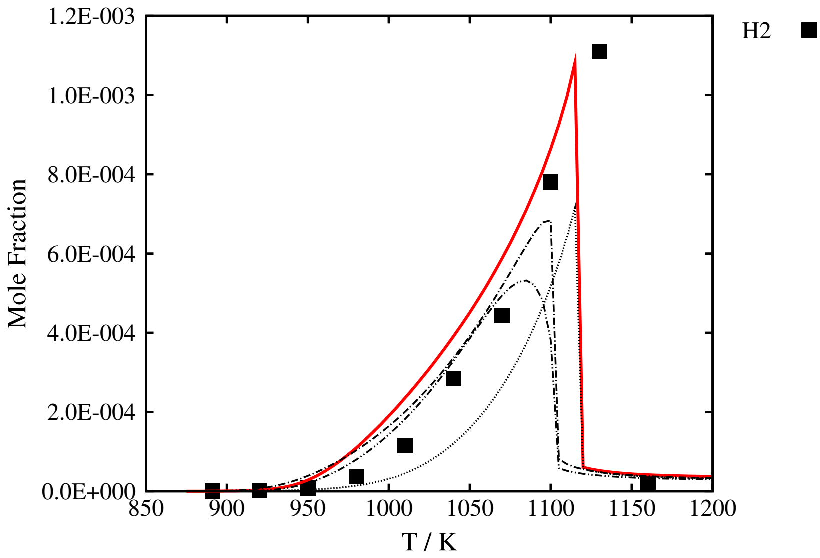
(j)

0.2% C_2H_5OH in N_2, $\Phi = 0.5$, $p = 1.0$ atm, $\tau = 0.07$ s

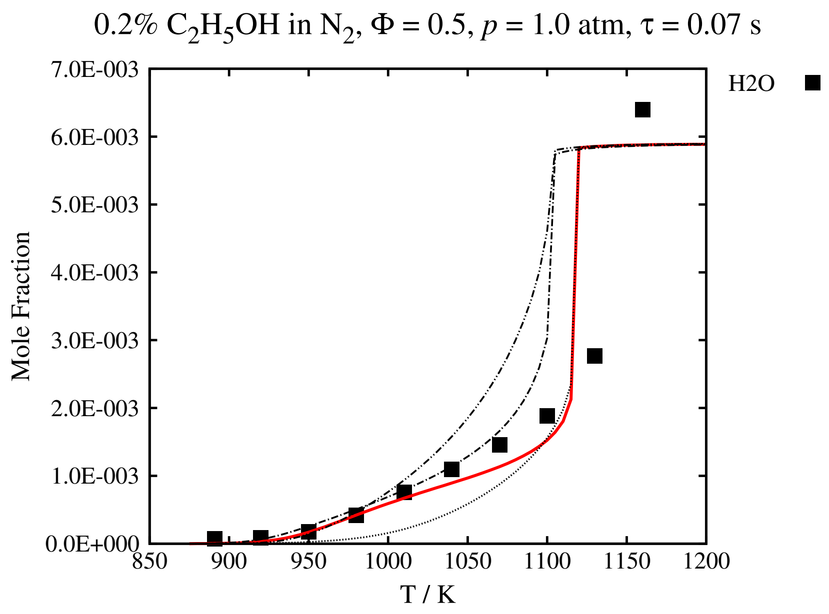


(k)

0.2% C_2H_5OH in N_2, $\Phi = 0.5$, $p = 1.0$ atm, $\tau = 0.07$ s



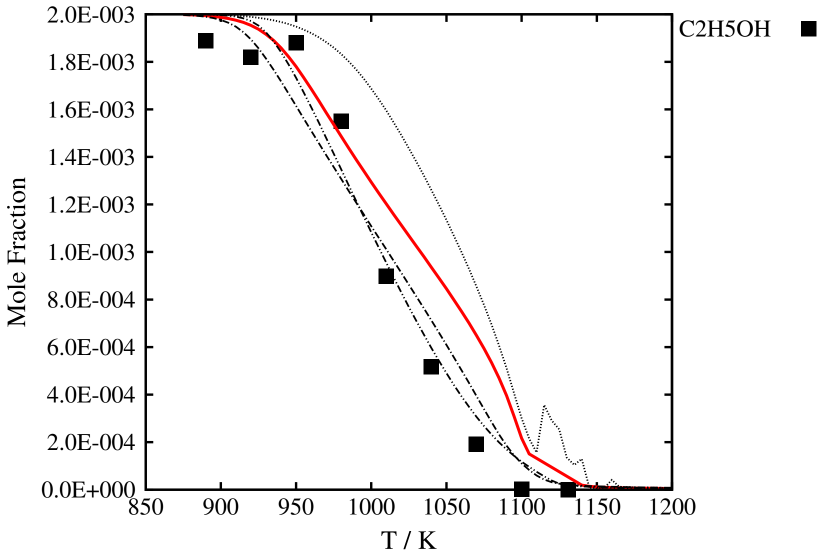
(l)



(m)

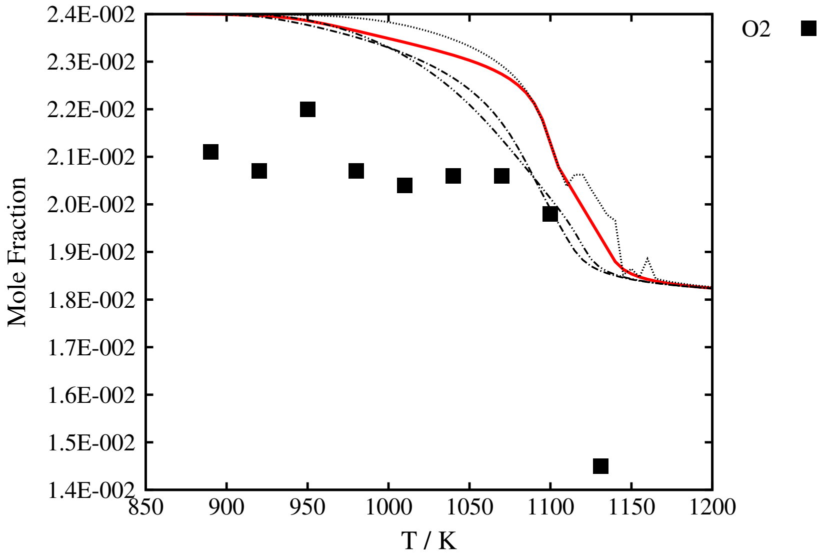
S80 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s

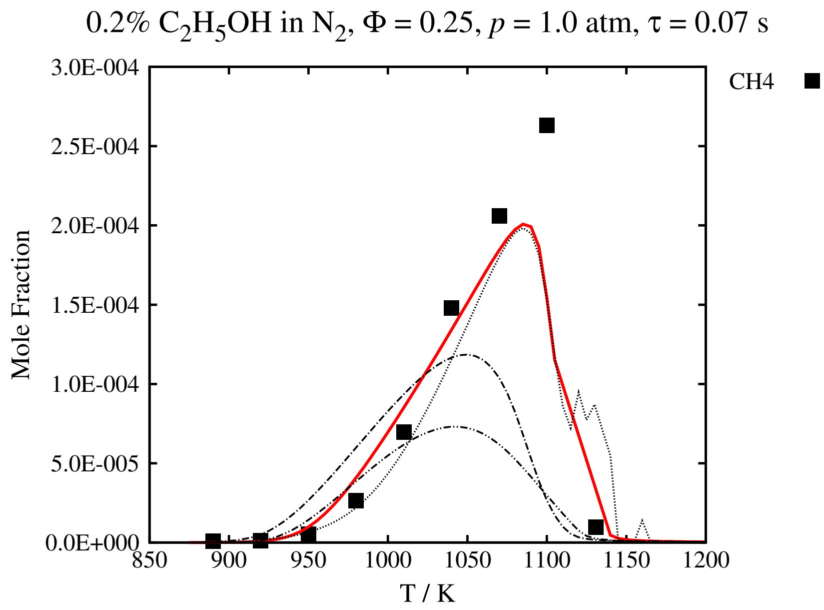


(a)

0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s

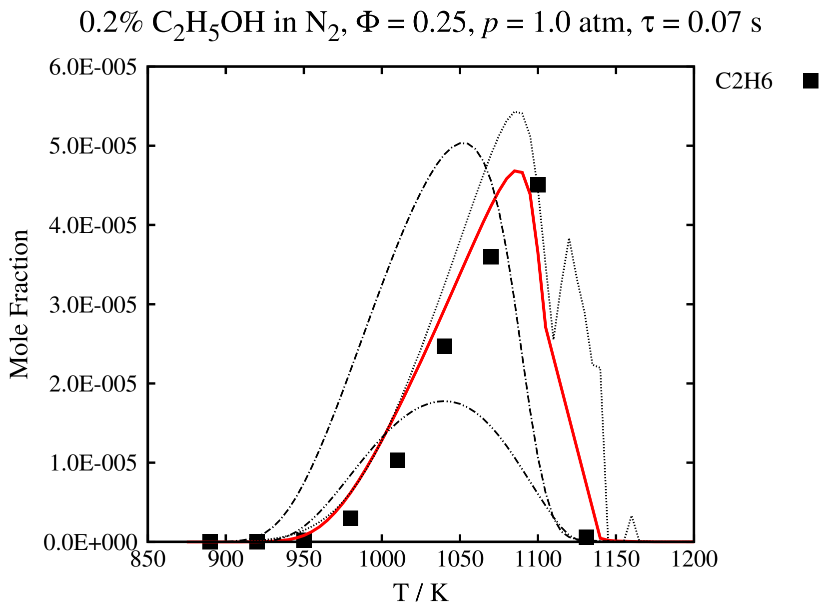


(b)



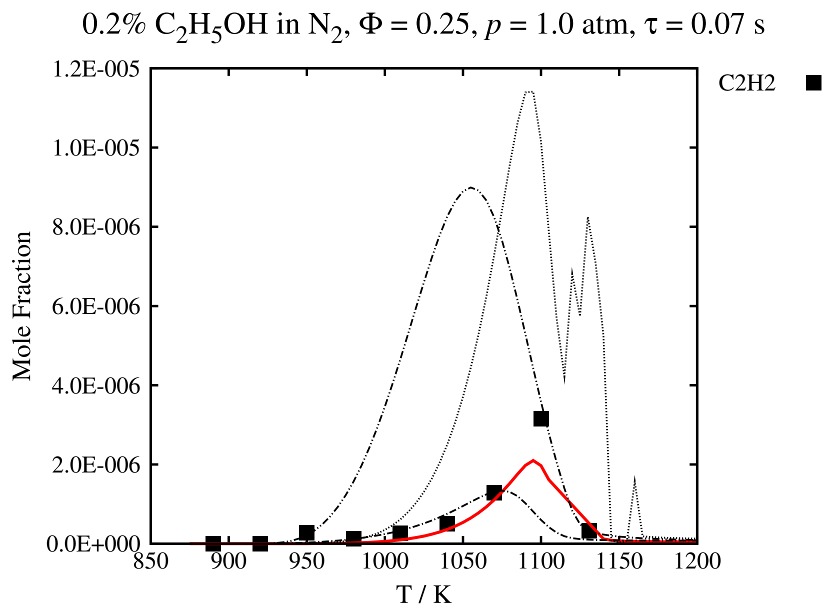
0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
CH4
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

(c)

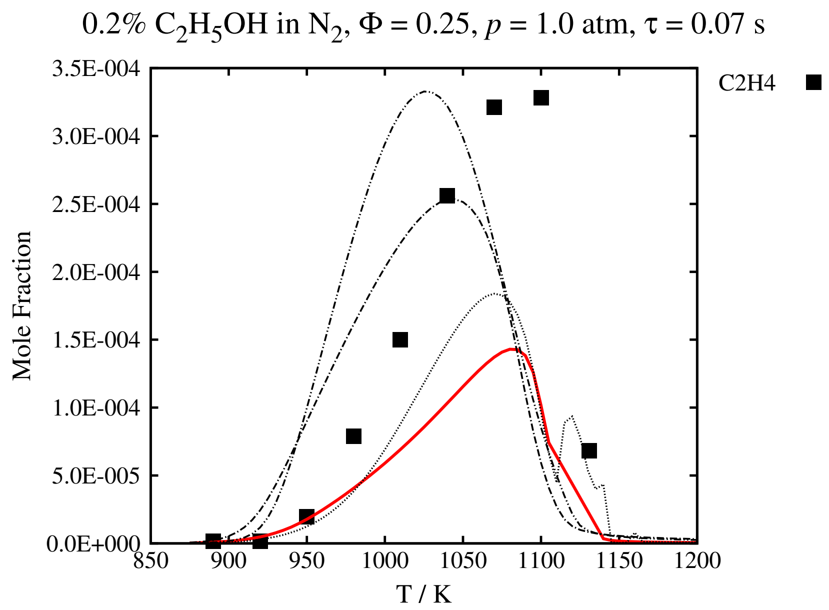


0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
C2H6
Mole Fraction
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

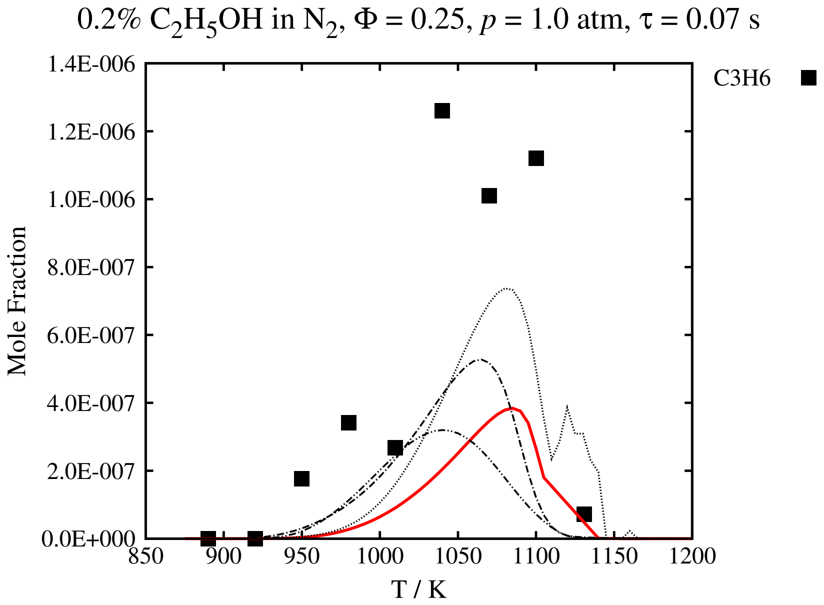
(d)


0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
C2H2
Mole Fraction
T / K
1.2E-005
1.0E-005
8.0E-006
6.0E-006
4.0E-006
2.0E-006
0.0E+000
850
900
950
1000
1050
1100
1150
1200

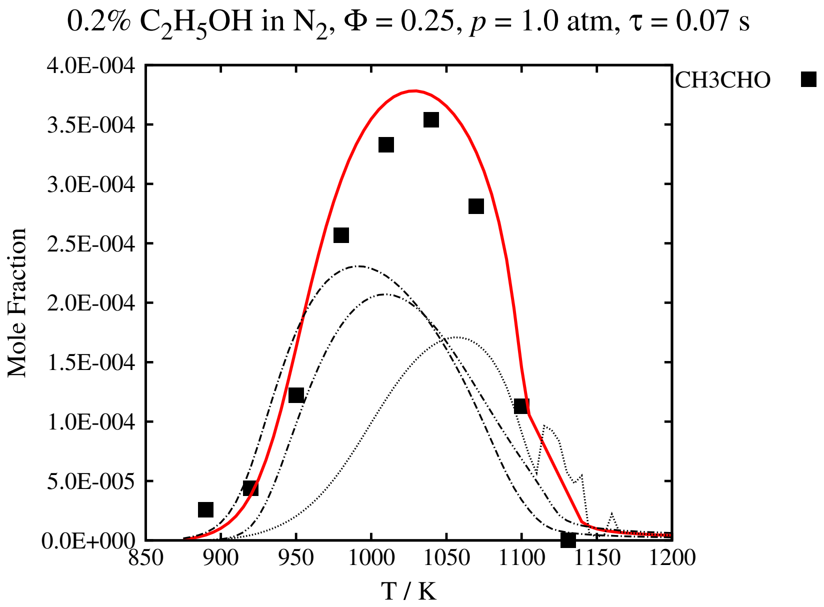
(e)


0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
C2H4
Mole Fraction
T / K
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200

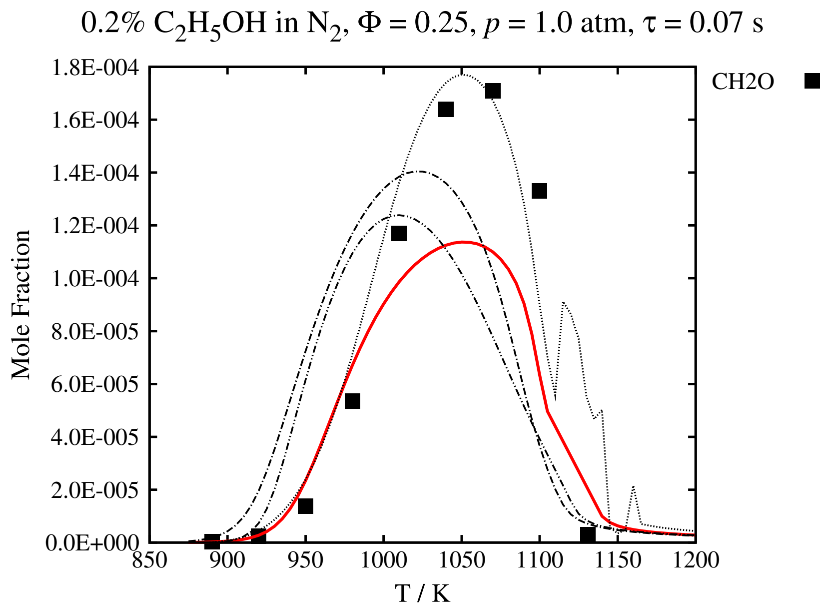
(f)


0.2% C2H5OH in N2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
C3H6
Mole Fraction
1.4E-006
1.2E-006
1.0E-006
8.0E-007
6.0E-007
4.0E-007
2.0E-007
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

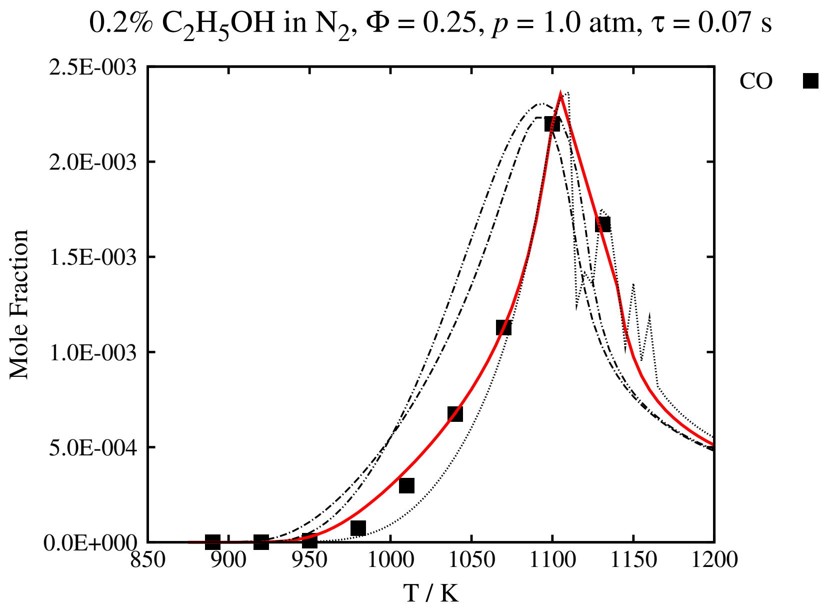
(g)


0.2% C2H5OH in N2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
CH3CHO
Mole Fraction
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

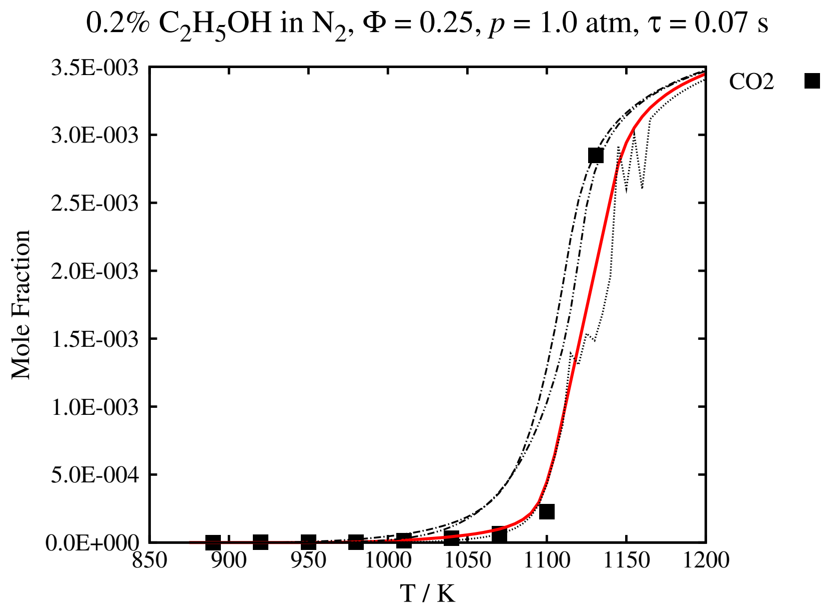
(h)


0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
CH2O
Mole Fraction
T / K
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200

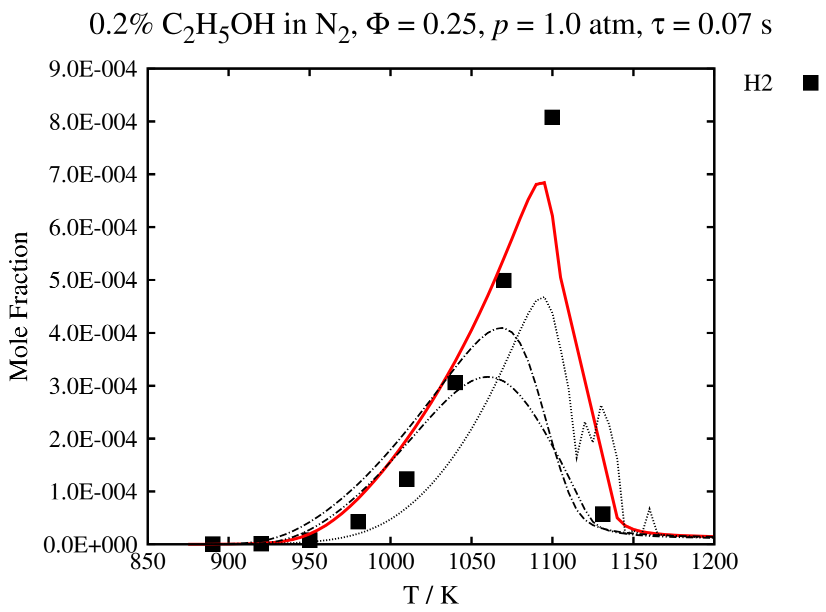
(i)


0.2% C_2H_5OH in N_2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
CO
Mole Fraction
T / K
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200

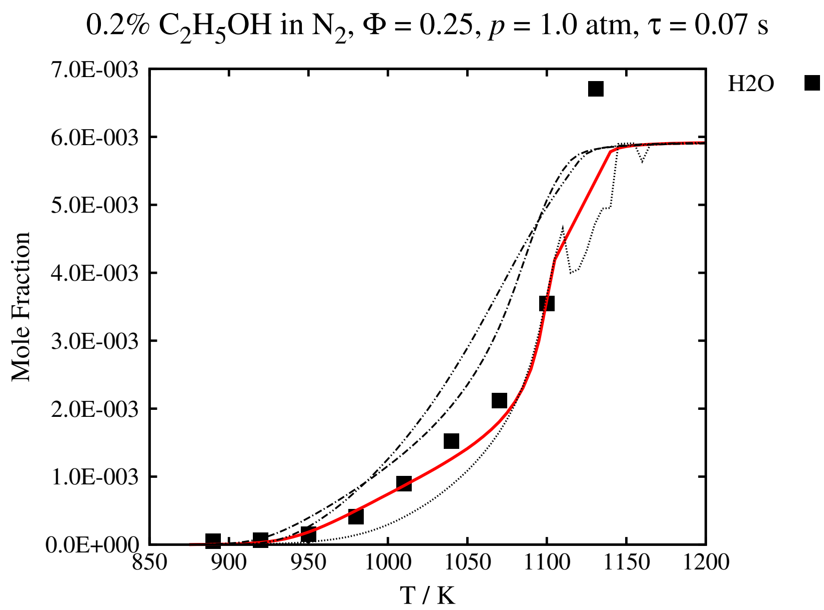
(j)


0.2% C2H5OH in N2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
CO2
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

(k)

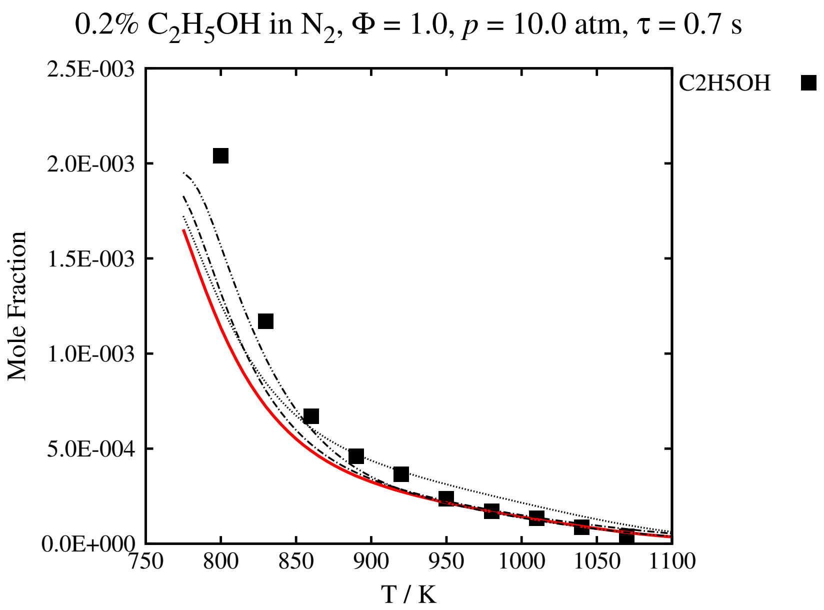

0.2% C2H5OH in N2, Φ = 0.25, p = 1.0 atm, τ = 0.07 s
H2
Mole Fraction
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
T / K

(l)

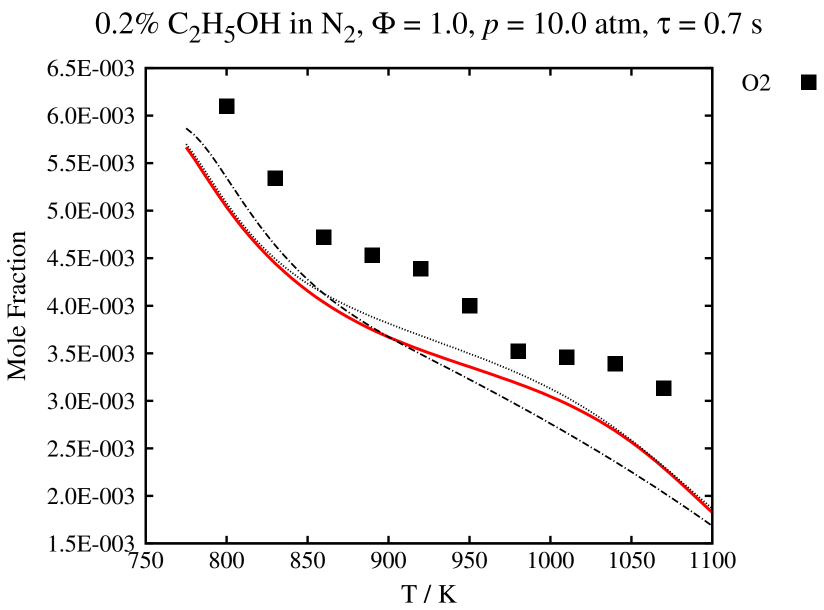


(m)

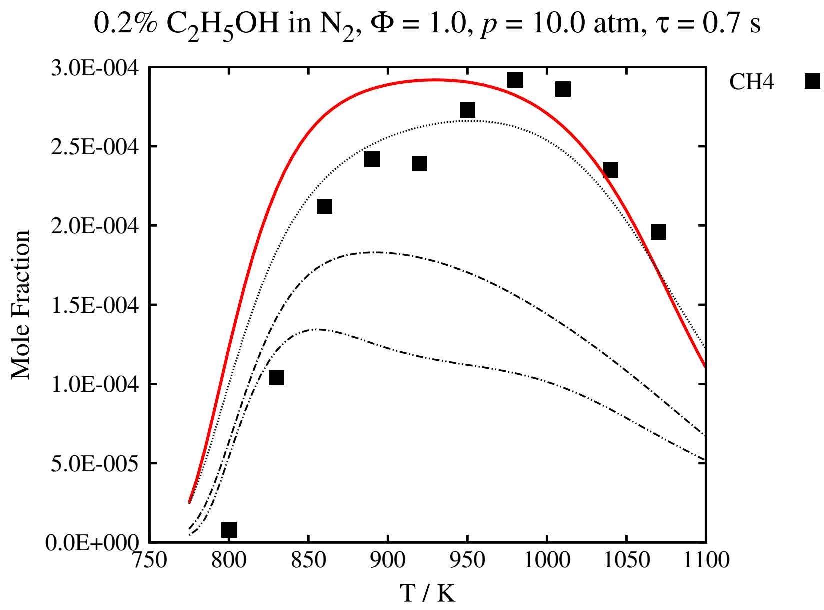
S81 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
C2H5OH
Mole Fraction
T / K
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100

(a)

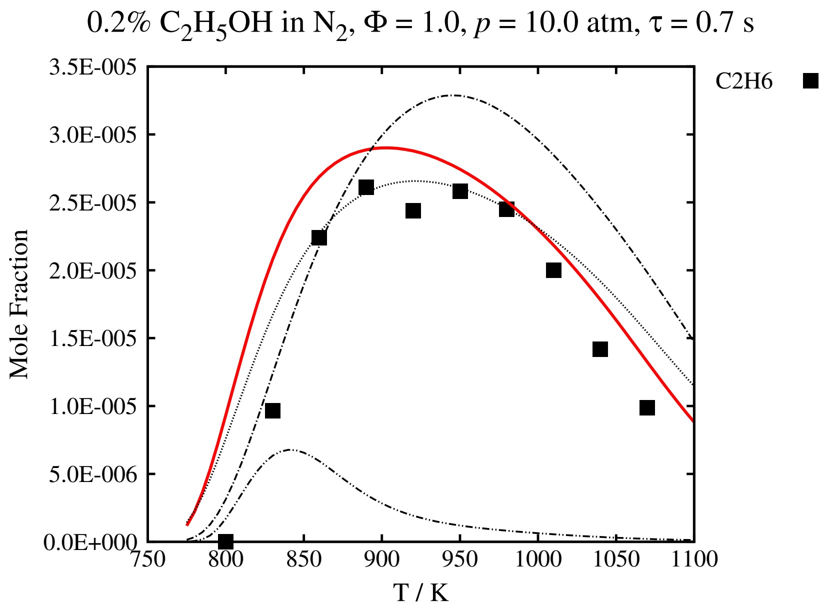

0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
O2
Mole Fraction
T / K
6.5E-003
6.0E-003
5.5E-003
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
750
800
850
900
950
1000
1050
1100

(b)



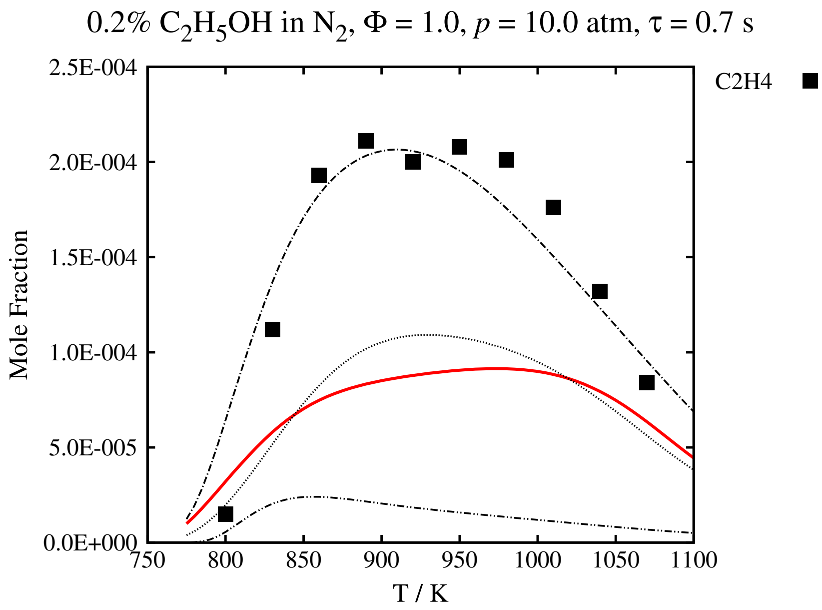
0.2% C_2H_5OH in N_2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
CH4
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

(c)

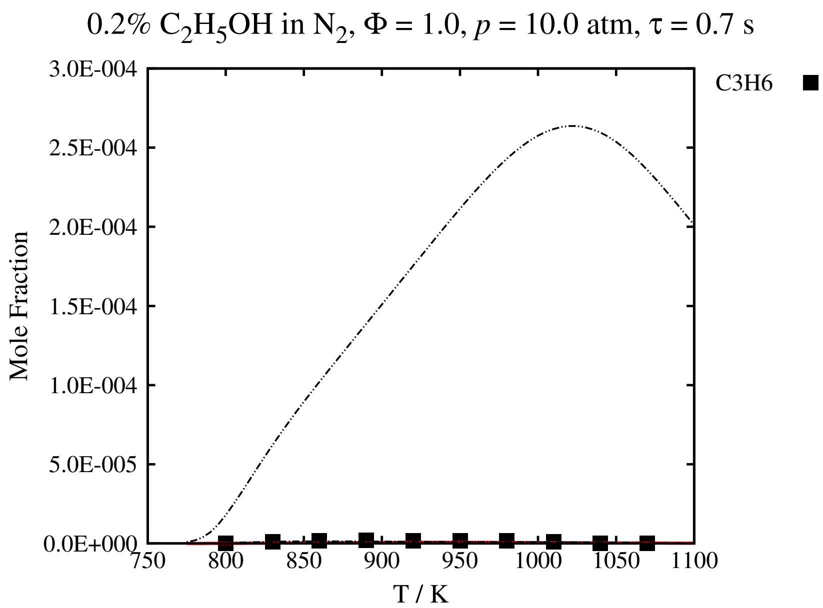


0.2% C_2H_5OH in N_2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
C2H6
Mole Fraction
3.5E-005
3.0E-005
2.5E-005
2.0E-005
1.5E-005
1.0E-005
5.0E-006
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

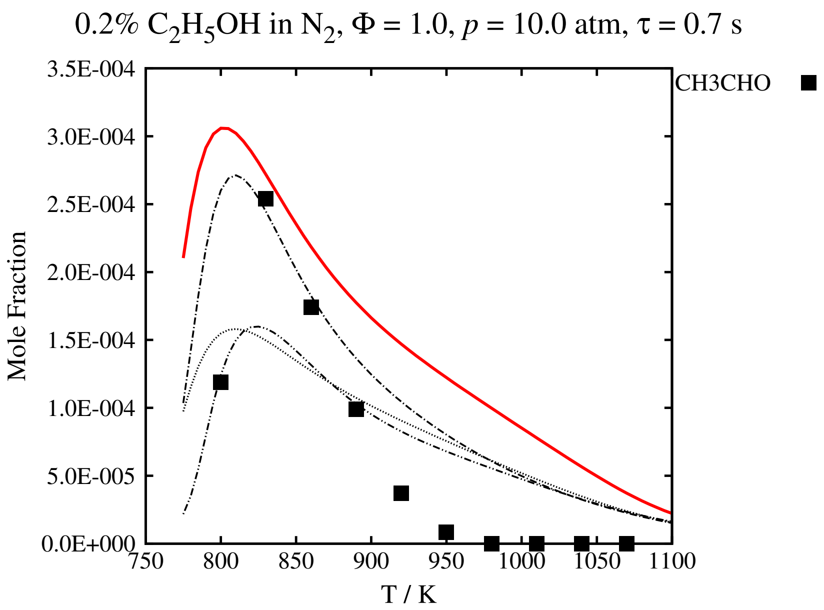
(d)


0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
C2H4
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

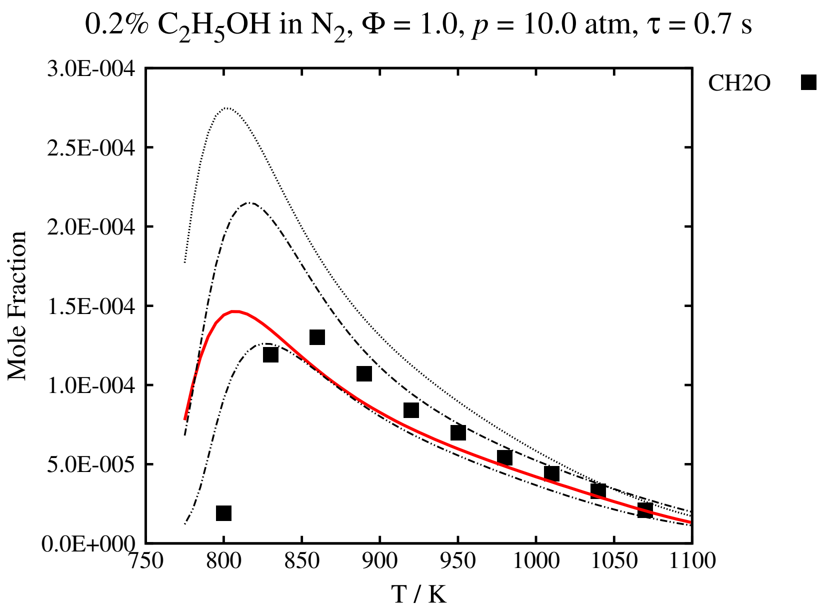
(e)


0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
C3H6
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

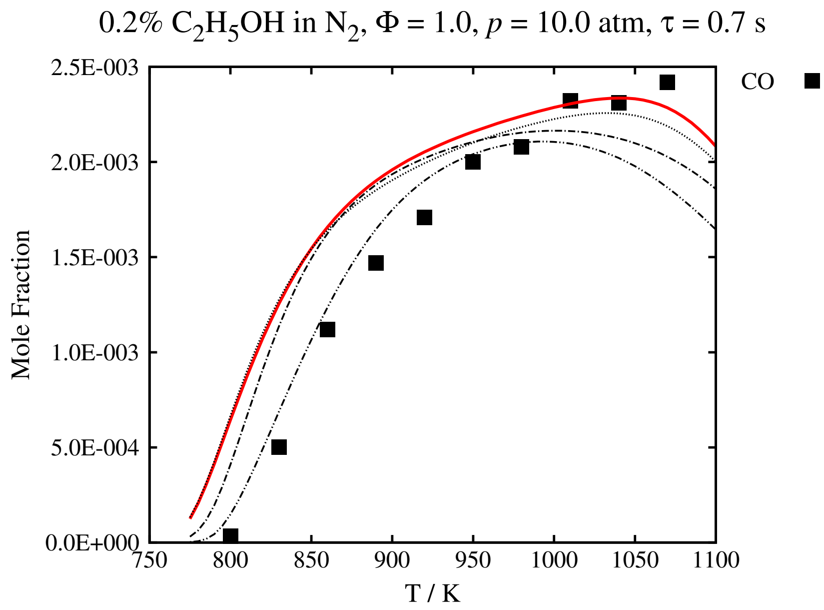
(f)


0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
CH3CHO
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

(g)

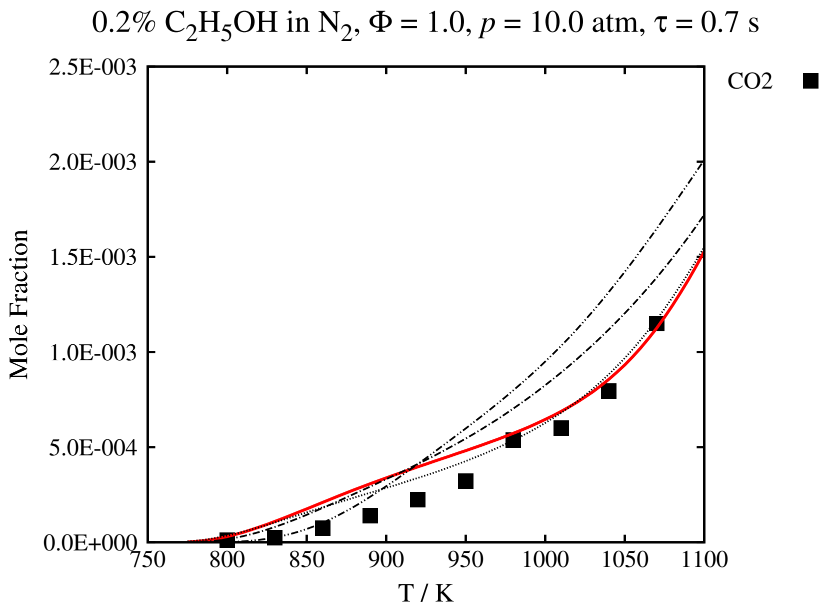

0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
CH2O
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

(h)



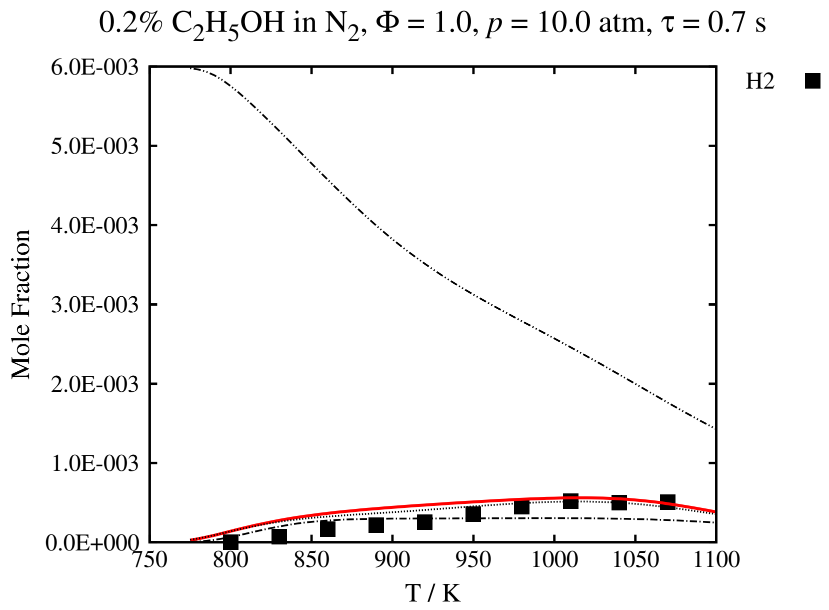
0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
CO
Mole Fraction
T / K
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100

(i)

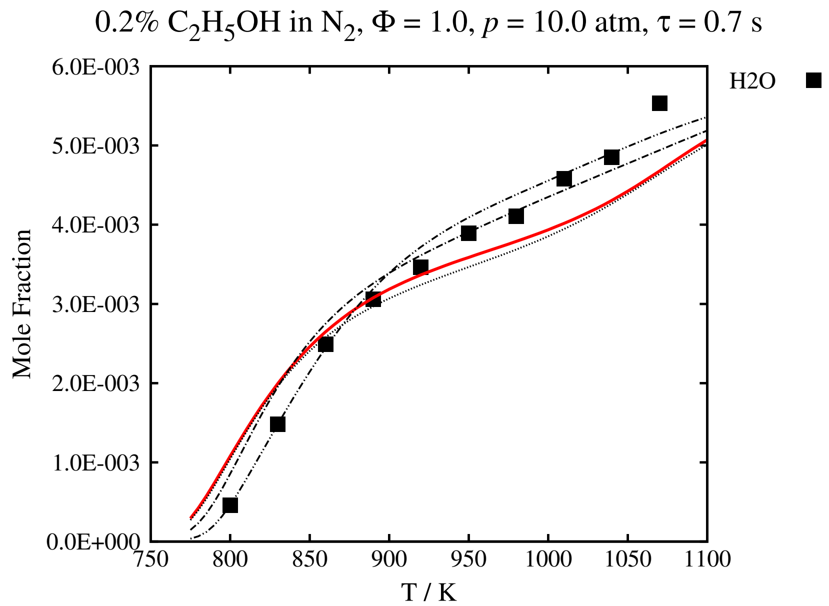


0.2% C2H5OH in N2, Φ = 1.0, p = 10.0 atm, τ = 0.7 s
CO2
Mole Fraction
T / K
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100

(j)

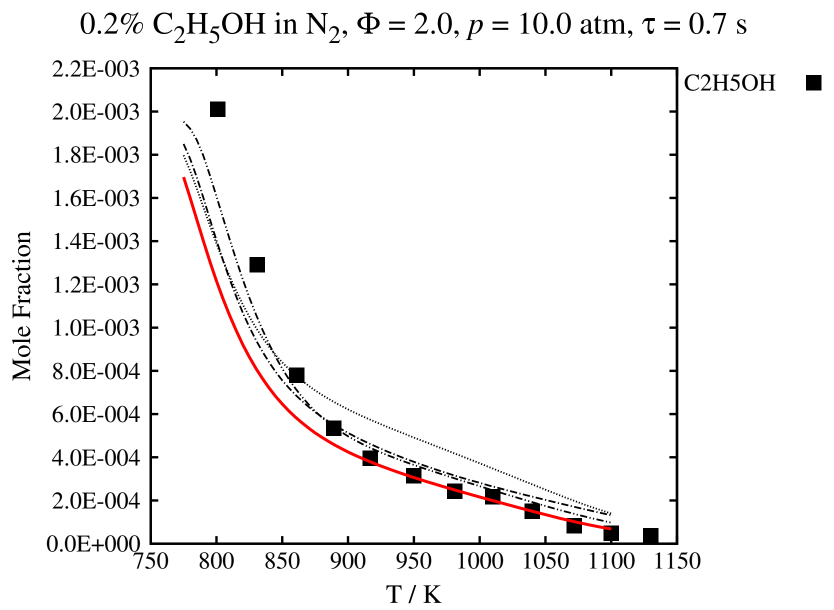


(k)



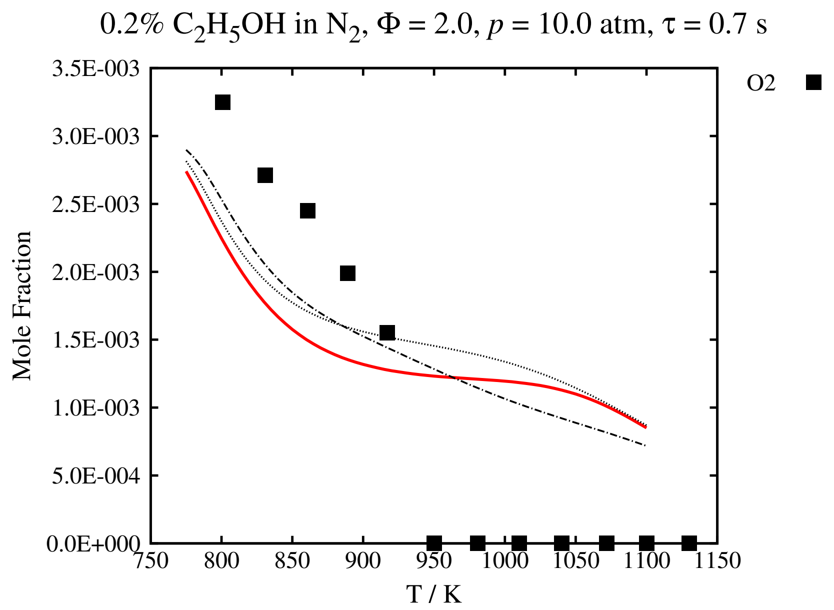
(l)

S82 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



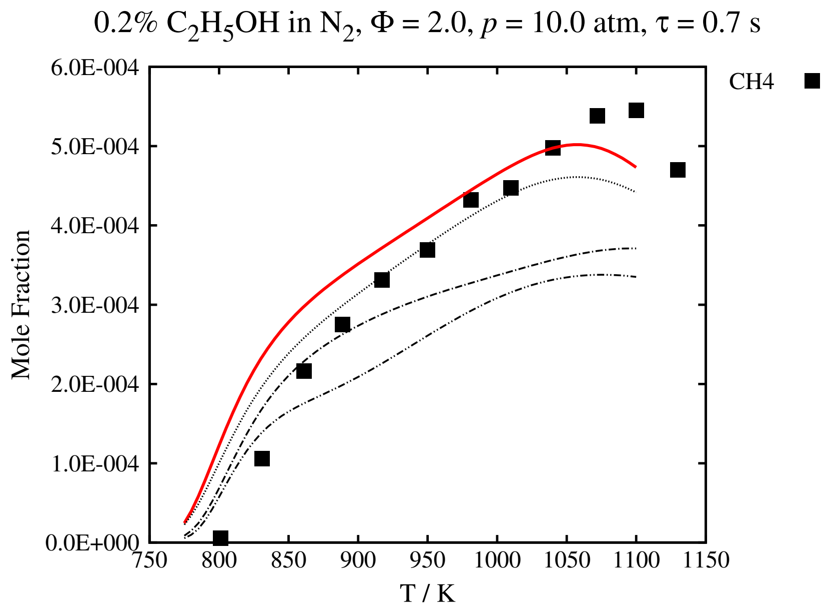
0.2% C2H5OH in N2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
C2H5OH
Mole Fraction
T / K
2.2E-003
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
1150

(a)

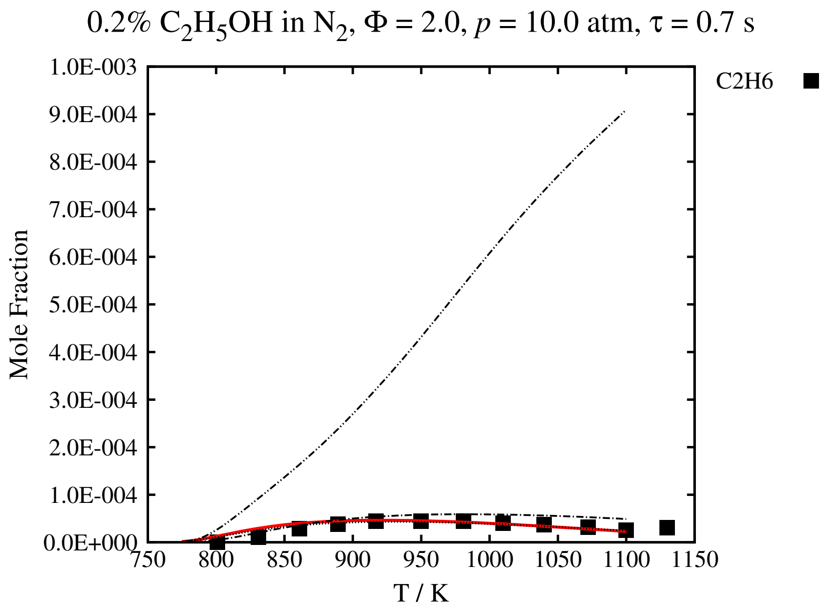


0.2% C2H5OH in N2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
O2
Mole Fraction
T / K
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
1150

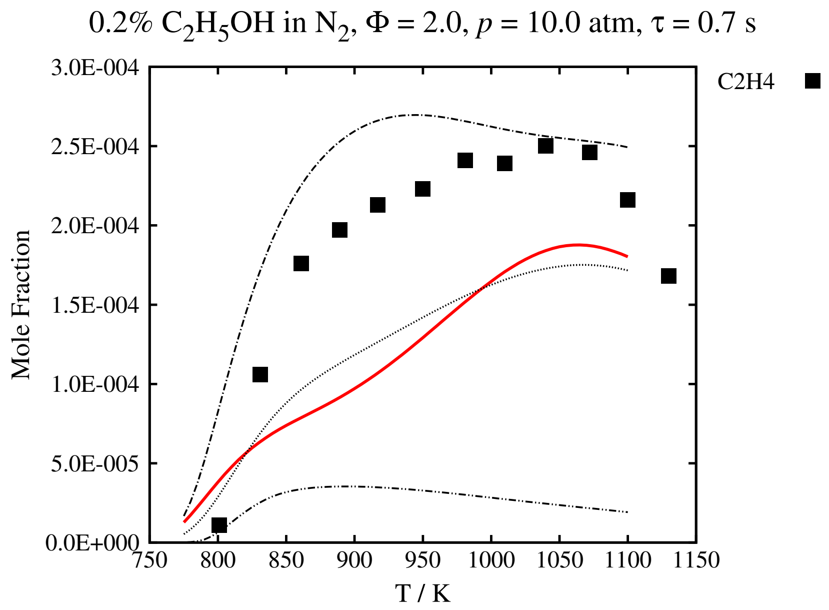
(b)


0.2% C_2H_5OH in N_2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
CH4
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
1150
T / K

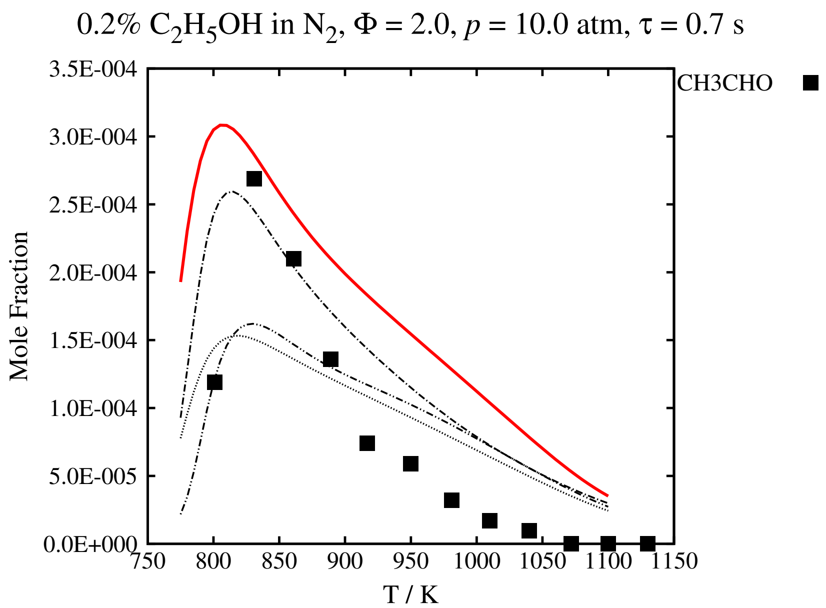
(c)


0.2% C_2H_5OH in N_2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
C2H6
Mole Fraction
1.0E-003
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
1150
T / K

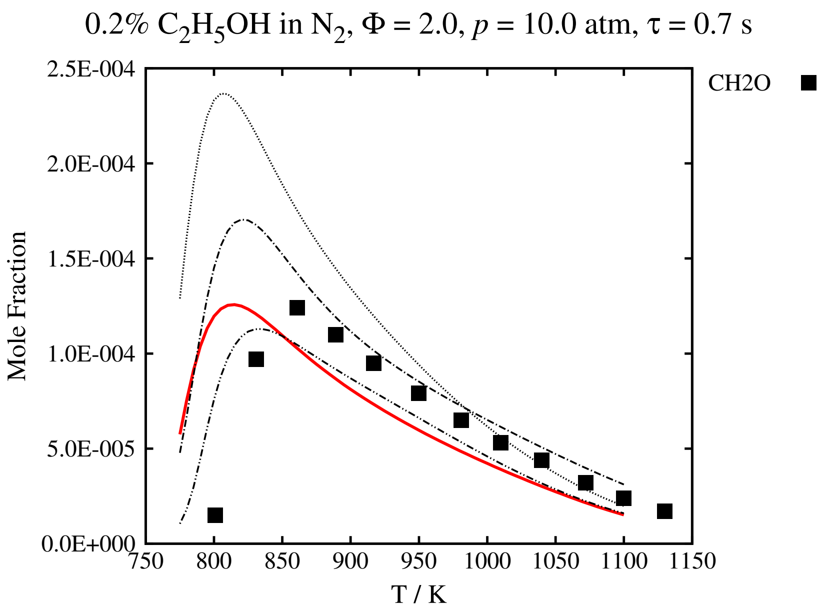
(d)


0.2% C2H5OH in N2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
C2H4
Mole Fraction
T / K
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750 800 850 900 950 1000 1050 1100 1150

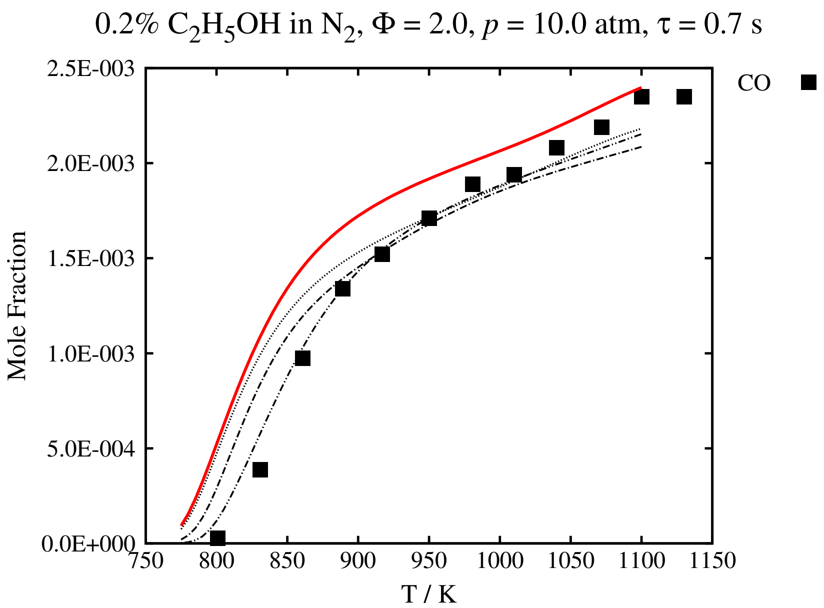
(e)


0.2% C2H5OH in N2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
CH3CHO
Mole Fraction
T / K
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750 800 850 900 950 1000 1050 1100 1150

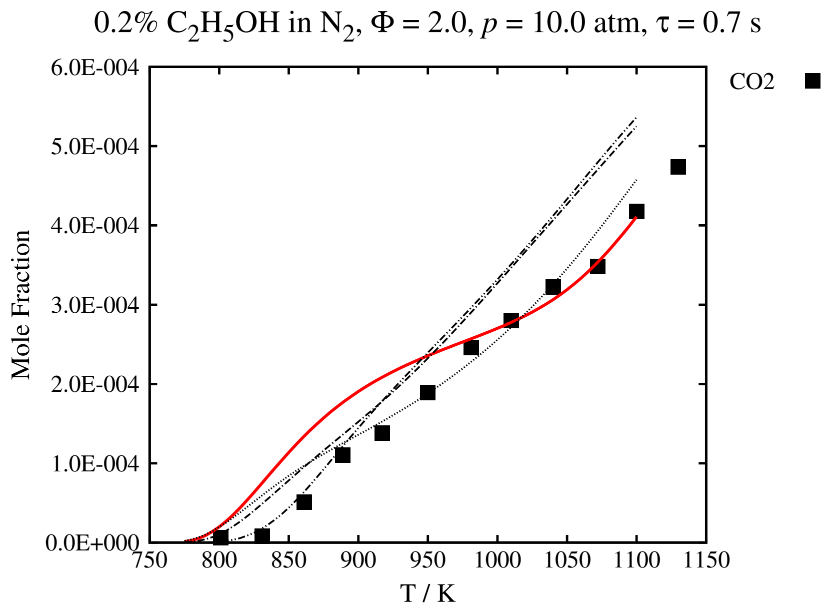
(f)


0.2% C_2H_5OH in N_2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
CH2O
Mole Fraction
T / K
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
1150

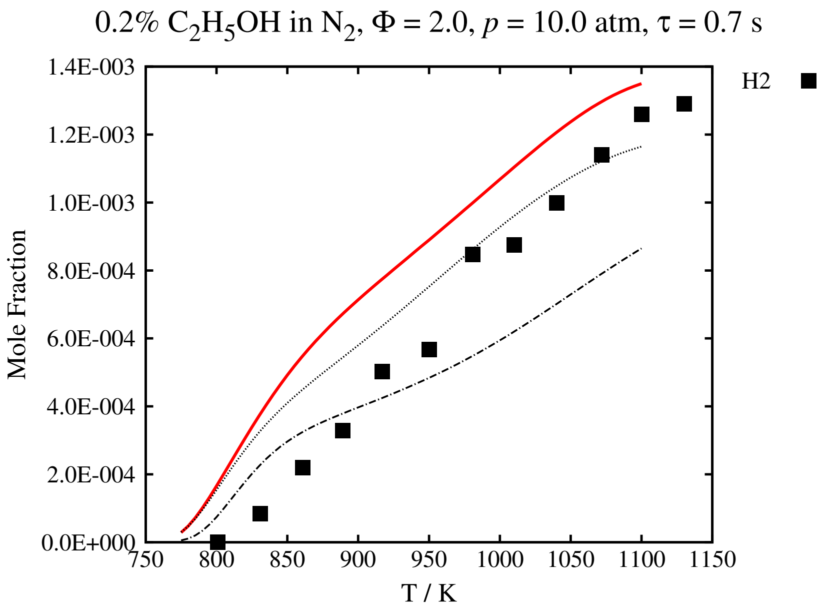
(g)


0.2% C_2H_5OH in N_2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
CO
Mole Fraction
T / K
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
1150

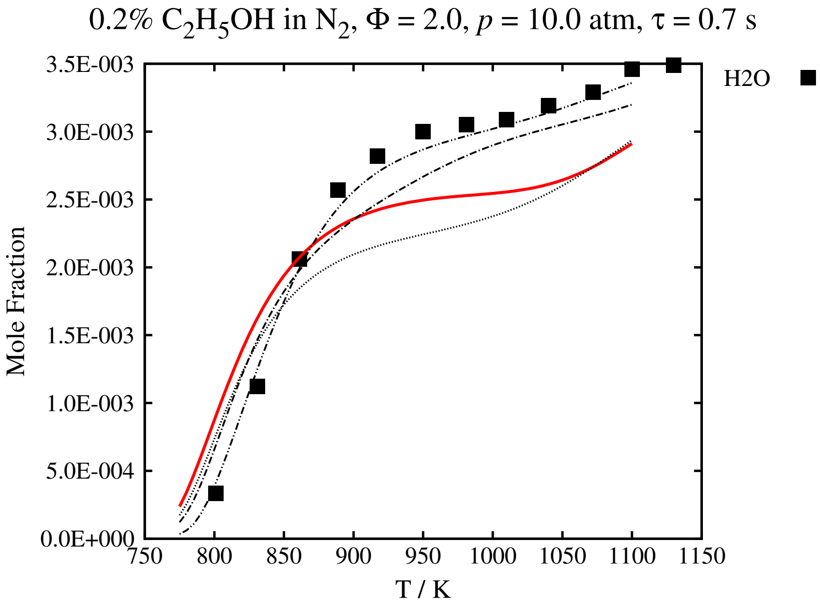
(h)


0.2% C_2H_5OH in N_2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
CO2
Mole Fraction
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
1150
T / K

(i)

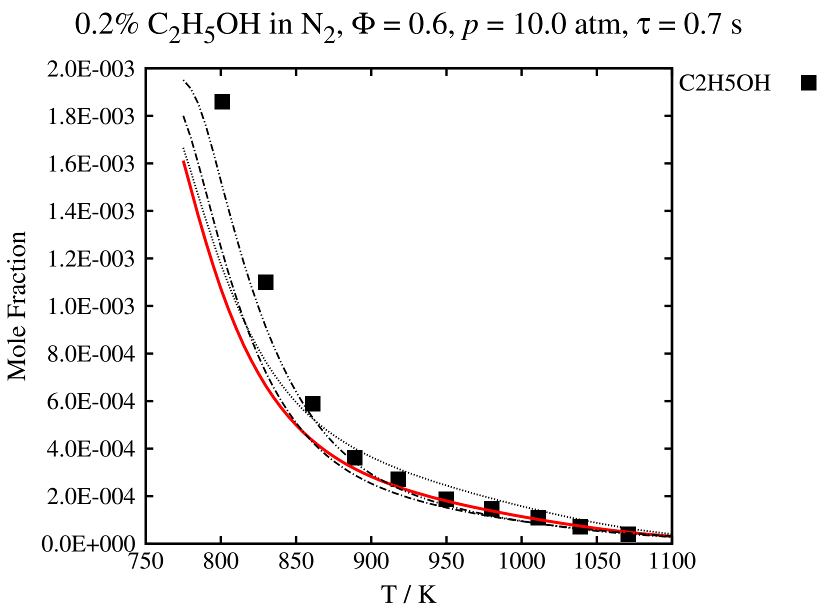

0.2% C_2H_5OH in N_2, Φ = 2.0, p = 10.0 atm, τ = 0.7 s
H2
Mole Fraction
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
1150
T / K

(j)

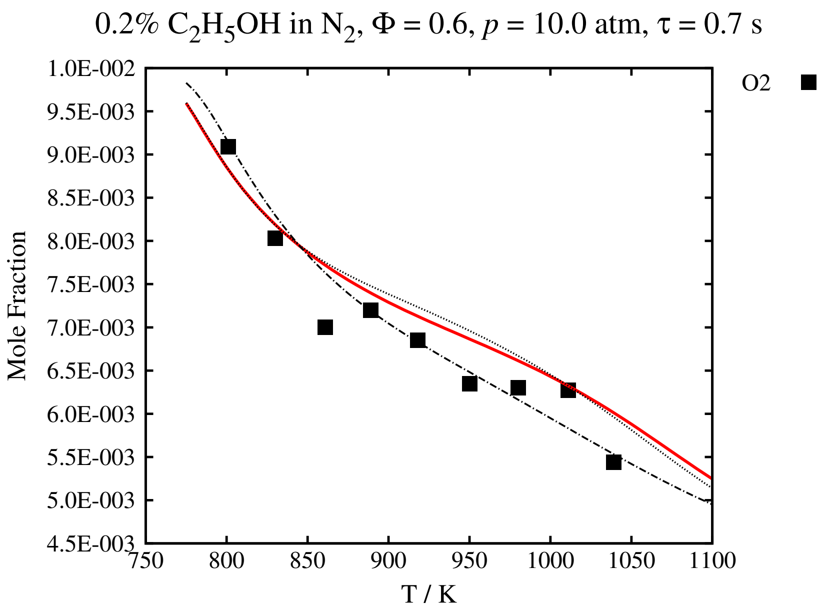


(k)

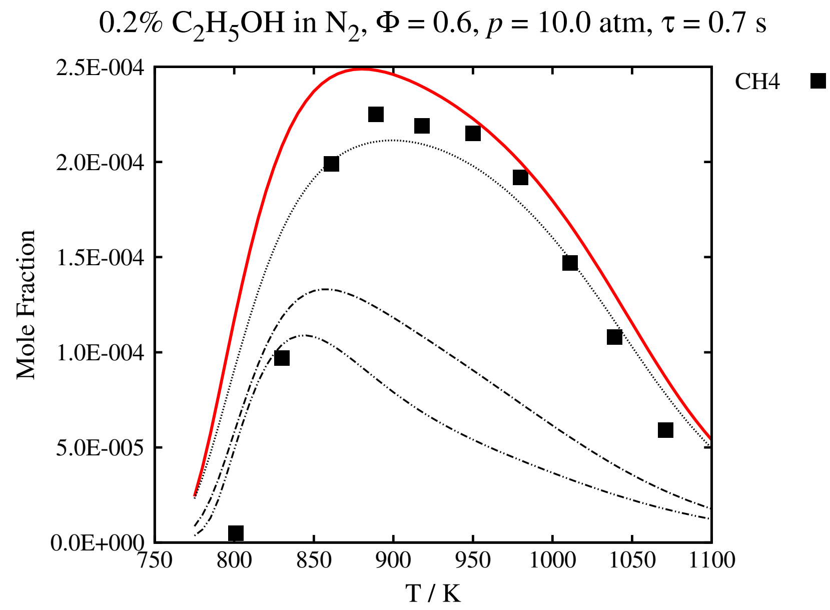
S83 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.2% C_2H_5OH in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
C2H5OH
Mole Fraction
2.0E-003
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

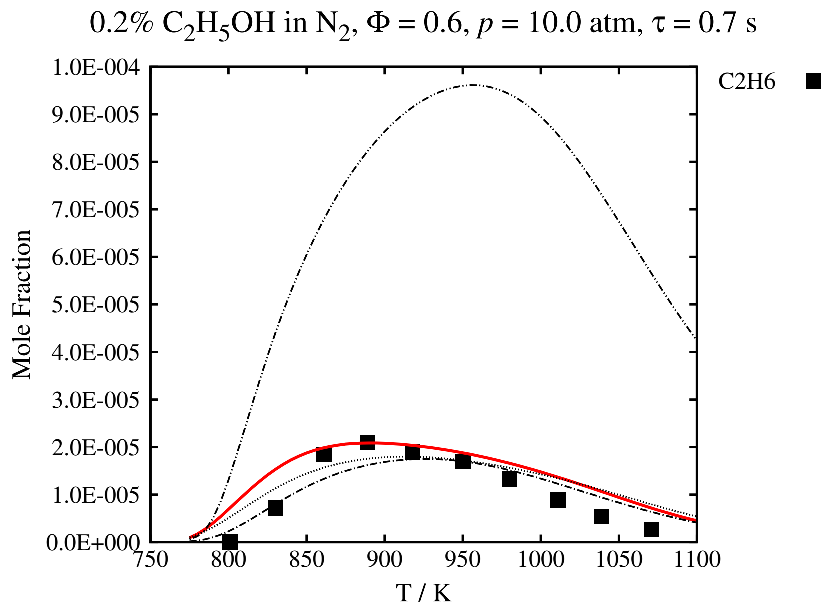
(a)


0.2% C_2H_5OH in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
O2
Mole Fraction
1.0E-002
9.5E-003
9.0E-003
8.5E-003
8.0E-003
7.5E-003
7.0E-003
6.5E-003
6.0E-003
5.5E-003
5.0E-003
4.5E-003
750
800
850
900
950
1000
1050
1100
T / K

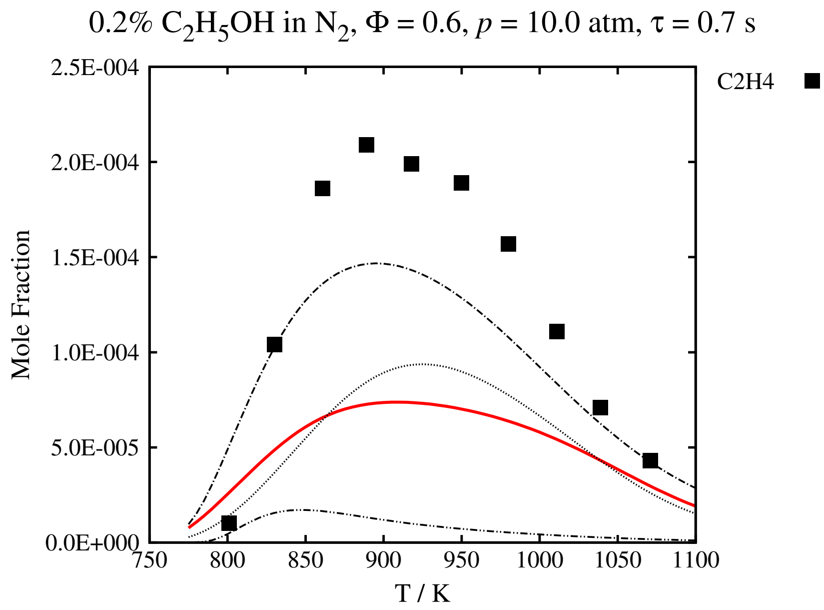
(b)


0.2% C2H5OH in N2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
CH4
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

(c)

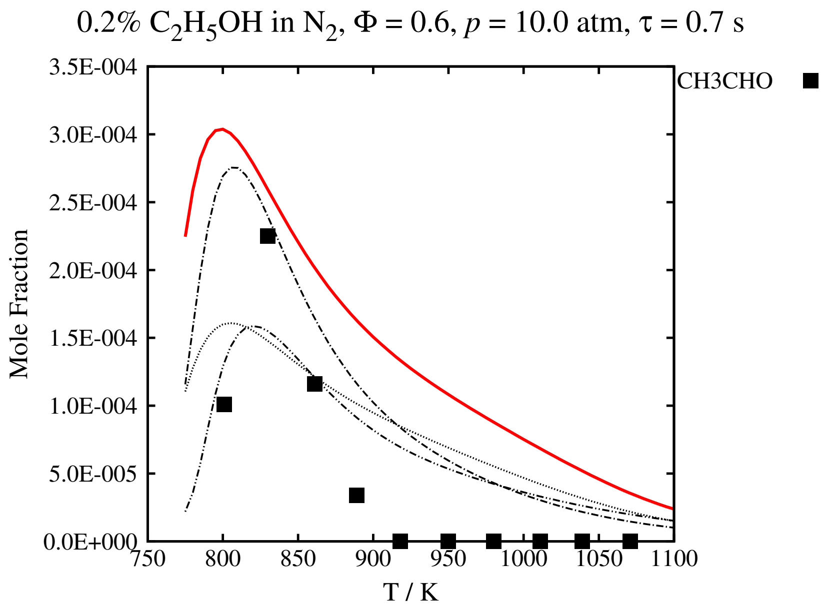

0.2% C2H5OH in N2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
C2H6
Mole Fraction
1.0E-004
9.0E-005
8.0E-005
7.0E-005
6.0E-005
5.0E-005
4.0E-005
3.0E-005
2.0E-005
1.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

(d)



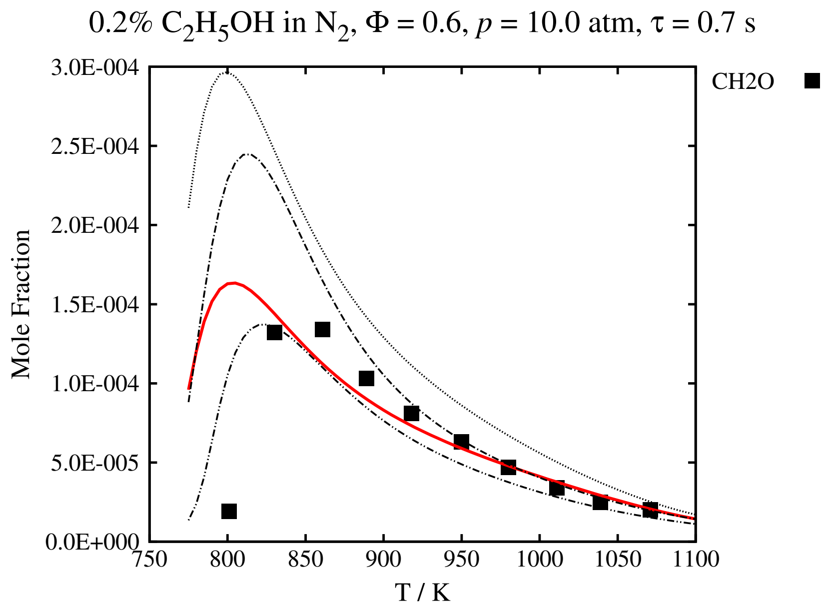
0.2% C_2H_5OH in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
C2H4
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
Mole Fraction
750
800
850
900
950
1000
1050
1100
T / K

(e)

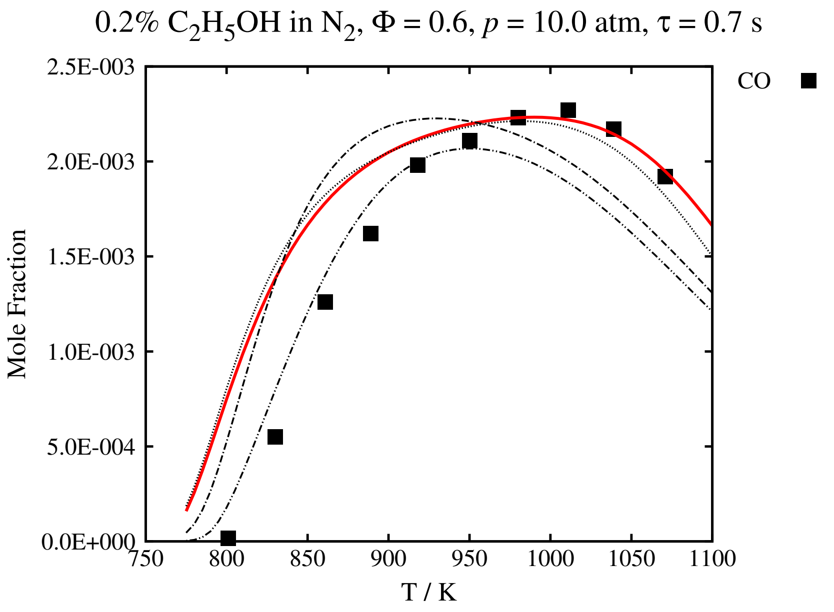


0.2% C_2H_5OH in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
CH3CHO
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
Mole Fraction
750
800
850
900
950
1000
1050
1100
T / K

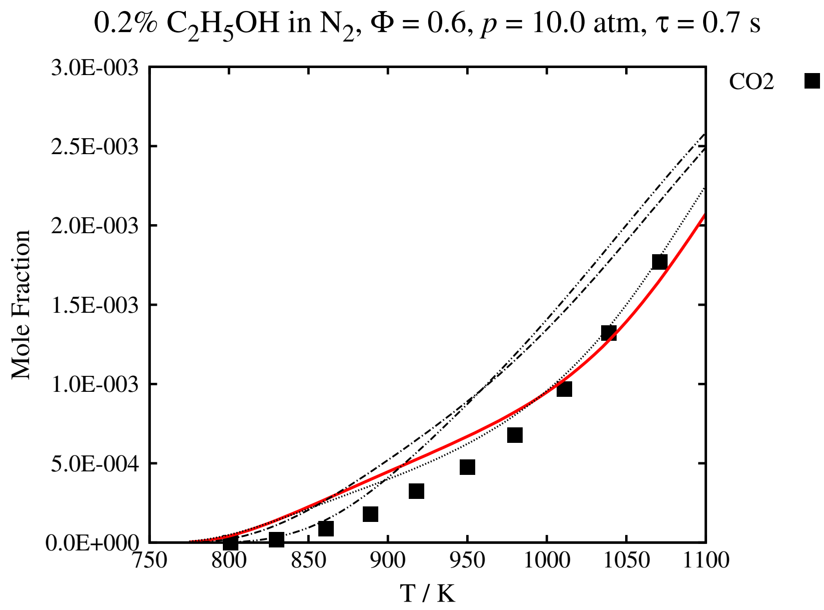
(f)


0.2% C_2H_5OH in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
CH2O
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

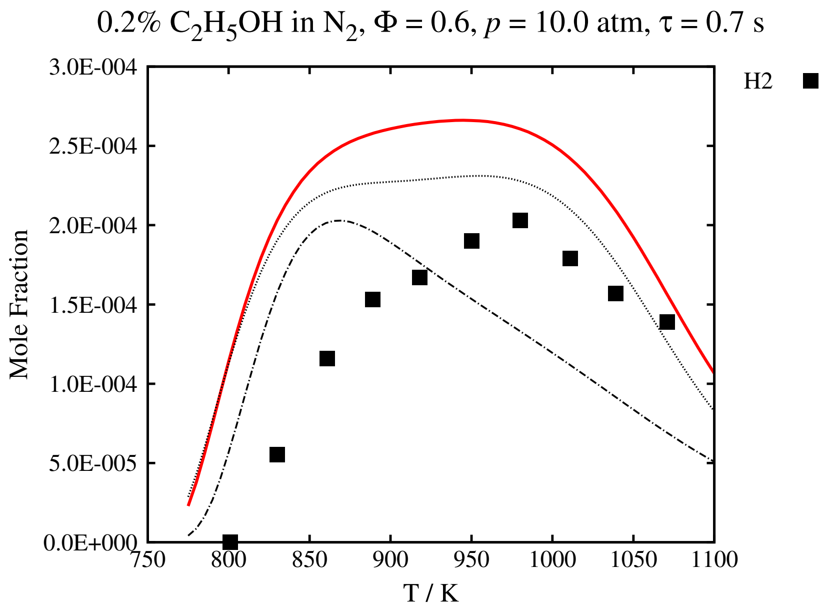
(g)


0.2% C_2H_5OH in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
CO
Mole Fraction
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

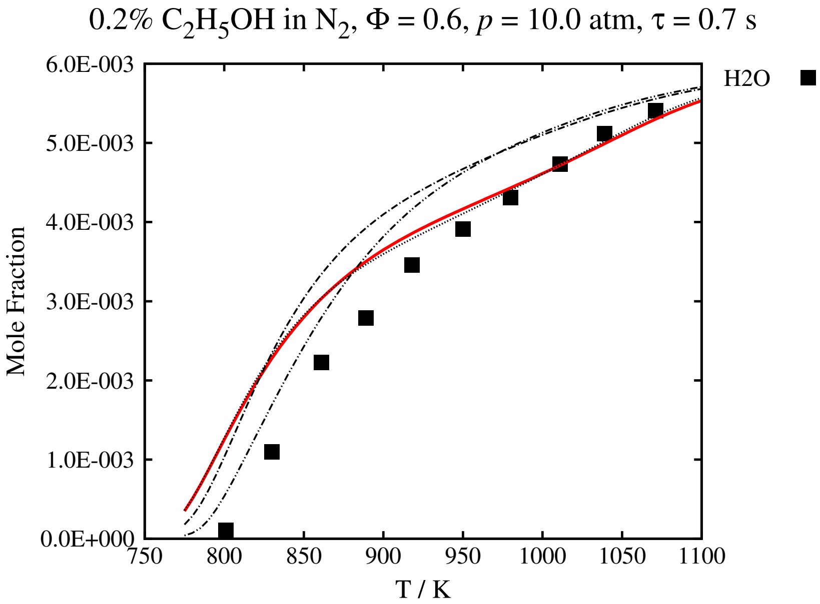
(h)


0.2% C2H5OH in N2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
CO2
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

(i)

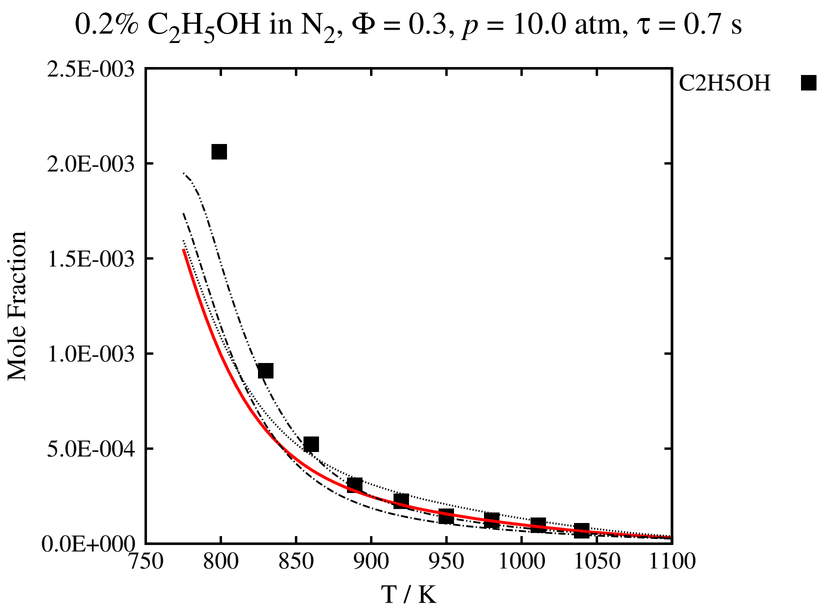

0.2% C2H5OH in N2, Φ = 0.6, p = 10.0 atm, τ = 0.7 s
H2
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

(j)

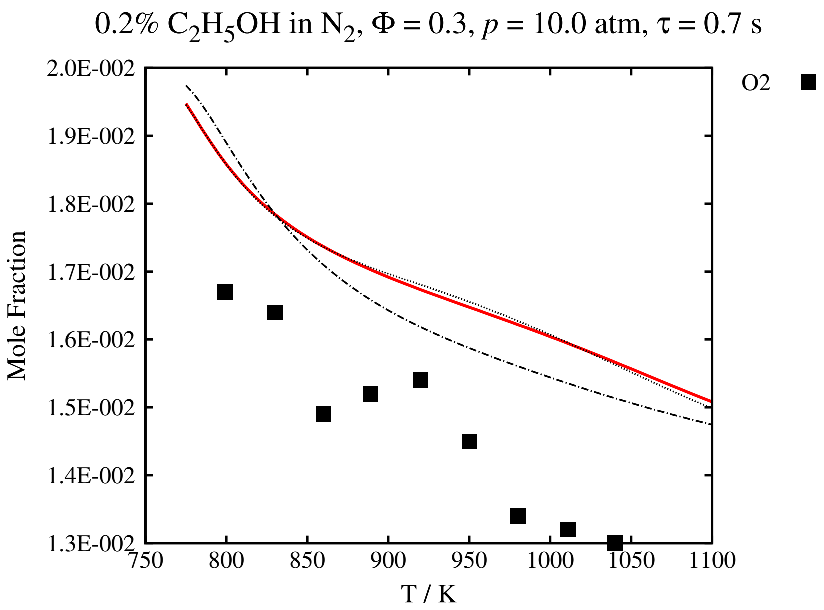


(k)

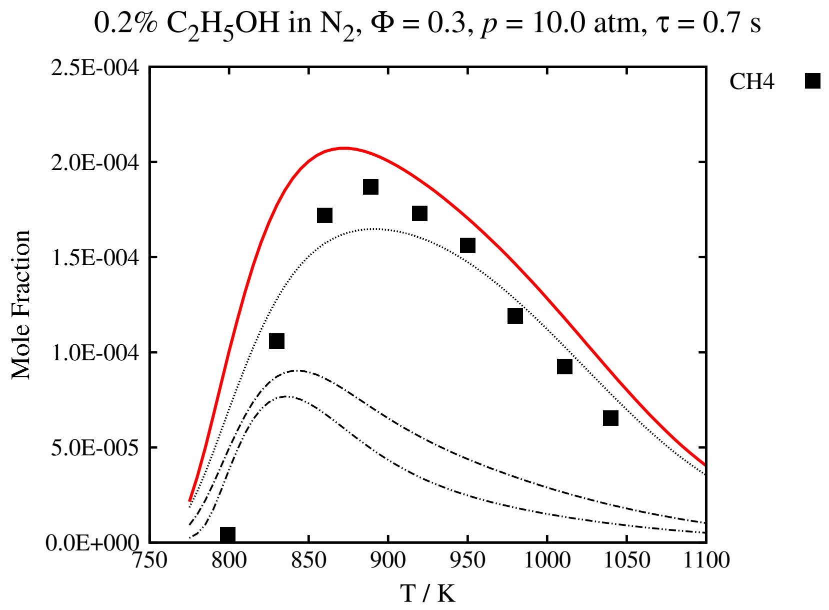
S84 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.2% C2H5OH in N2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
C2H5OH
Mole Fraction
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

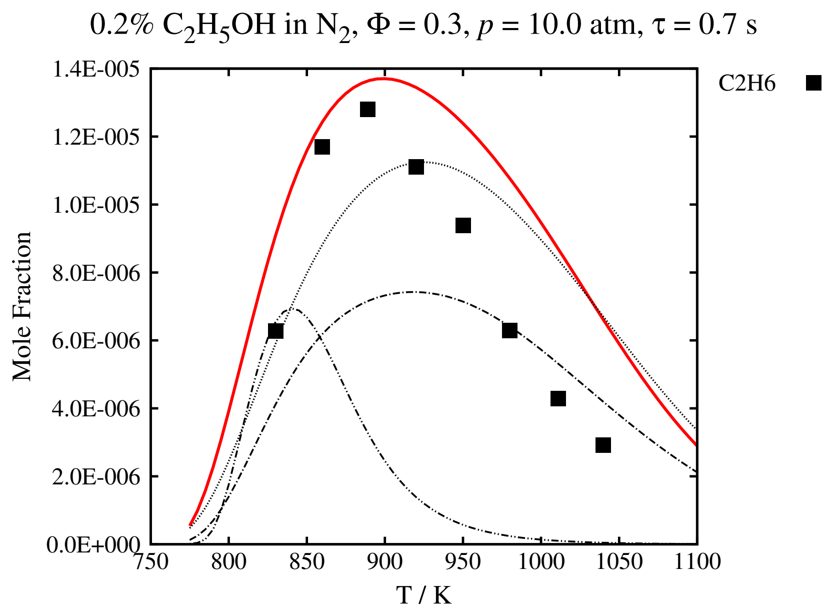
(a)


0.2% C2H5OH in N2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
O2
Mole Fraction
2.0E-002
1.9E-002
1.8E-002
1.7E-002
1.6E-002
1.5E-002
1.4E-002
1.3E-002
750
800
850
900
950
1000
1050
1100
T / K

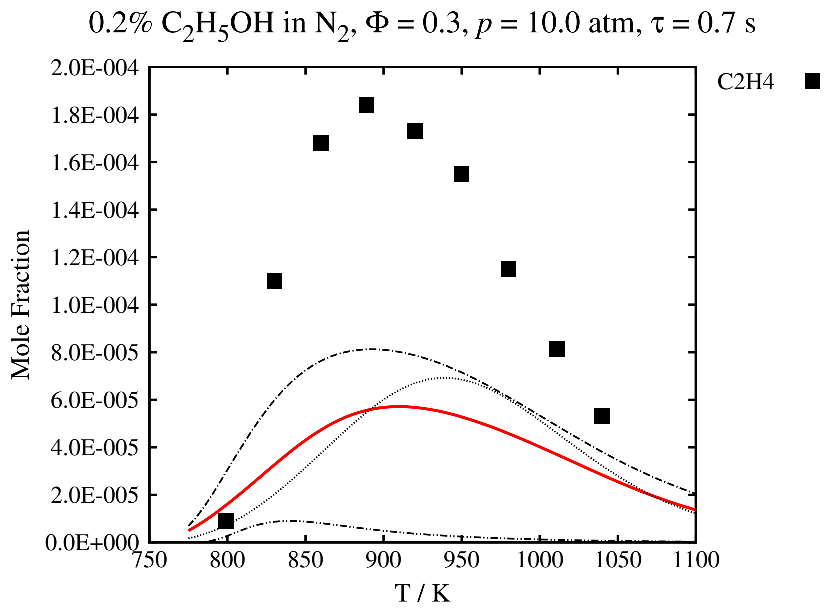
(b)


0.2% C_2H_5OH in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
CH4
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

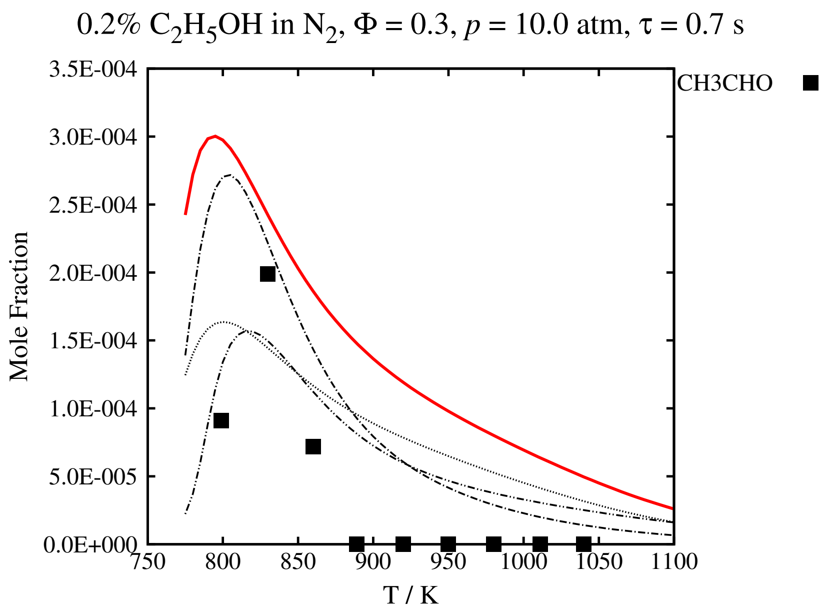
(c)


0.2% C_2H_5OH in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
C2H6
Mole Fraction
1.4E-005
1.2E-005
1.0E-005
8.0E-006
6.0E-006
4.0E-006
2.0E-006
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

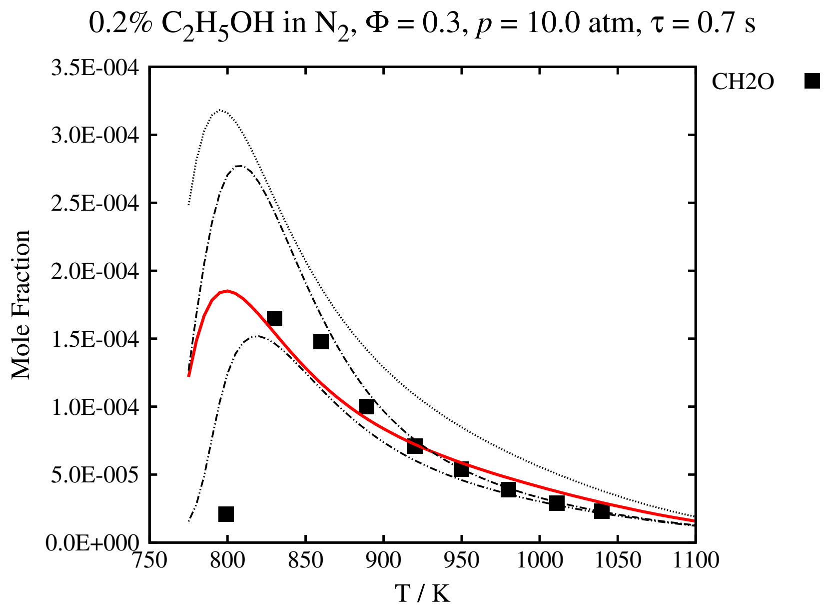
(d)


0.2% C2H5OH in N2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
C2H4
Mole Fraction
2.0E-004
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

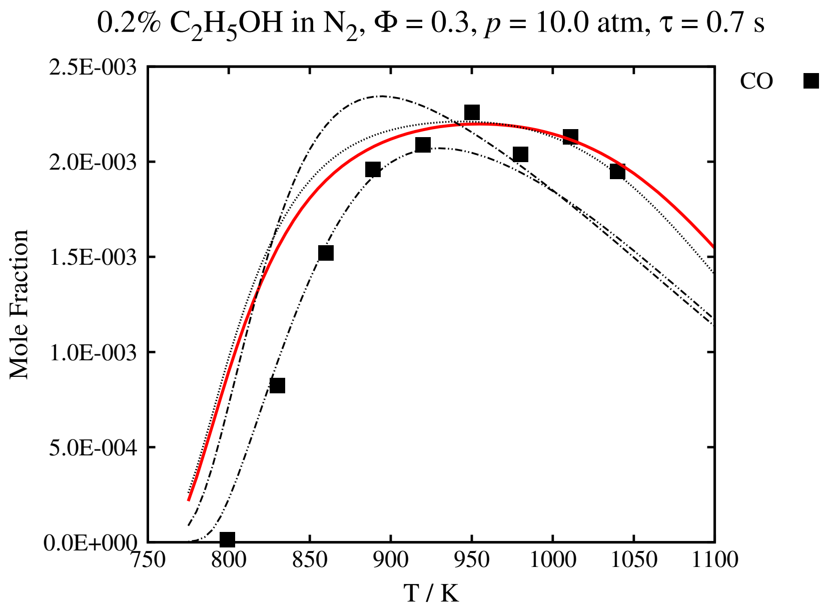
(e)


0.2% C2H5OH in N2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
CH3CHO
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

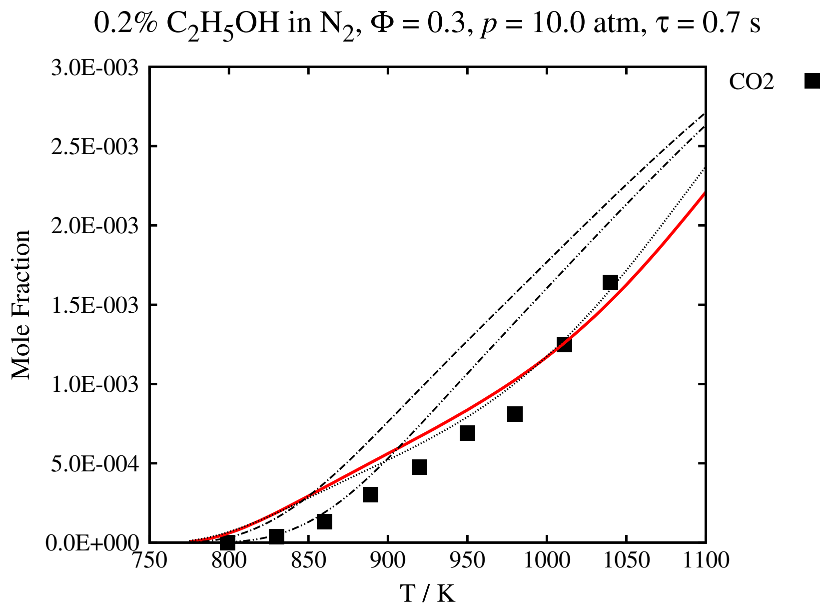
(f)


0.2% C2H5OH in N2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
CH2O
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

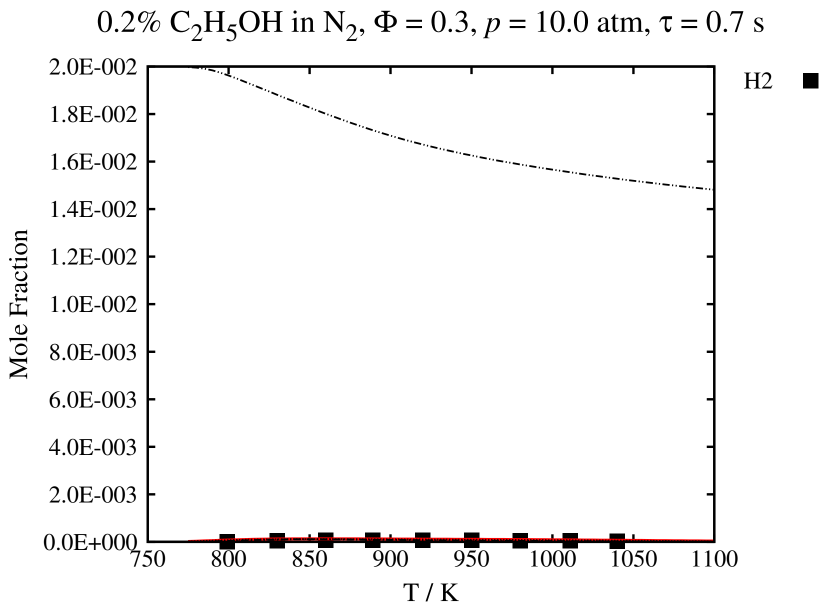
(g)


0.2% C2H5OH in N2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
CO
Mole Fraction
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100
T / K

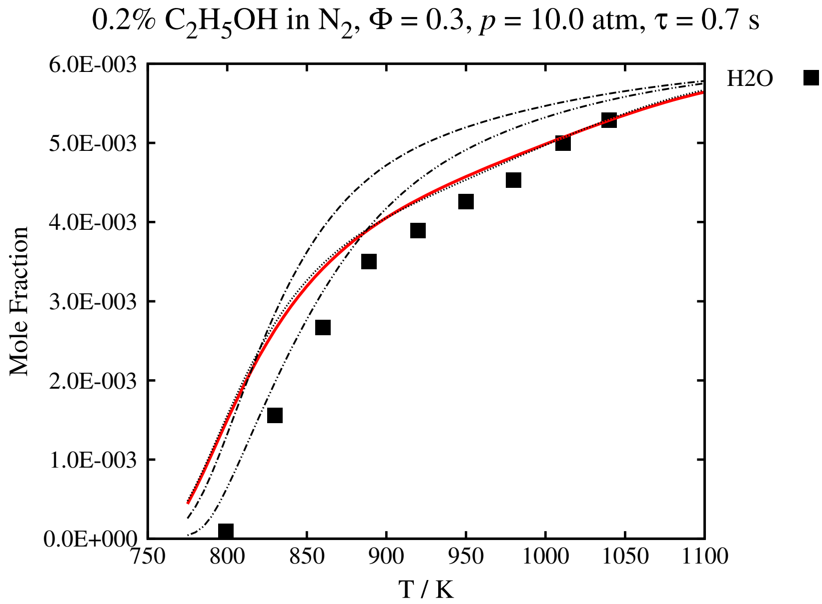
(h)


0.2% C_2H_5OH in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
Mole Fraction
T / K
CO2
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
750
800
850
900
950
1000
1050
1100

(i)

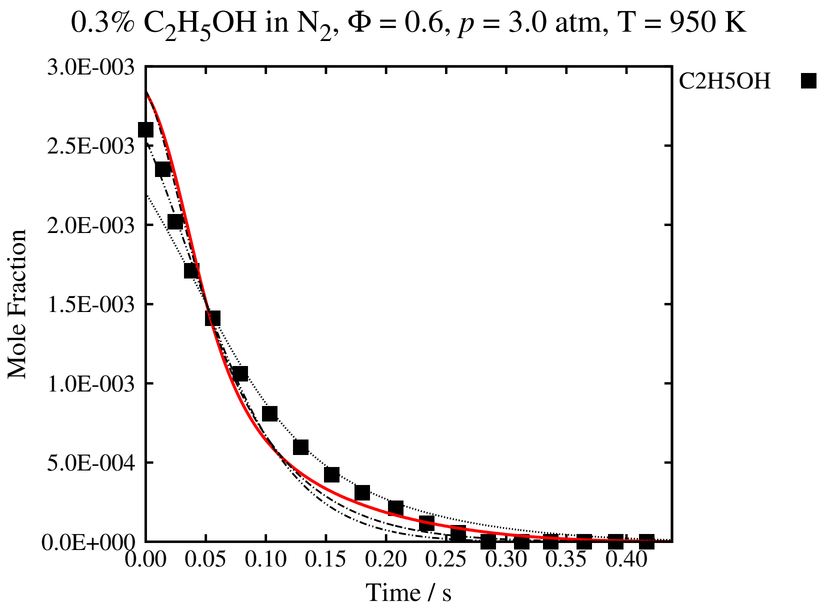

0.2% C_2H_5OH in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.7 s
Mole Fraction
T / K
H2
2.0E-002
1.8E-002
1.6E-002
1.4E-002
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
750
800
850
900
950
1000
1050
1100

(j)

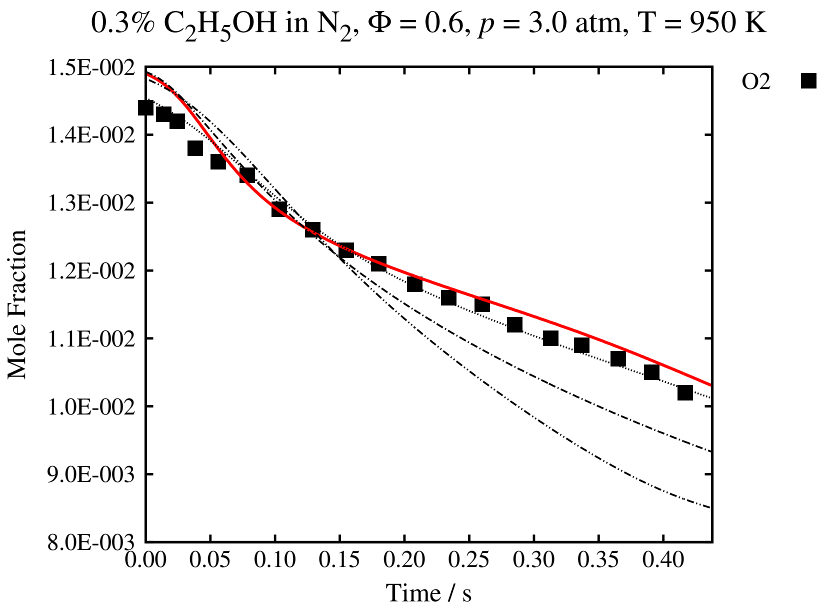


(k)

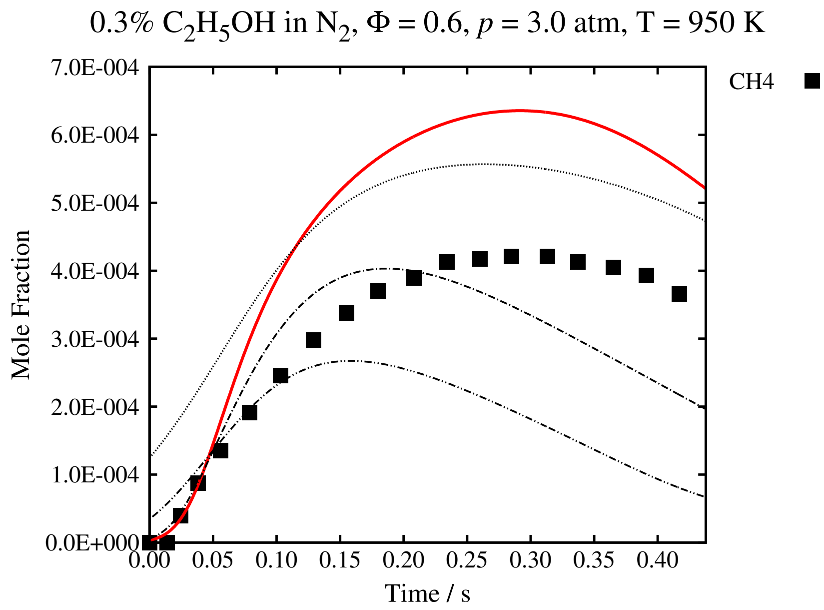
S85 Jet-stirred reactor species profiles of ethanol/oxygen/argon mixtures. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.3% C2H5OH in N2, Φ = 0.6, p = 3.0 atm, T = 950 K
C2H5OH
Mole Fraction
Time / s
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40

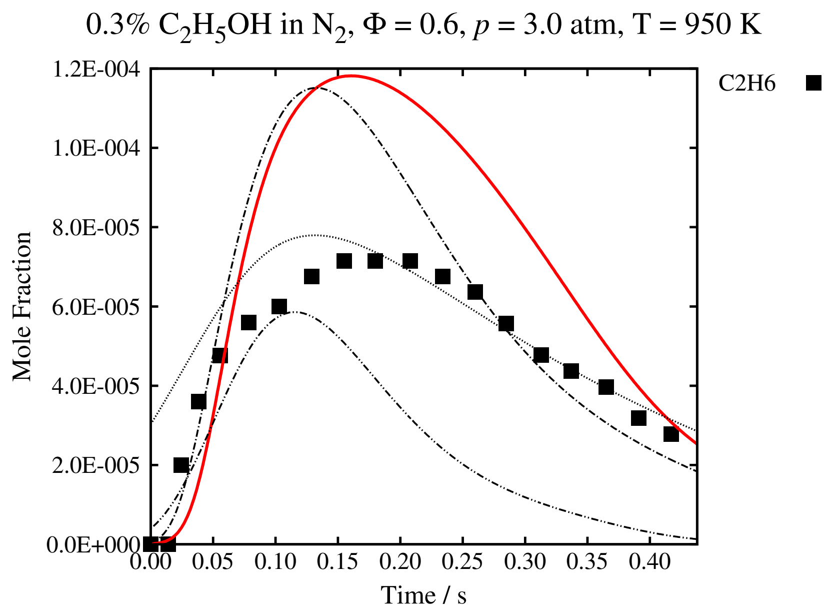
(a)


0.3% C2H5OH in N2, Φ = 0.6, p = 3.0 atm, T = 950 K
O2
Mole Fraction
Time / s
1.5E-002
1.4E-002
1.3E-002
1.2E-002
1.1E-002
1.0E-002
9.0E-003
8.0E-003
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40

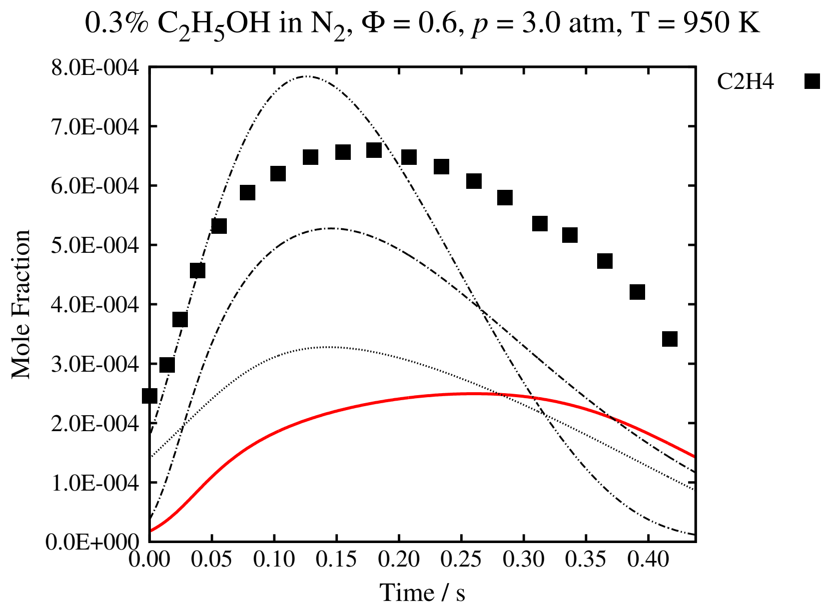
(b)


0.3% C_2H_5OH in N_2, Φ = 0.6, p = 3.0 atm, T = 950 K
CH4
Mole Fraction
Time / s
0.0E+000
1.0E-004
2.0E-004
3.0E-004
4.0E-004
5.0E-004
6.0E-004
7.0E-004
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40

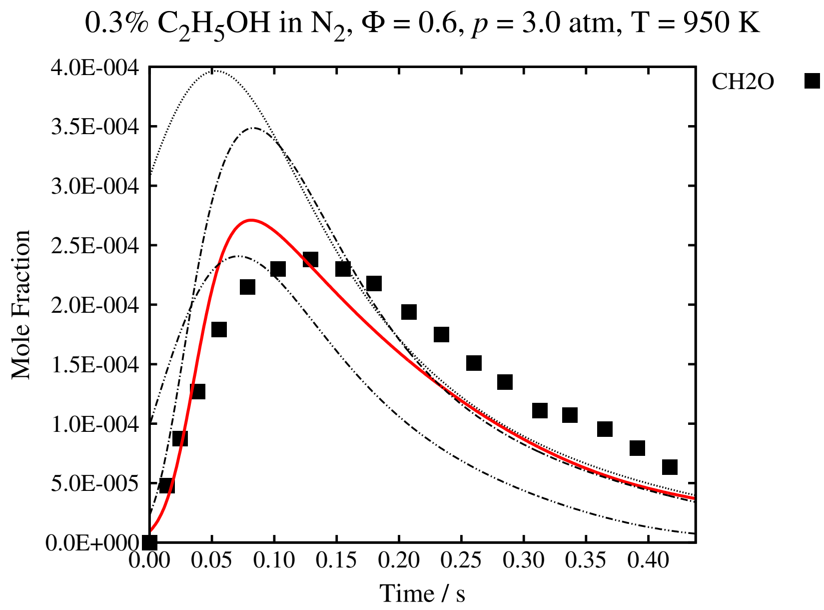
(c)


0.3% C_2H_5OH in N_2, Φ = 0.6, p = 3.0 atm, T = 950 K
C2H6
Mole Fraction
Time / s
0.0E+000
2.0E-005
4.0E-005
6.0E-005
8.0E-005
1.0E-004
1.2E-004
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40

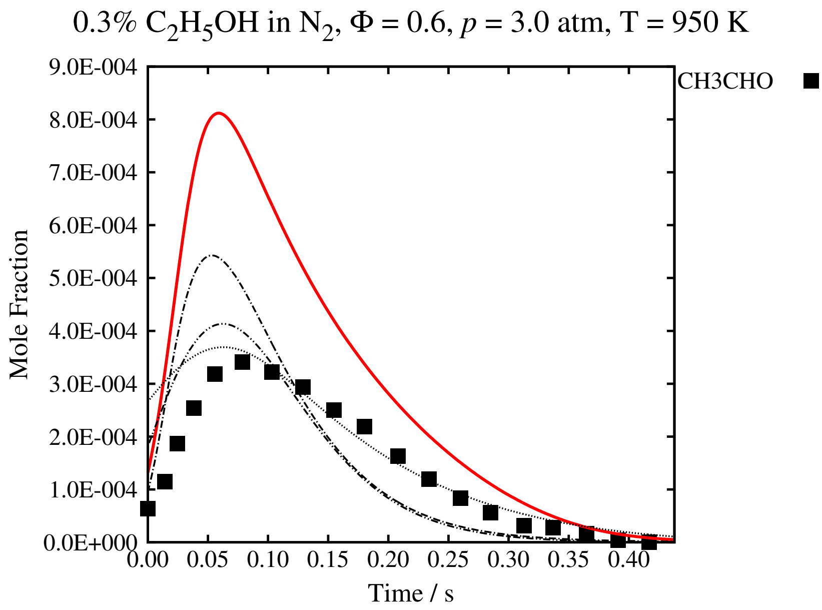
(d)


0.3% C_2H_5OH in N_2, Φ = 0.6, p = 3.0 atm, T = 950 K
C2H4
Mole Fraction
Time / s
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40

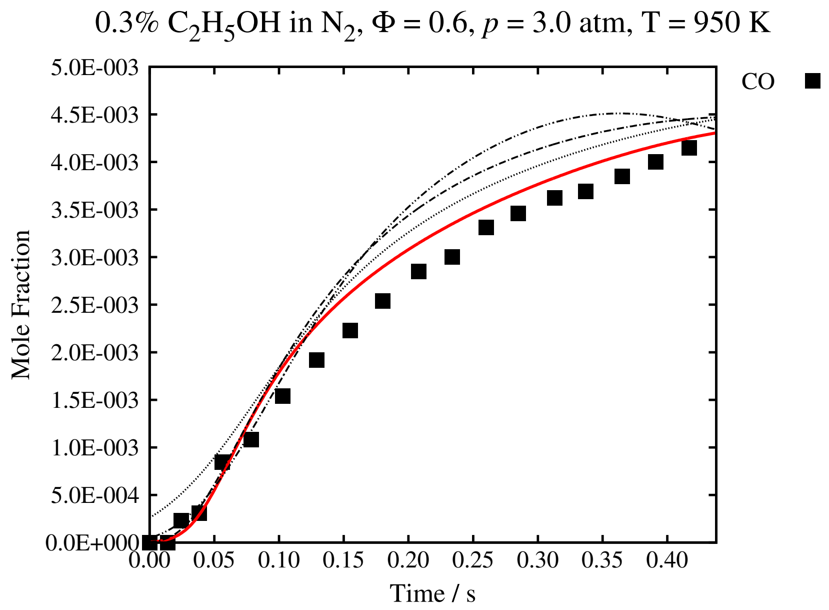
(e)


0.3% C_2H_5OH in N_2, $\Phi = 0.6$, $p = 3.0$ atm, T = 950 K
CH2O
Mole Fraction
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

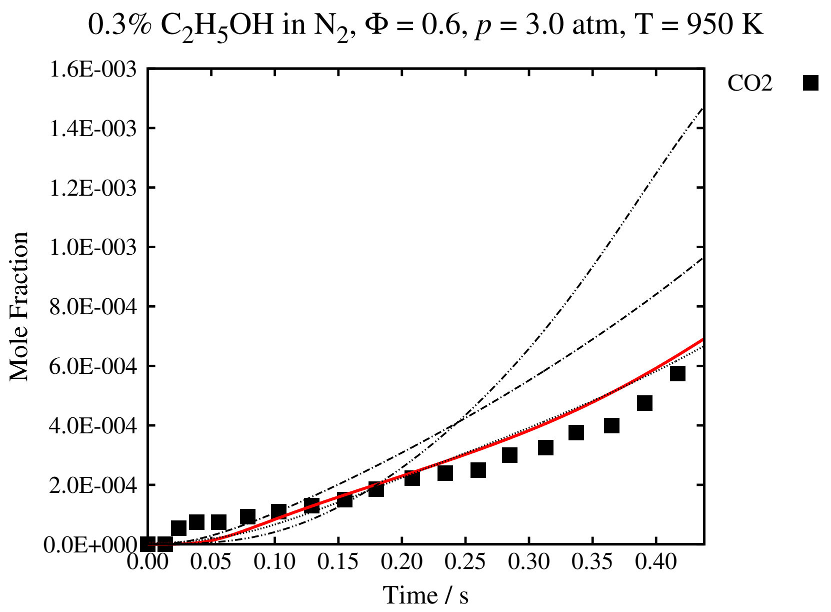
(f)


0.3% C_2H_5OH in N_2, $\Phi = 0.6$, $p = 3.0$ atm, T = 950 K
CH3CHO
Mole Fraction
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

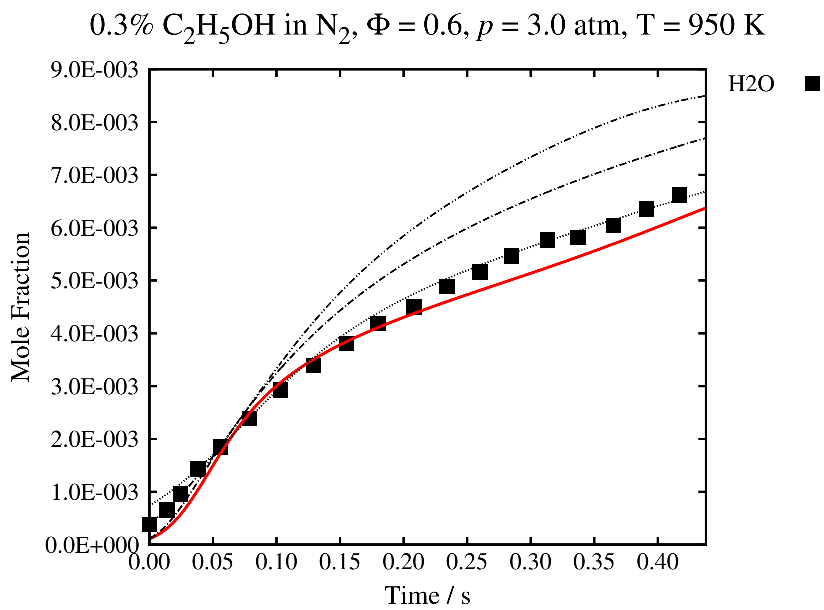
(g)


0.3% C2H5OH in N2, Φ = 0.6, p = 3.0 atm, T = 950 K
CO
Mole Fraction
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
Time / s

(h)

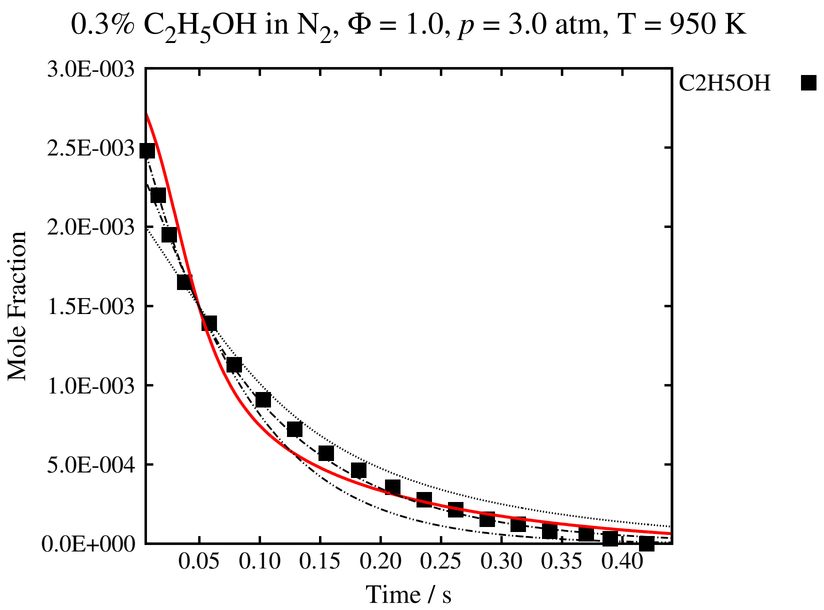

0.3% C2H5OH in N2, Φ = 0.6, p = 3.0 atm, T = 950 K
CO2
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
Time / s

(i)

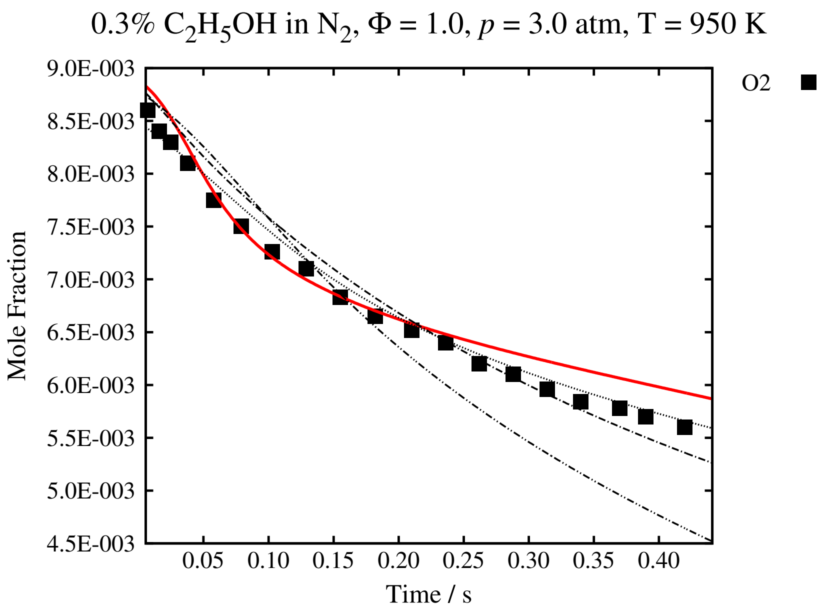


(j)

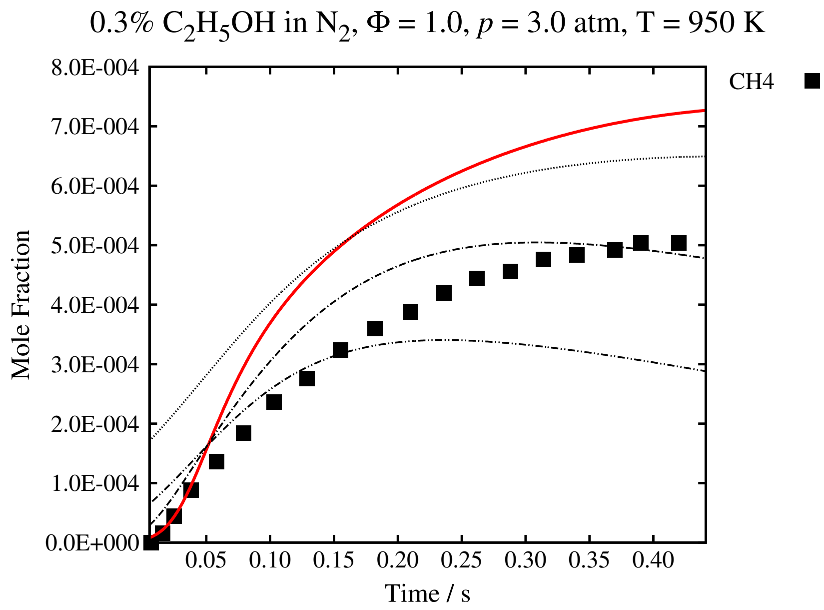
S86 Flow reactor species profiles of ethanol/oxygen/nitrogen mixtures. Symbols are experimental data [56] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.3% C_2H_5OH in N_2, Φ = 1.0, p = 3.0 atm, T = 950 K
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
Mole Fraction
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s
C2H5OH

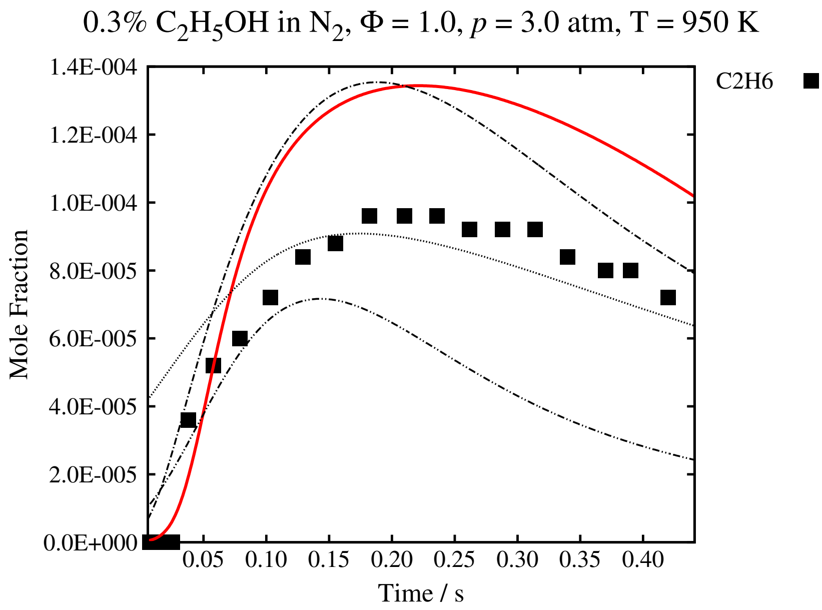
(a)


0.3% C_2H_5OH in N_2, Φ = 1.0, p = 3.0 atm, T = 950 K
9.0E-003
8.5E-003
8.0E-003
7.5E-003
7.0E-003
6.5E-003
6.0E-003
5.5E-003
5.0E-003
4.5E-003
Mole Fraction
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s
O2

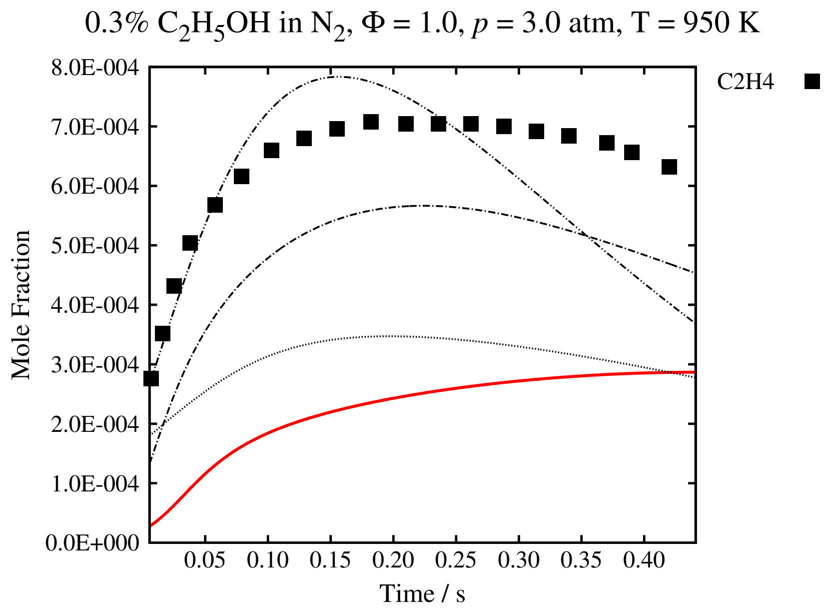
(b)


0.3% C_2H_5OH in N_2, Φ = 1.0, *p* = 3.0 atm, T = 950 K
CH4
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

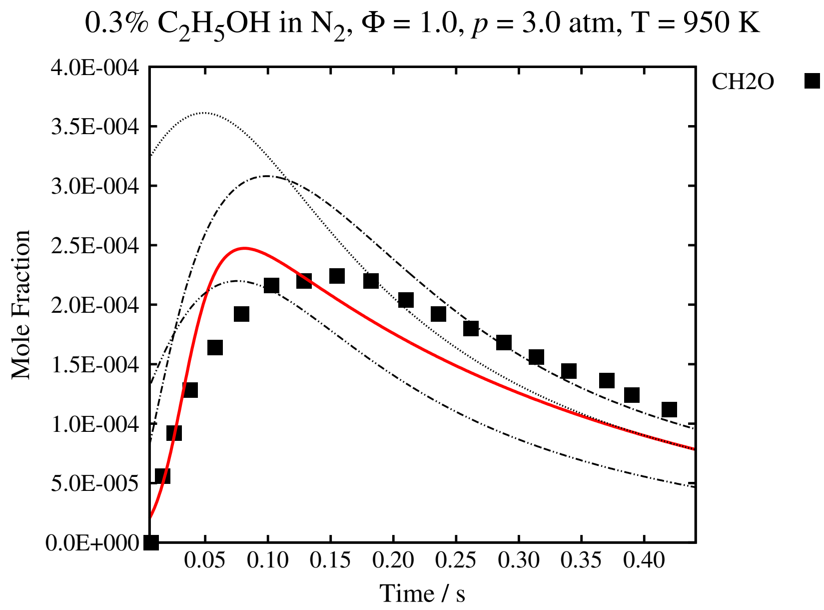
(c)


0.3% C_2H_5OH in N_2, Φ = 1.0, *p* = 3.0 atm, T = 950 K
C2H6
Mole Fraction
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

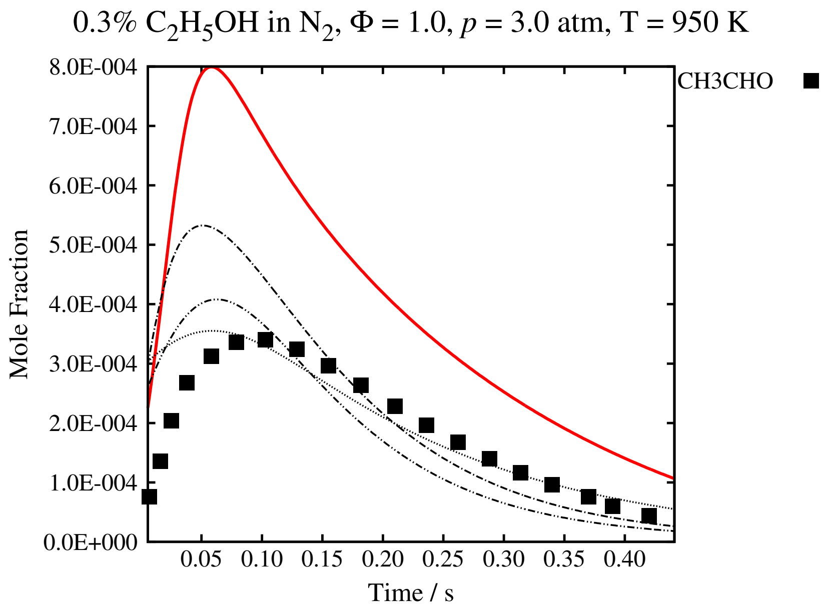
(d)


0.3% C_2H_5OH in N_2, Φ = 1.0, p = 3.0 atm, T = 950 K
C2H4
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
Time / s

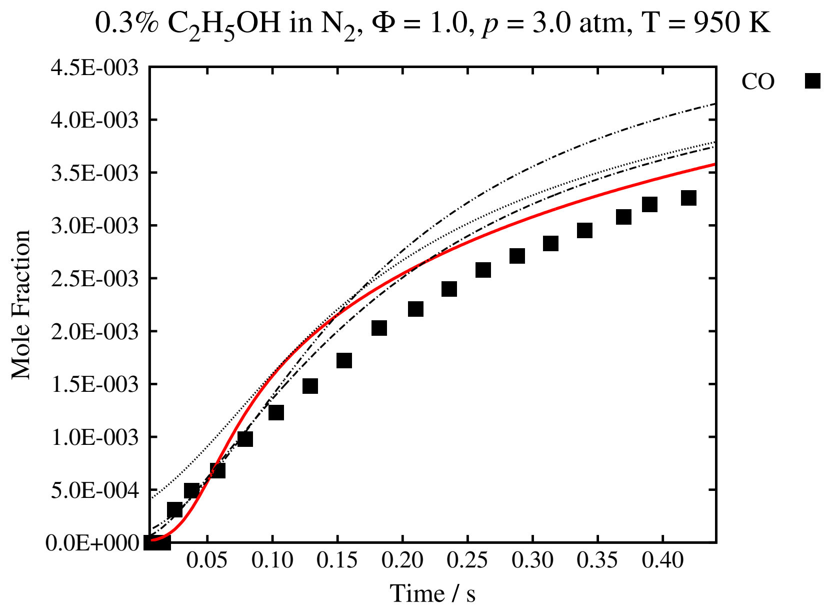
(e)


0.3% C_2H_5OH in N_2, Φ = 1.0, p = 3.0 atm, T = 950 K
CH2O
Mole Fraction
Time / s

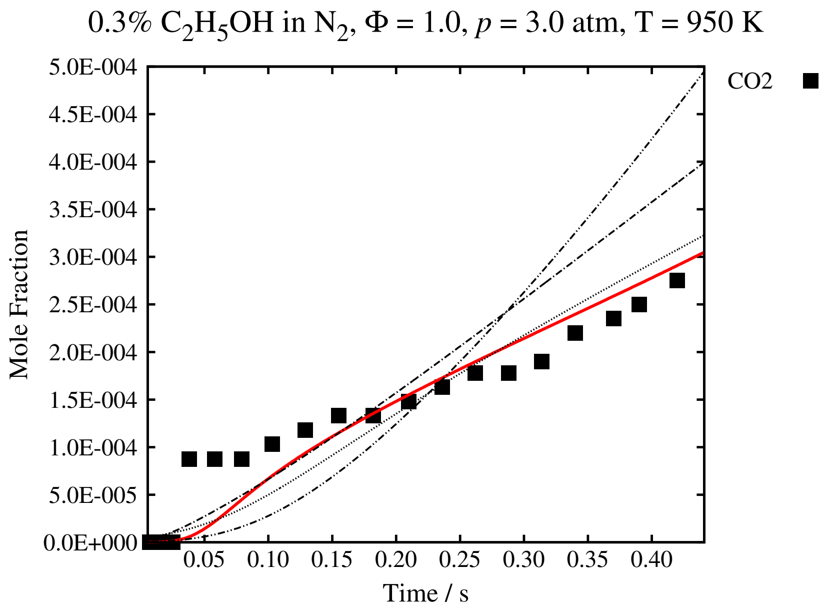
(f)


0.3% C_2H_5OH in N_2, Φ = 1.0, p = 3.0 atm, T = 950 K
CH3CHO
Mole Fraction
Time / s

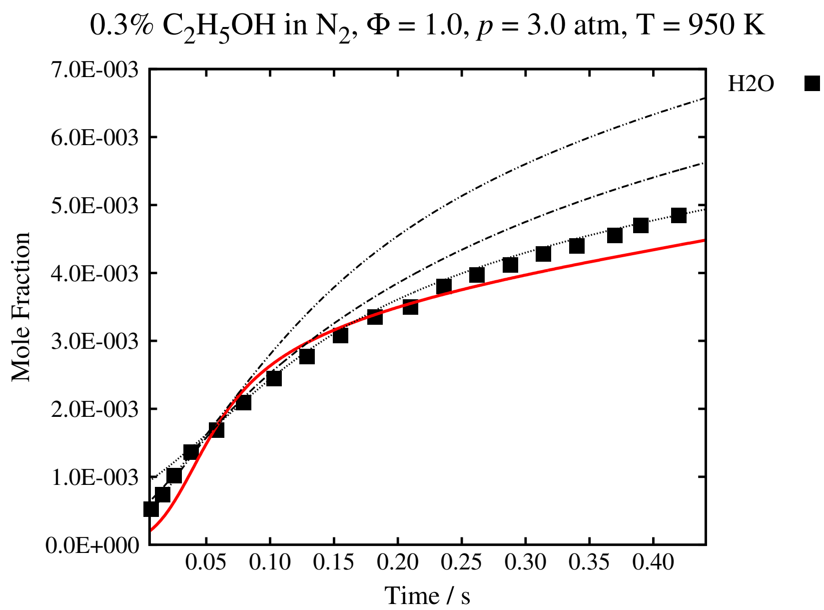
(g)


0.3% C_2H_5OH in N_2, Φ = 1.0, p = 3.0 atm, T = 950 K
CO
Mole Fraction
Time / s
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40

(h)

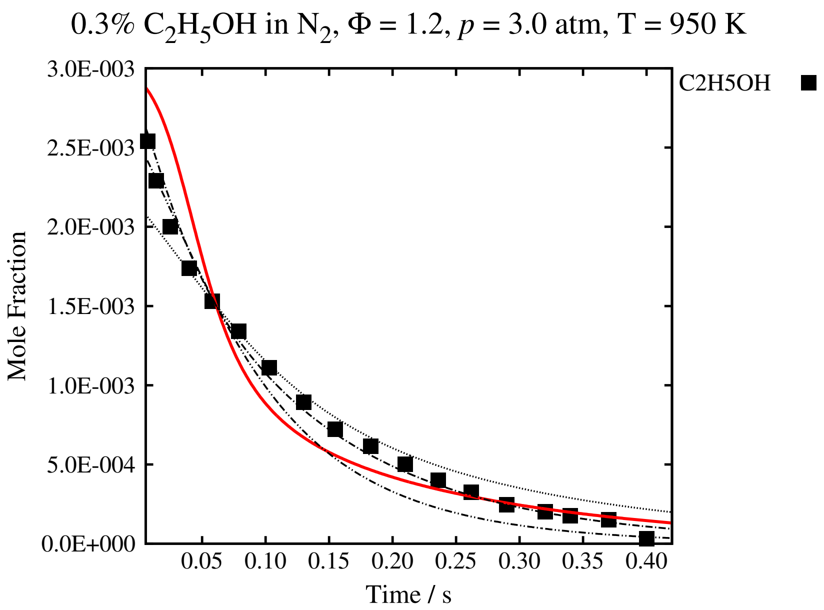

0.3% C_2H_5OH in N_2, Φ = 1.0, p = 3.0 atm, T = 950 K
CO2
Mole Fraction
Time / s
5.0E-004
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40

(i)

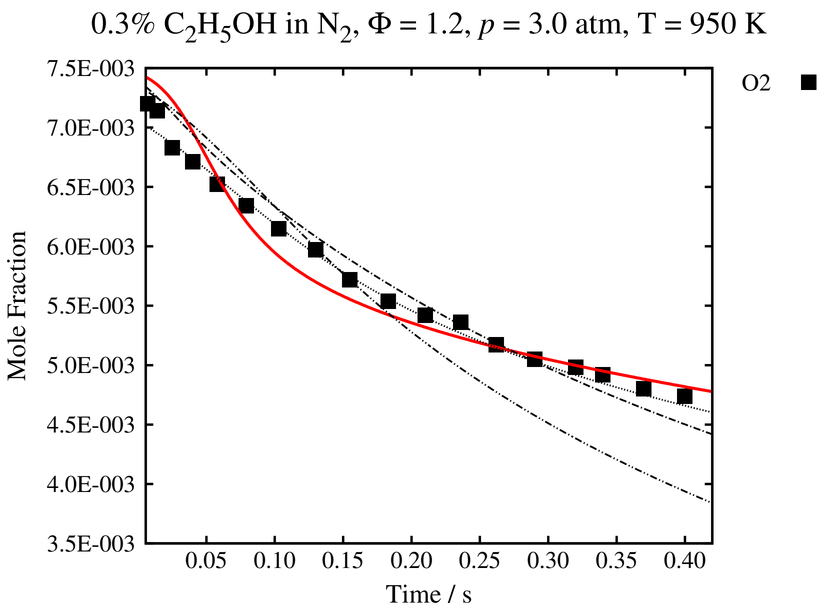


(j)

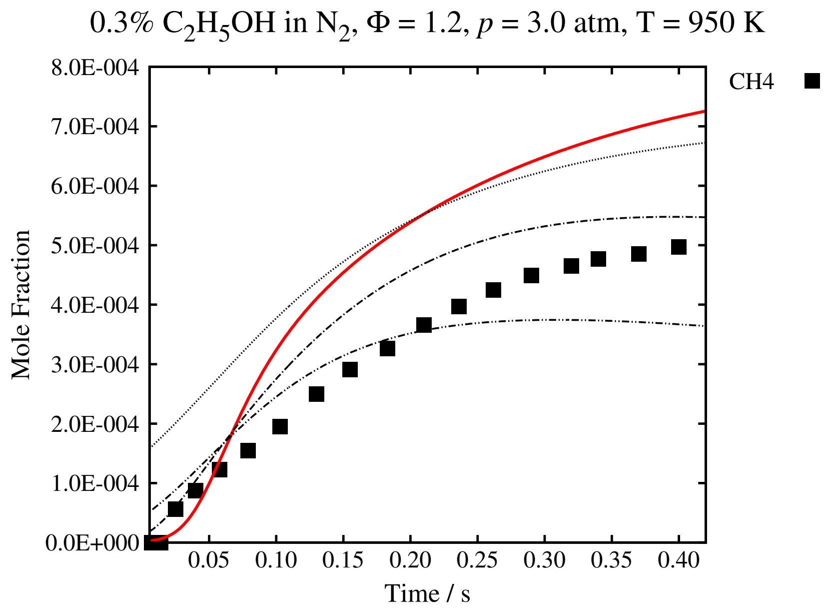
S87 Flow reactor species profiles of ethanol/oxygen/nitrogen mixtures. Symbols are experimental data [56] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.3% C_2H_5OH in N_2, Φ = 1.2, p = 3.0 atm, T = 950 K
C2H5OH
Mole Fraction
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
Time / s

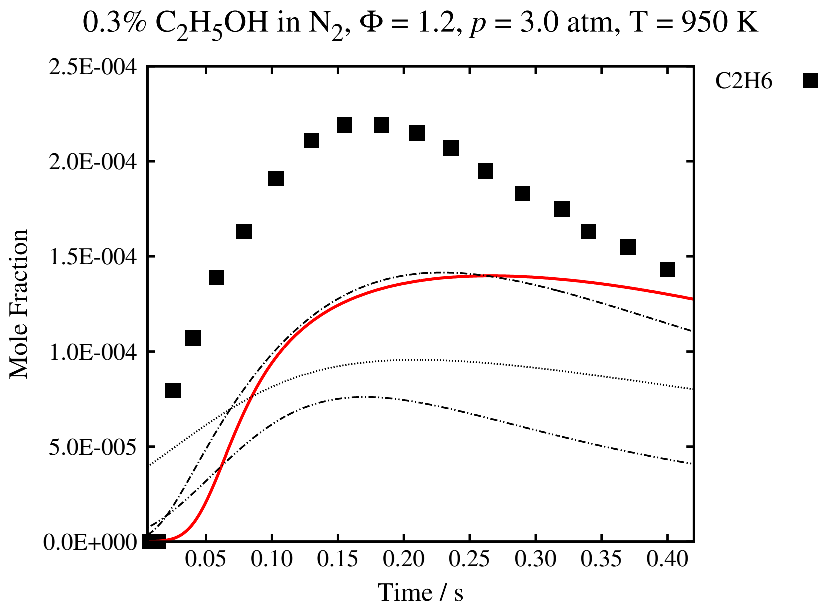
(a)


0.3% C_2H_5OH in N_2, Φ = 1.2, p = 3.0 atm, T = 950 K
O2
Mole Fraction
7.5E-003
7.0E-003
6.5E-003
6.0E-003
5.5E-003
5.0E-003
4.5E-003
4.0E-003
3.5E-003
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
Time / s

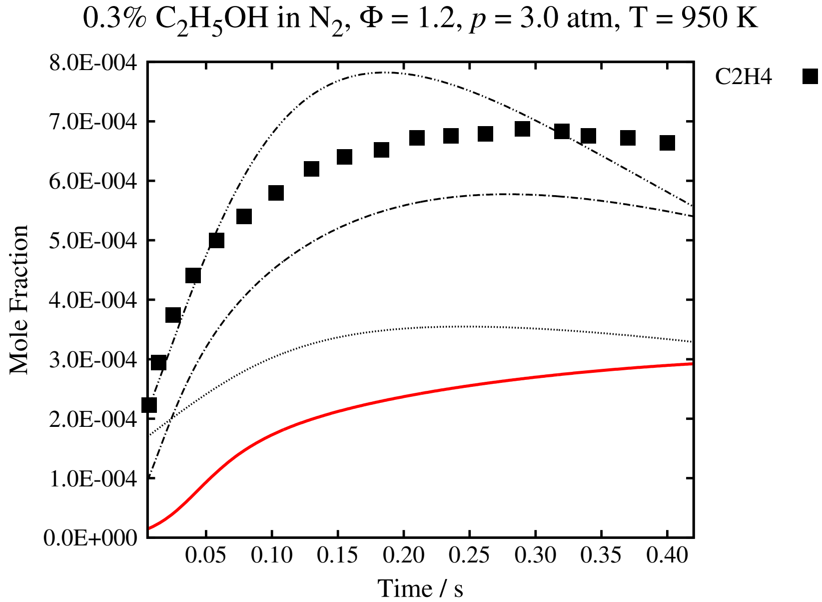
(b)


0.3% C2H5OH in N2, Φ = 1.2, p = 3.0 atm, T = 950 K
CH4
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

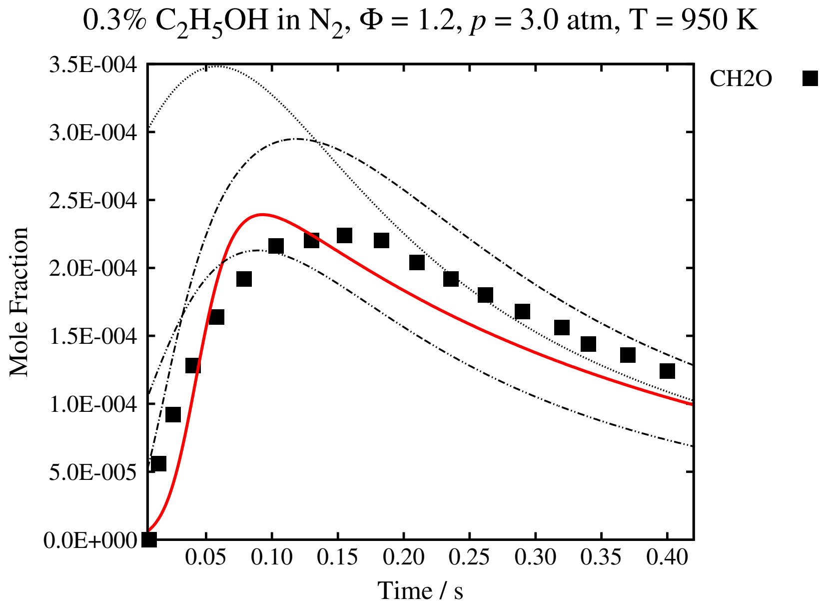
(c)


0.3% C2H5OH in N2, Φ = 1.2, p = 3.0 atm, T = 950 K
C2H6
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

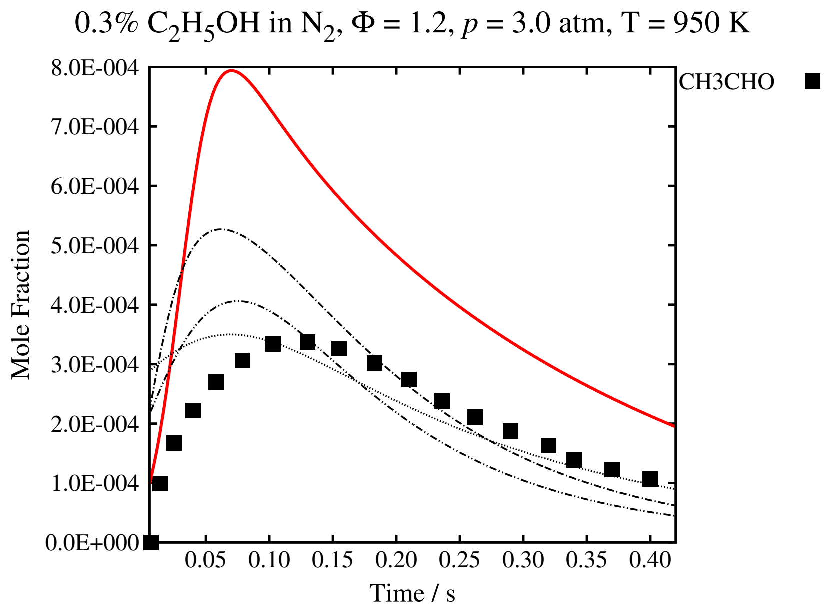
(d)


0.3% C2H5OH in N2, Φ = 1.2, p = 3.0 atm, T = 950 K
C2H4
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
Time / s

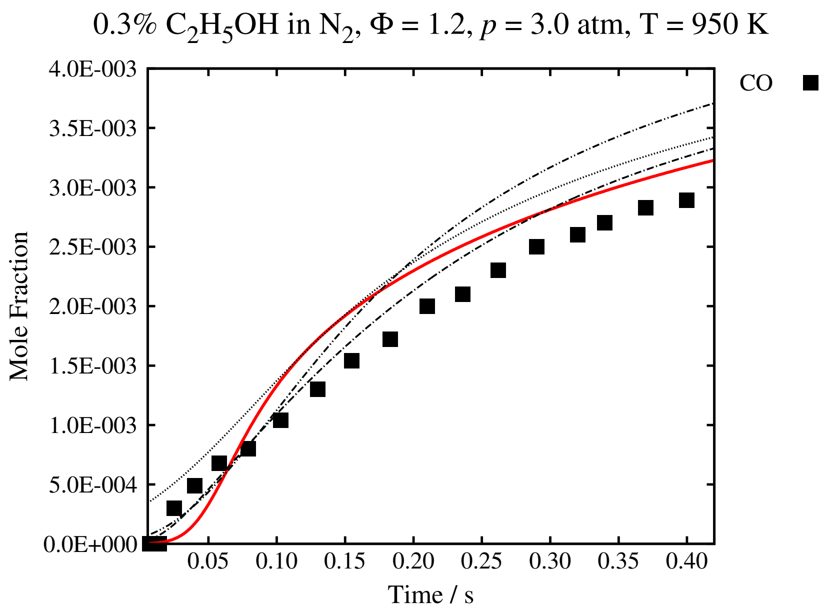
(e)


0.3% C2H5OH in N2, Φ = 1.2, p = 3.0 atm, T = 950 K
CH2O
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
Time / s

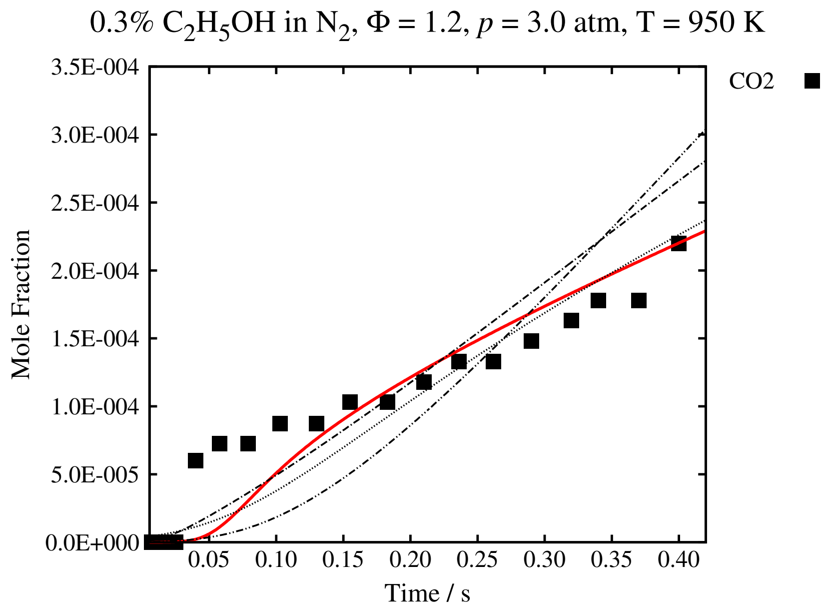
(f)


0.3% C2H5OH in N2, Φ = 1.2, p = 3.0 atm, T = 950 K
CH3CHO
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

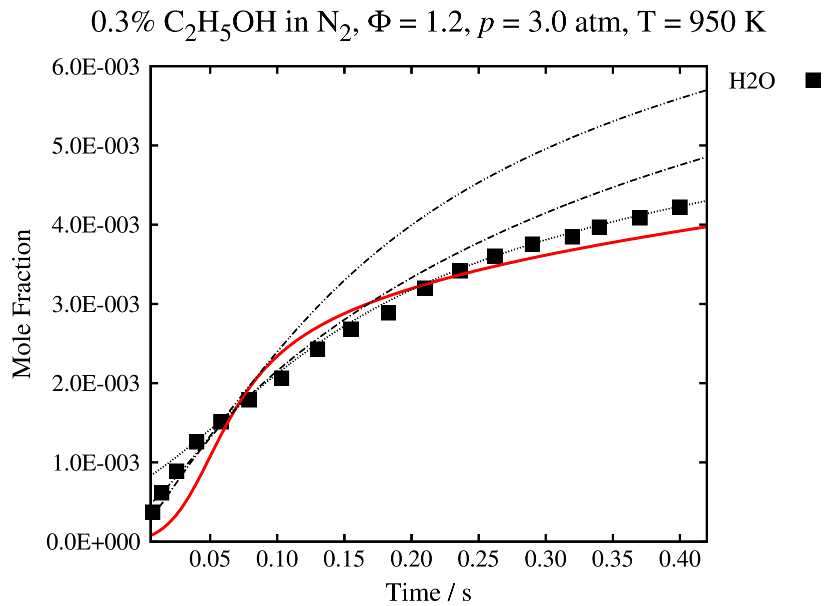
(g)


0.3% C2H5OH in N2, Φ = 1.2, p = 3.0 atm, T = 950 K
CO
Mole Fraction
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40
Time / s

(h)



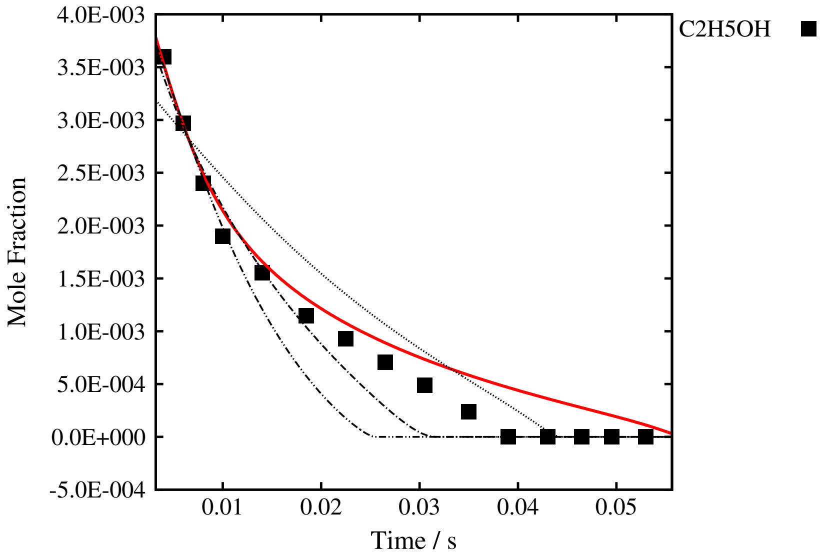
(i)



(j)

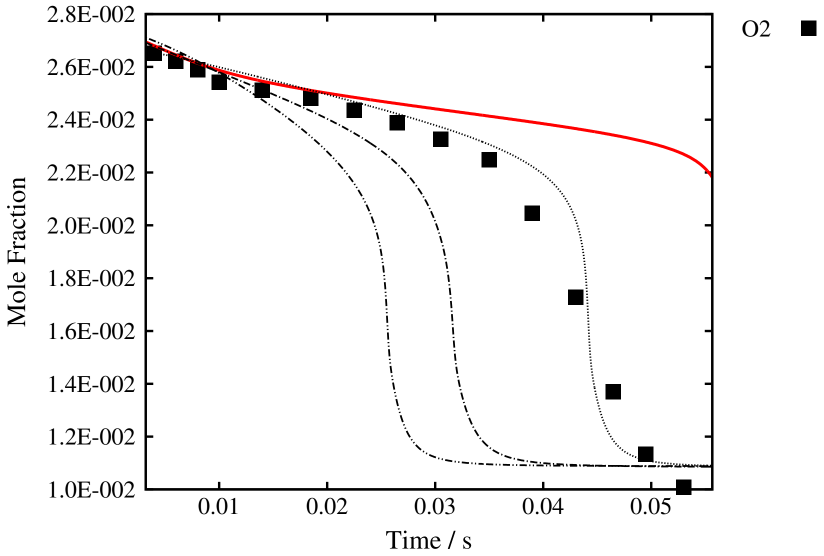
S88 Flow reactor species profiles of ethanol/oxygen/nitrogen mixtures. Symbols are experimental data [56] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

0.565% C_2H_5OH in N_2, Φ = 0.61, p = 1.0 atm, T = 1092 K

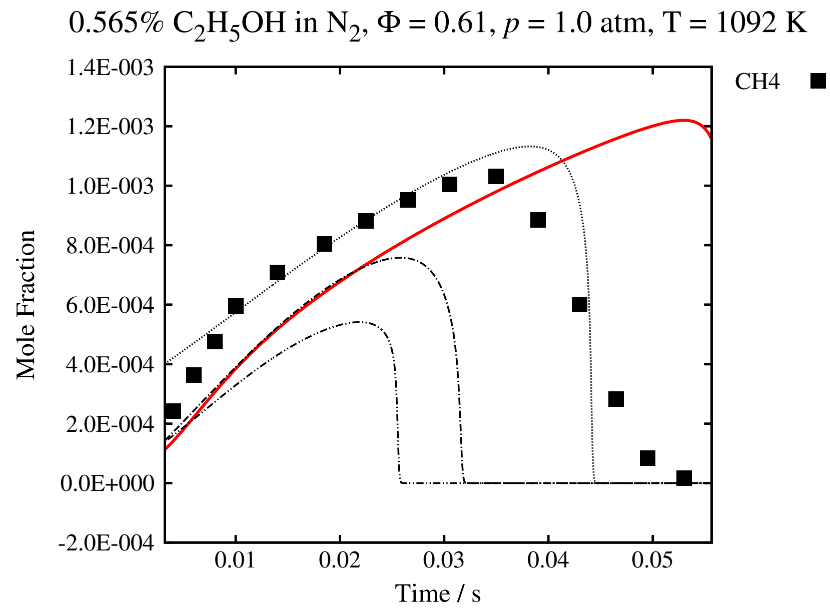


(a)

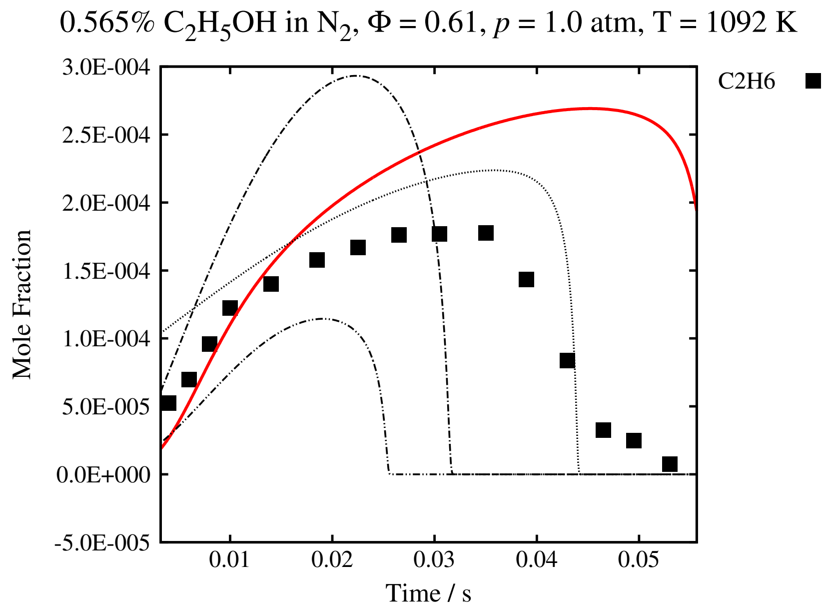
0.565% C_2H_5OH in N_2, Φ = 0.61, p = 1.0 atm, T = 1092 K



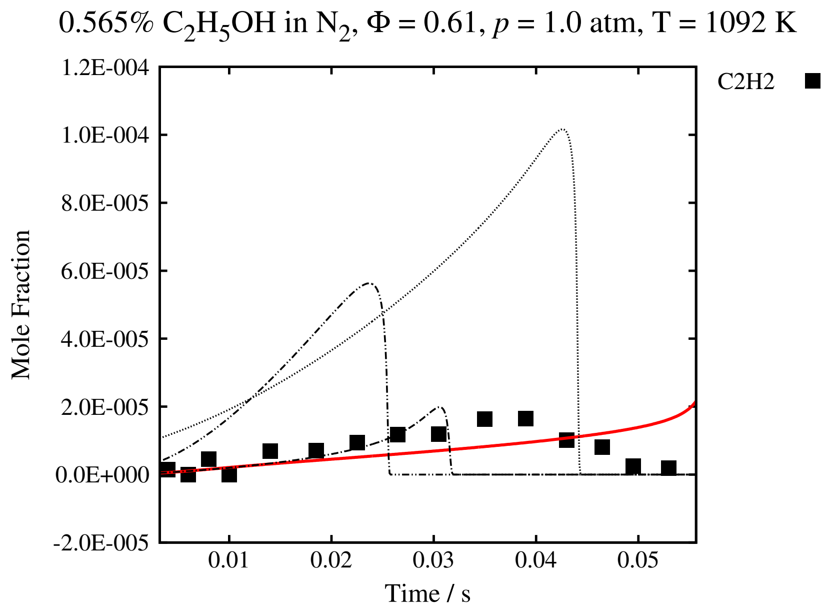
(b)


0.565% C2H5OH in N2, Φ = 0.61, p = 1.0 atm, T = 1092 K
CH4
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
-2.0E-004
Mole Fraction
0.01
0.02
0.03
0.04
0.05
Time / s

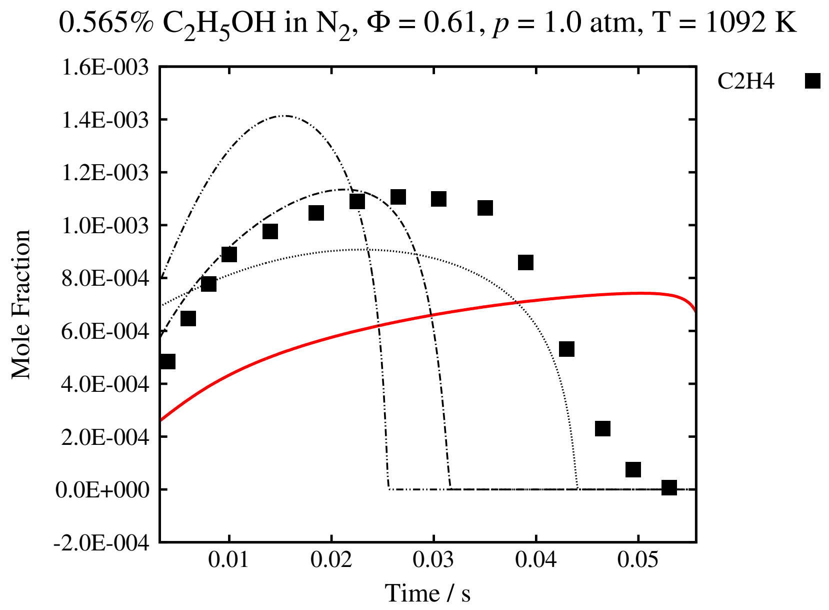
(c)


0.565% C2H5OH in N2, Φ = 0.61, p = 1.0 atm, T = 1092 K
C2H6
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
-5.0E-005
Mole Fraction
0.01
0.02
0.03
0.04
0.05
Time / s

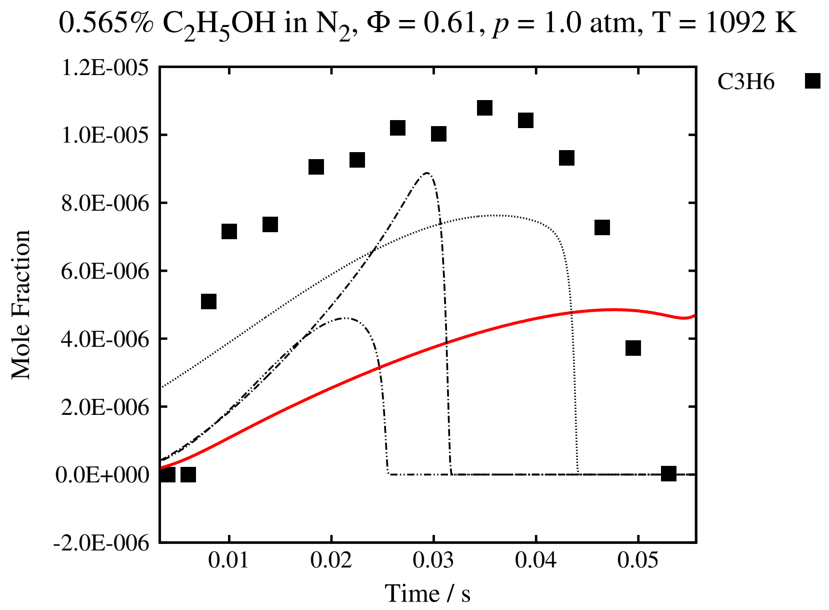
(d)


0.565% C2H5OH in N2, Φ = 0.61, p = 1.0 atm, T = 1092 K
C2H2
Mole Fraction
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
-2.0E-005
0.01
0.02
0.03
0.04
0.05
Time / s

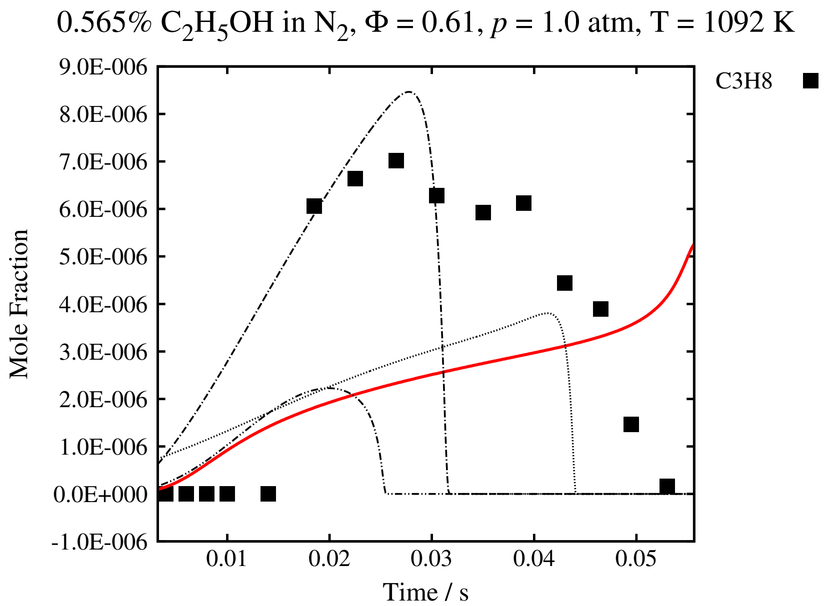
(e)


0.565% C2H5OH in N2, Φ = 0.61, p = 1.0 atm, T = 1092 K
C2H4
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
-2.0E-004
0.01
0.02
0.03
0.04
0.05
Time / s

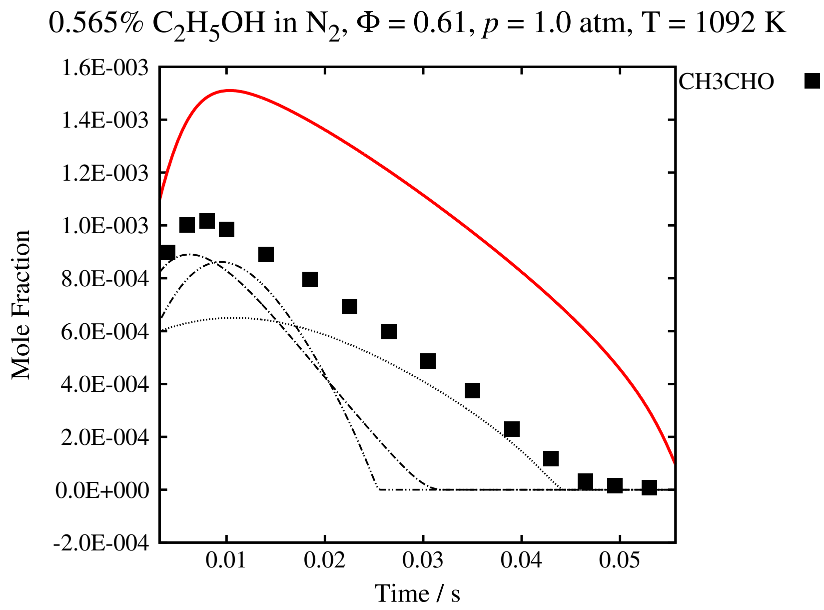
(f)


0.565% C_2H_5OH in N_2, Φ = 0.61, p = 1.0 atm, T = 1092 K
C3H6
Mole Fraction
Time / s
1.2E-005
1.0E-005
8.0E-006
6.0E-006
4.0E-006
2.0E-006
0.0E+000
-2.0E-006
0.01
0.02
0.03
0.04
0.05

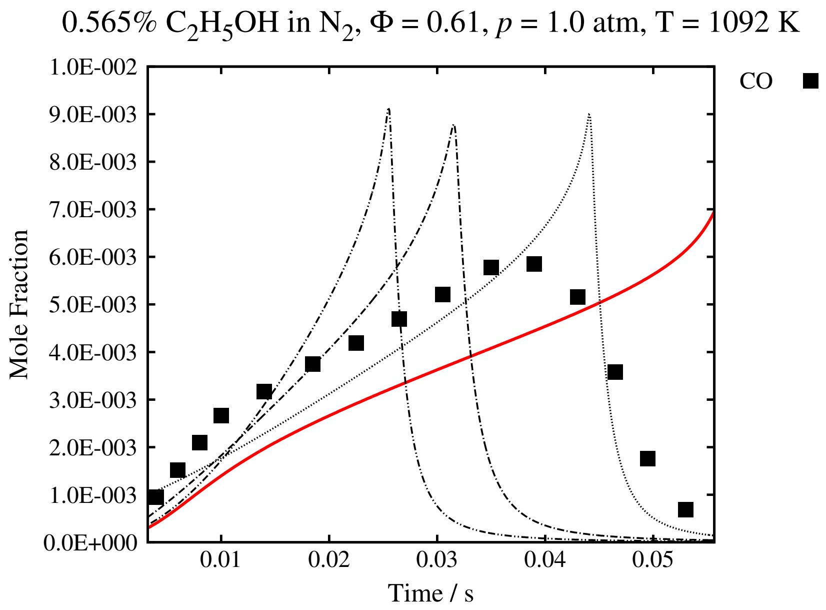
(g)


0.565% C_2H_5OH in N_2, Φ = 0.61, p = 1.0 atm, T = 1092 K
C3H8
Mole Fraction
Time / s
9.0E-006
8.0E-006
7.0E-006
6.0E-006
5.0E-006
4.0E-006
3.0E-006
2.0E-006
1.0E-006
0.0E+000
-1.0E-006
0.01
0.02
0.03
0.04
0.05

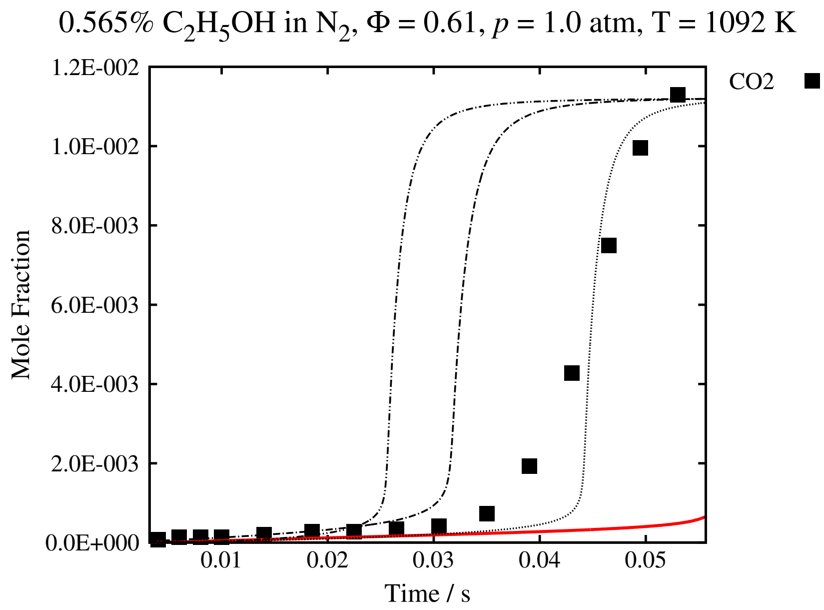
(h)


0.565% C2H5OH in N2, Φ = 0.61, p = 1.0 atm, T = 1092 K
CH3CHO
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
-2.0E-004
0.01
0.02
0.03
0.04
0.05
Time / s

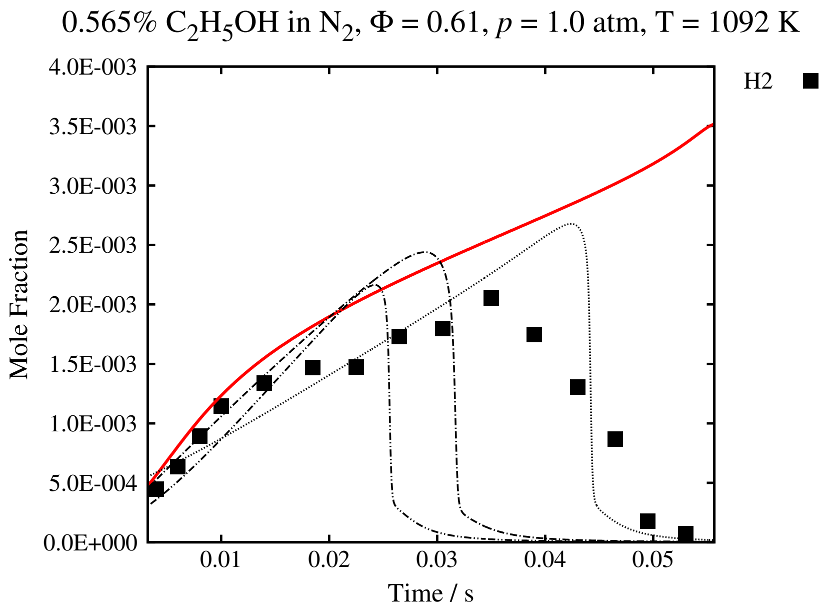
(i)


0.565% C2H5OH in N2, Φ = 0.61, p = 1.0 atm, T = 1092 K
CO
Mole Fraction
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05
Time / s

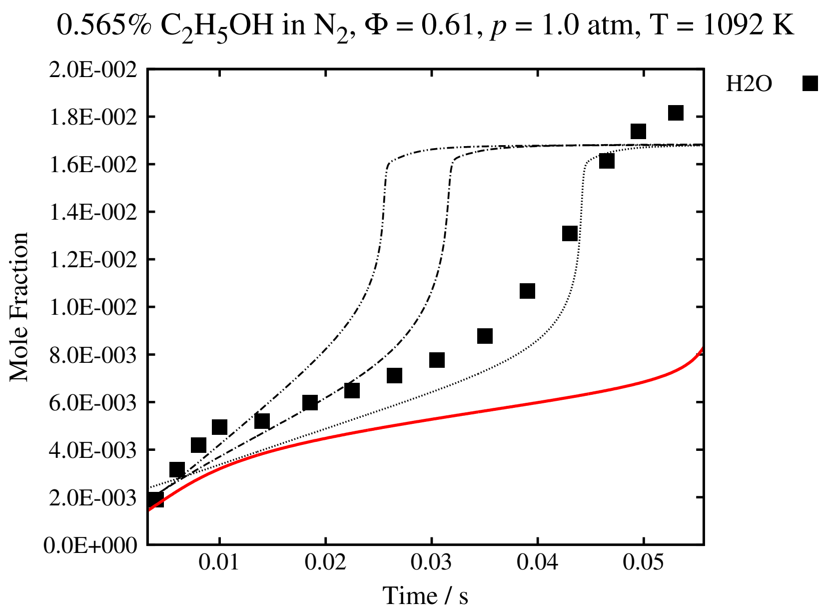
(j)


0.565% C_2H_5OH in N_2, $\Phi = 0.61$, $p = 1.0$ atm, T = 1092 K
CO2
Mole Fraction
Time / s
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05

(k)

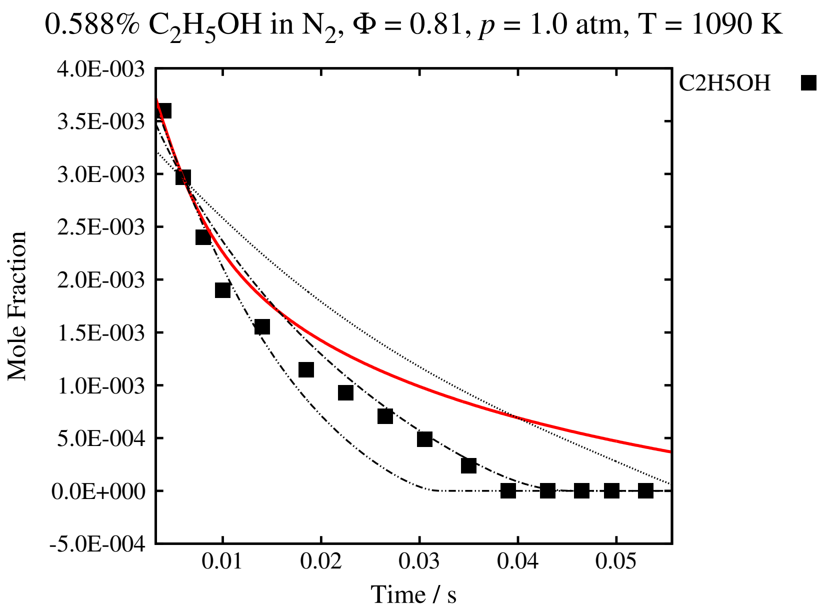

0.565% C_2H_5OH in N_2, $\Phi = 0.61$, $p = 1.0$ atm, T = 1092 K
H2
Mole Fraction
Time / s
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05

(l)

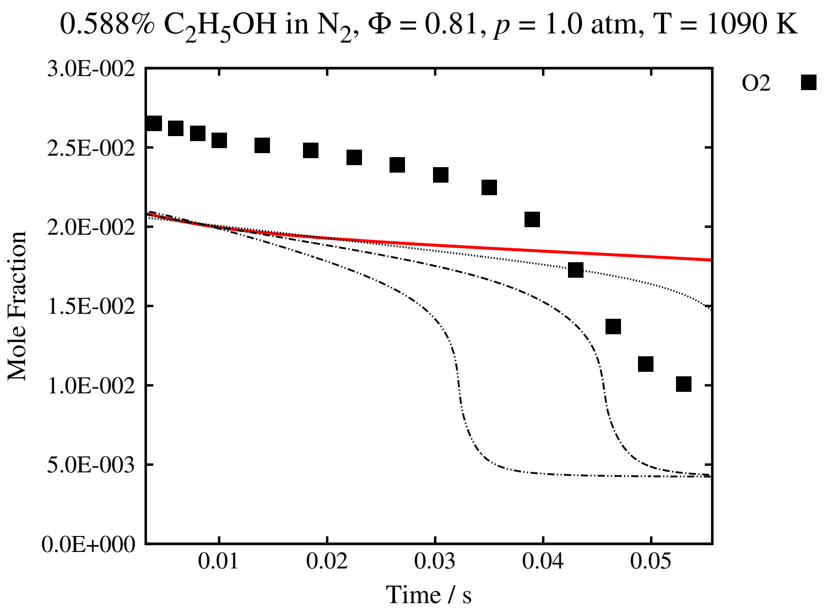


(m)

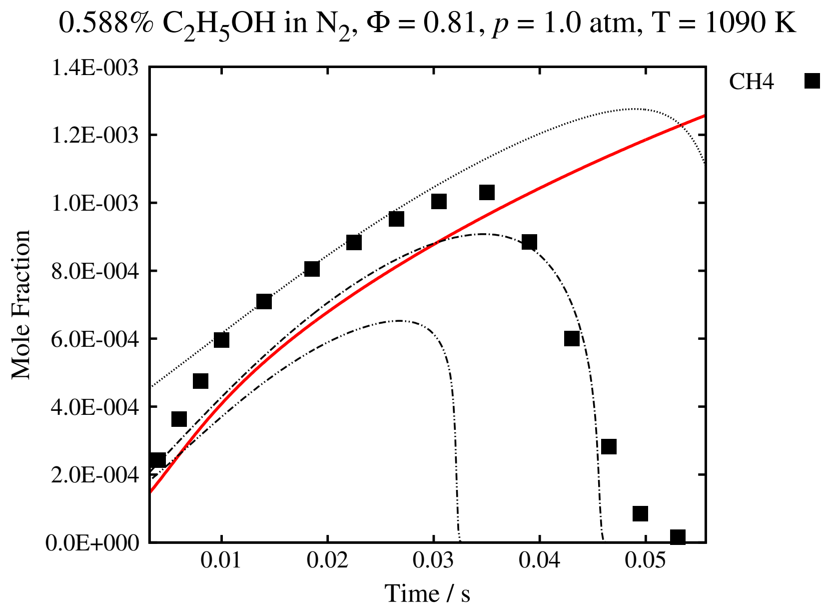
S89 Flow reactor species profiles of ethanol/oxygen/nitrogen mixtures. Symbols are experimental data [57] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.588% C2H5OH in N2, Φ = 0.81, p = 1.0 atm, T = 1090 K
C2H5OH
Mole Fraction
Time / s
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
-5.0E-004
0.01
0.02
0.03
0.04
0.05

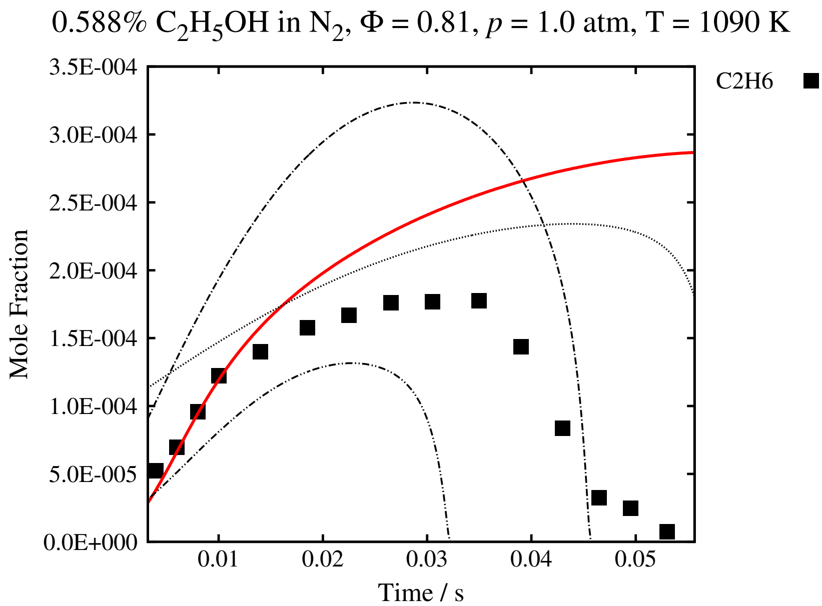
(a)


0.588% C2H5OH in N2, Φ = 0.81, p = 1.0 atm, T = 1090 K
O2
Mole Fraction
Time / s
3.0E-002
2.5E-002
2.0E-002
1.5E-002
1.0E-002
5.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05

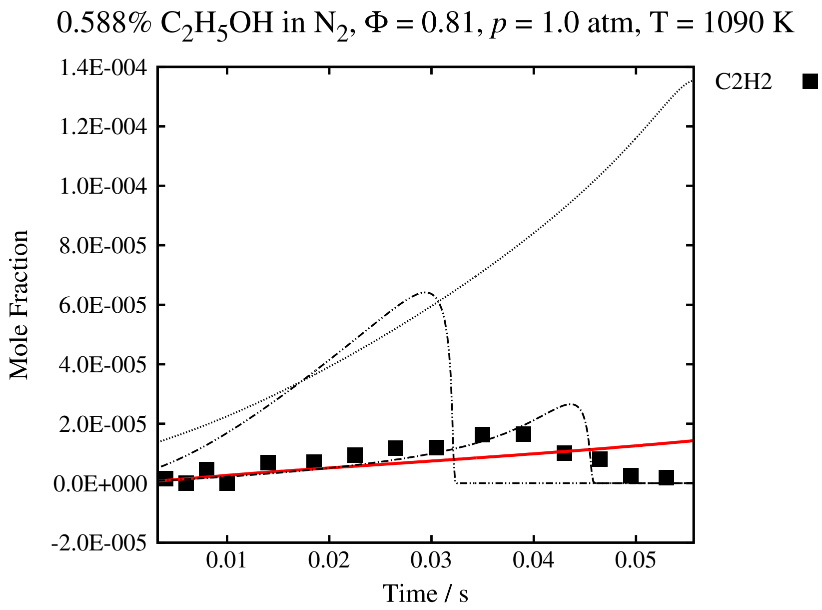
(b)


0.588% C2H5OH in N2, Φ = 0.81, p = 1.0 atm, T = 1090 K
CH4
Mole Fraction
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05
Time / s

(c)

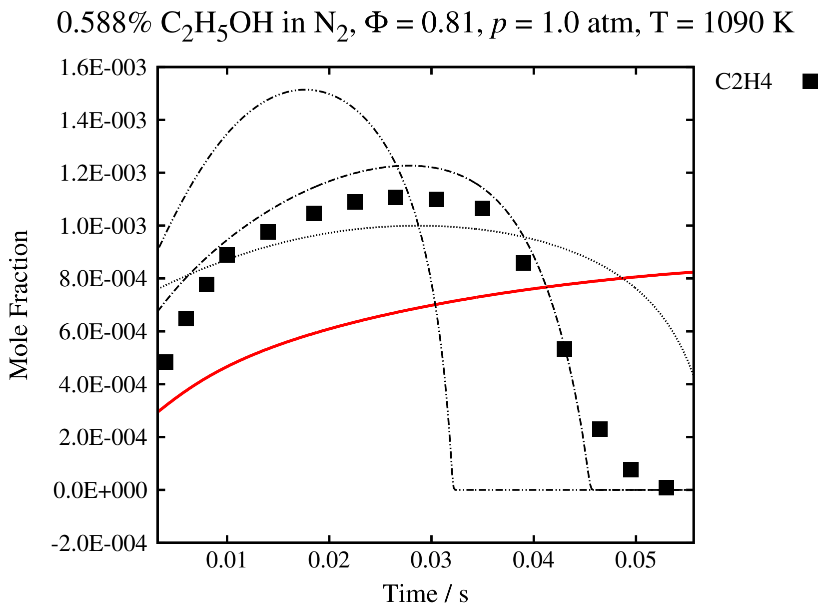

0.588% C2H5OH in N2, Φ = 0.81, p = 1.0 atm, T = 1090 K
C2H6
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.01
0.02
0.03
0.04
0.05
Time / s

(d)



0.588% C_2H_5OH in N_2, Φ = 0.81, *p* = 1.0 atm, T = 1090 K
C2H2
Mole Fraction
Time / s
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
-2.0E-005
0.01
0.02
0.03
0.04
0.05

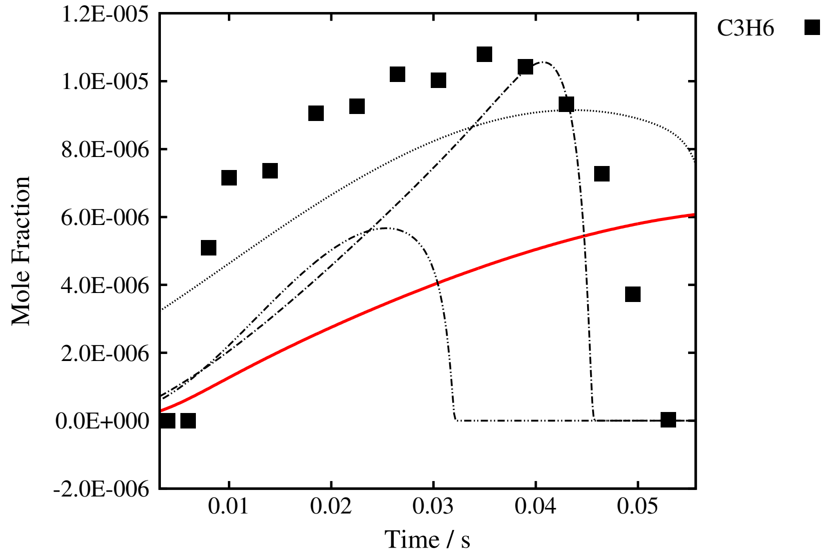
(e)



0.588% C_2H_5OH in N_2, Φ = 0.81, *p* = 1.0 atm, T = 1090 K
C2H4
Mole Fraction
Time / s
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
-2.0E-004
0.01
0.02
0.03
0.04
0.05

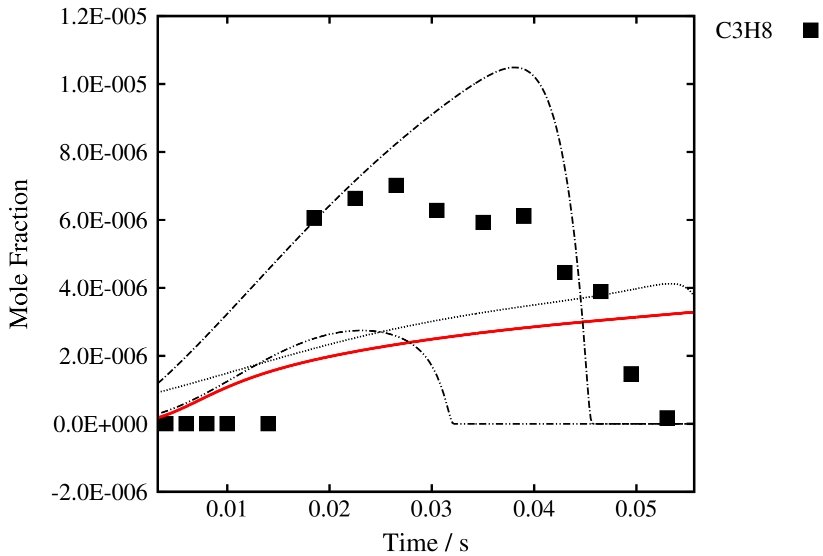
(f)

0.588% C_2H_5OH in N_2, Φ = 0.81, p = 1.0 atm, T = 1090 K

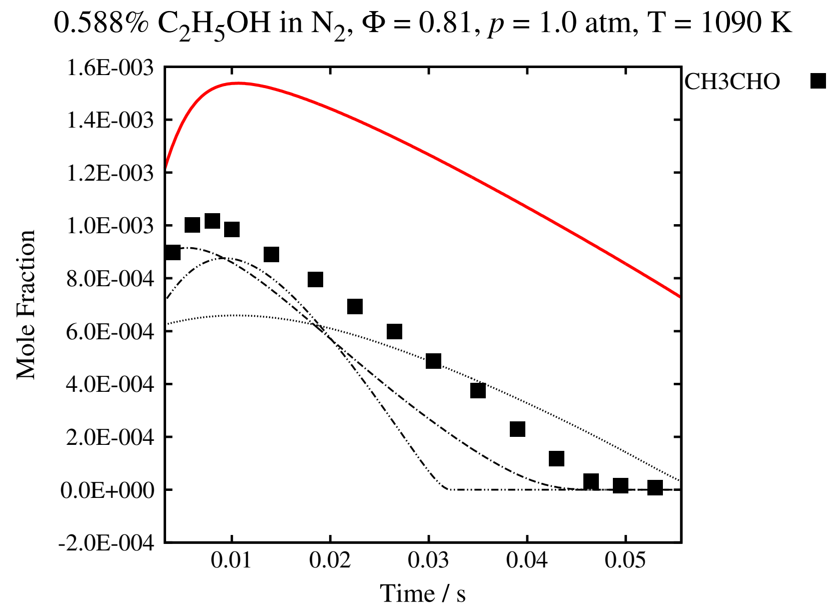


(g)

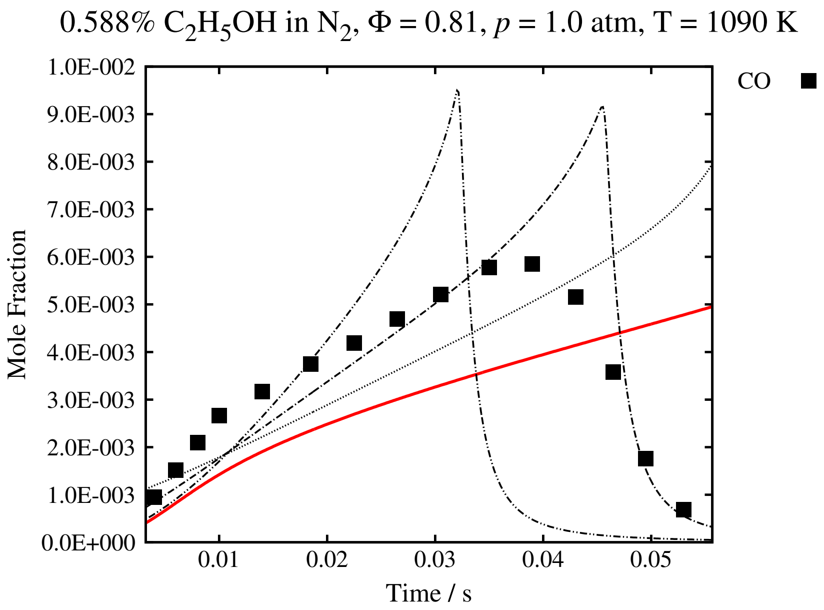
0.588% C_2H_5OH in N_2, Φ = 0.81, p = 1.0 atm, T = 1090 K



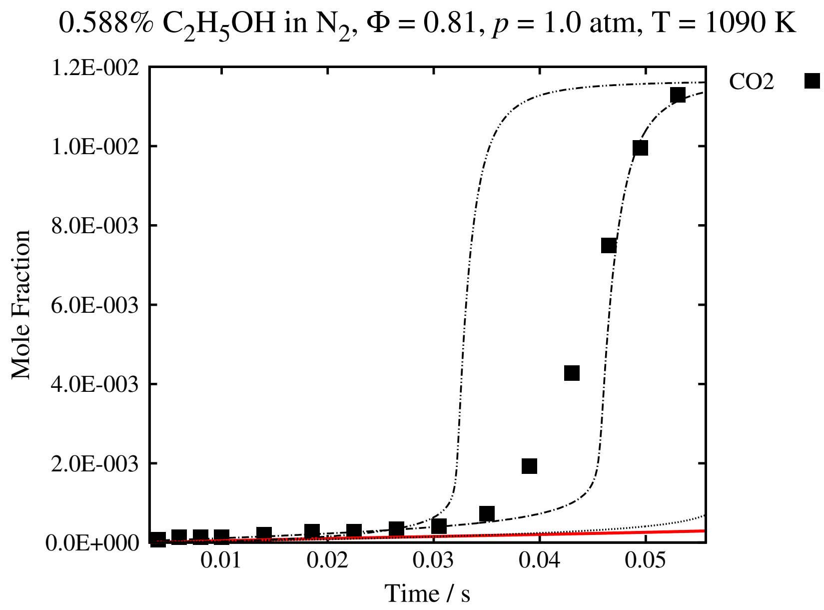
(h)


0.588% C_2H_5OH in N_2, Φ = 0.81, p = 1.0 atm, T = 1090 K
CH3CHO
Mole Fraction
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
-2.0E-004
0.01
0.02
0.03
0.04
0.05
Time / s

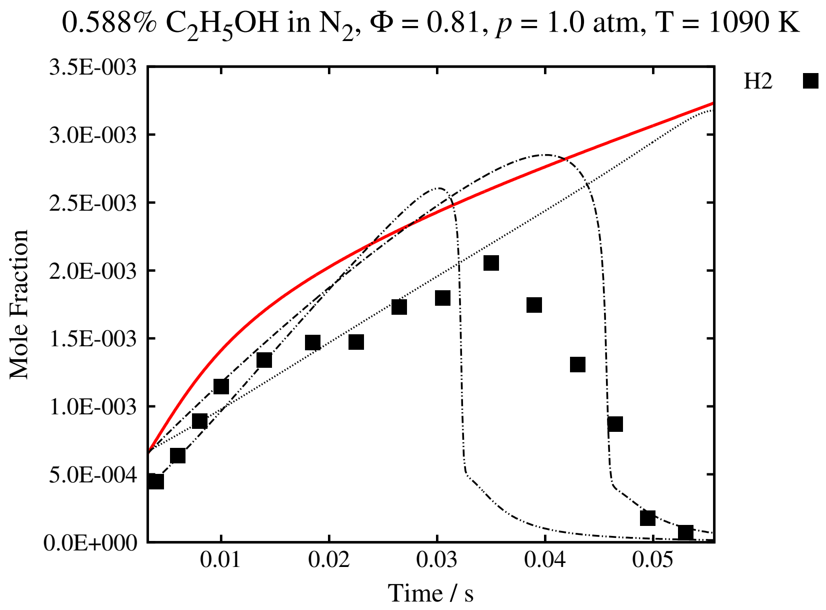
(i)


0.588% C_2H_5OH in N_2, Φ = 0.81, p = 1.0 atm, T = 1090 K
CO
Mole Fraction
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05
Time / s

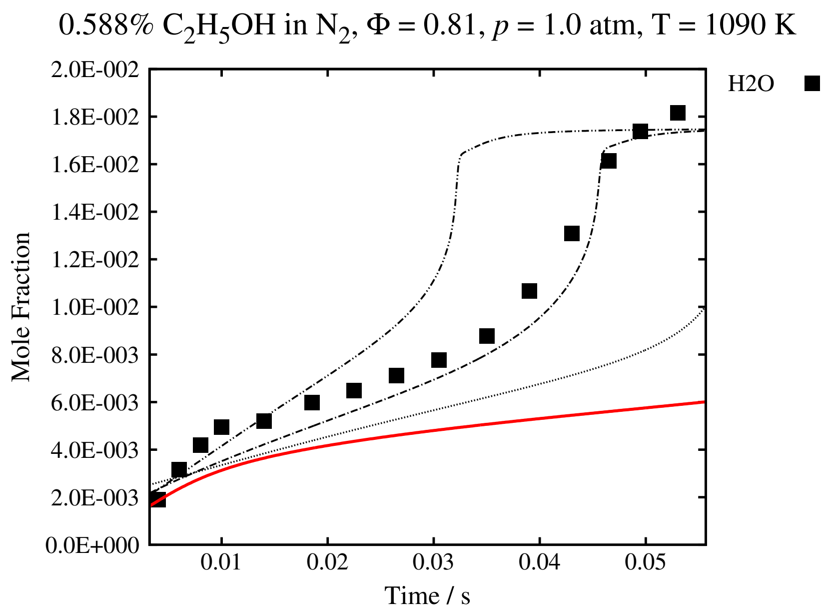
(j)


0.588% C2H5OH in N2, Φ = 0.81, p = 1.0 atm, T = 1090 K
Mole Fraction
Time / s
CO2
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
0.01
0.02
0.03
0.04
0.05

(k)

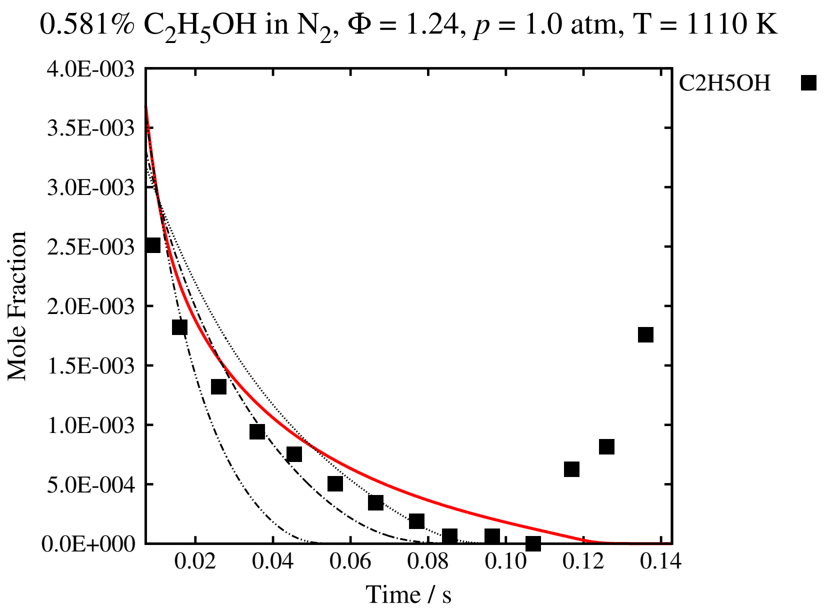

0.588% C2H5OH in N2, Φ = 0.81, p = 1.0 atm, T = 1090 K
Mole Fraction
Time / s
H2
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.01
0.02
0.03
0.04
0.05

(l)

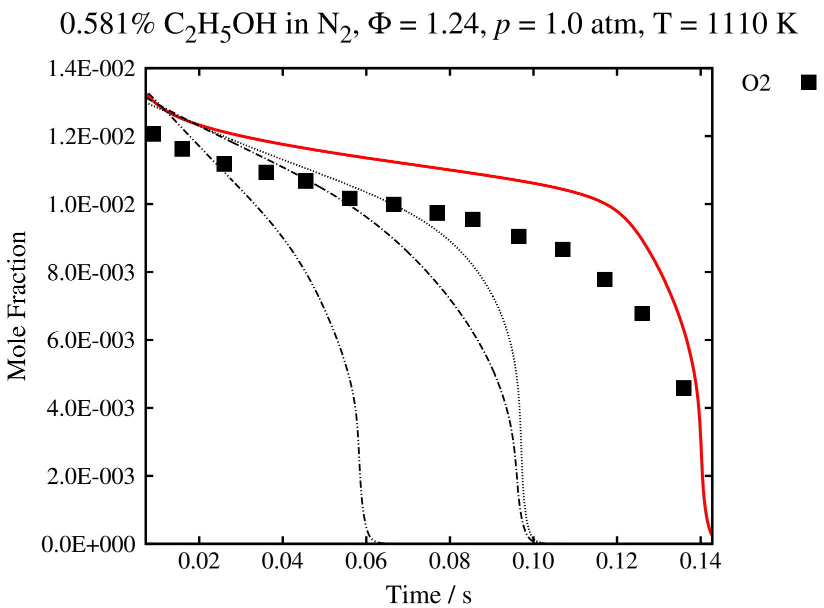


(m)

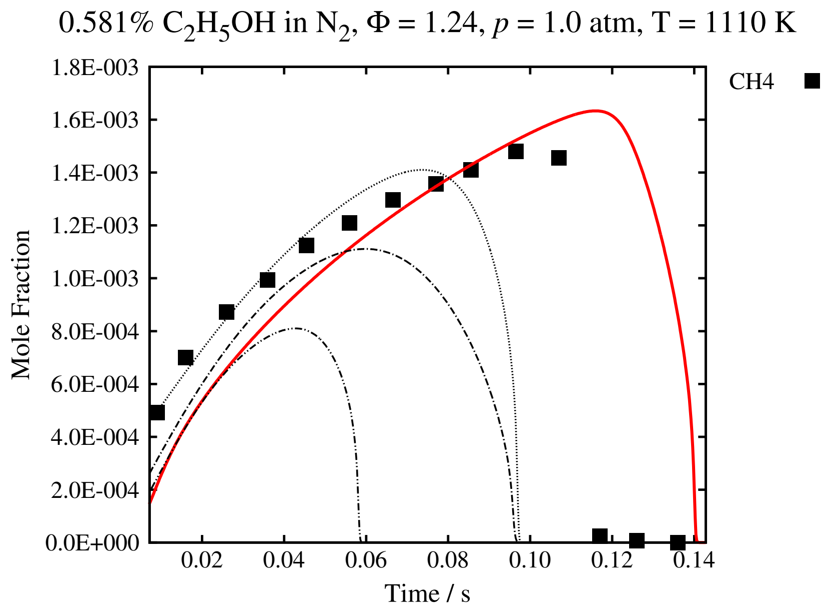
S90 Flow reactor species profiles of ethanol/oxygen/nitrogen mixtures. Symbols are experimental data [57] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.581% C2H5OH in N2, Φ = 1.24, p = 1.0 atm, T = 1110 K
C2H5OH
Mole Fraction
Time / s

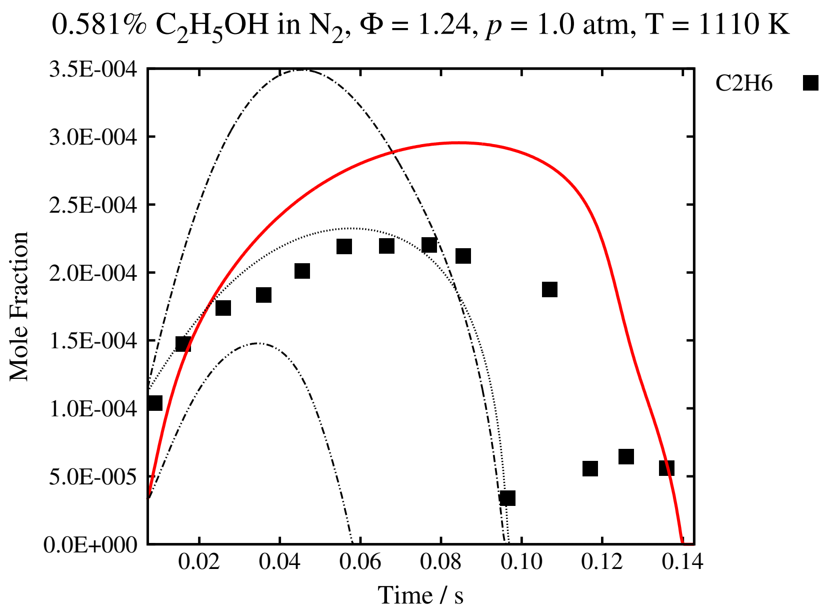
(a)


0.581% C2H5OH in N2, Φ = 1.24, p = 1.0 atm, T = 1110 K
O2
Mole Fraction
Time / s

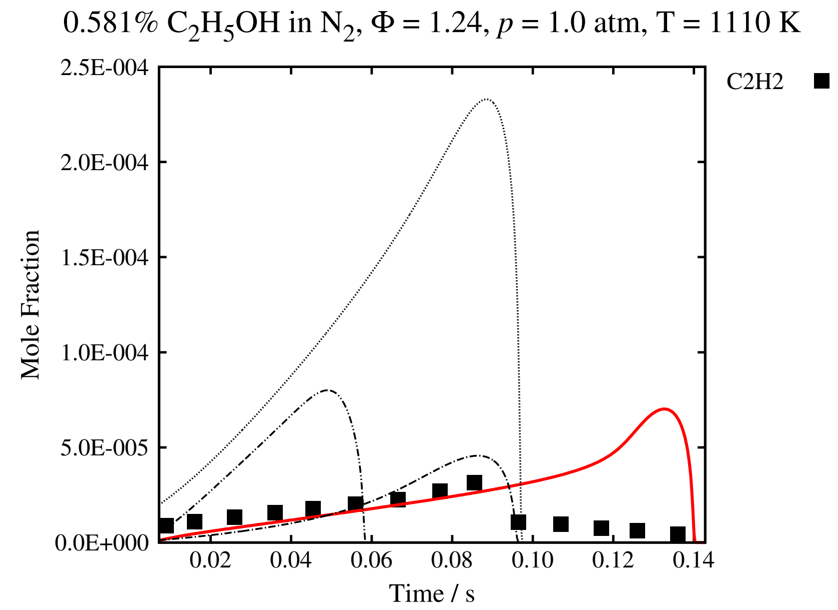
(b)


0.581% C2H5OH in N2, Φ = 1.24, p = 1.0 atm, T = 1110 K
CH4
Mole Fraction
1.8E-003
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

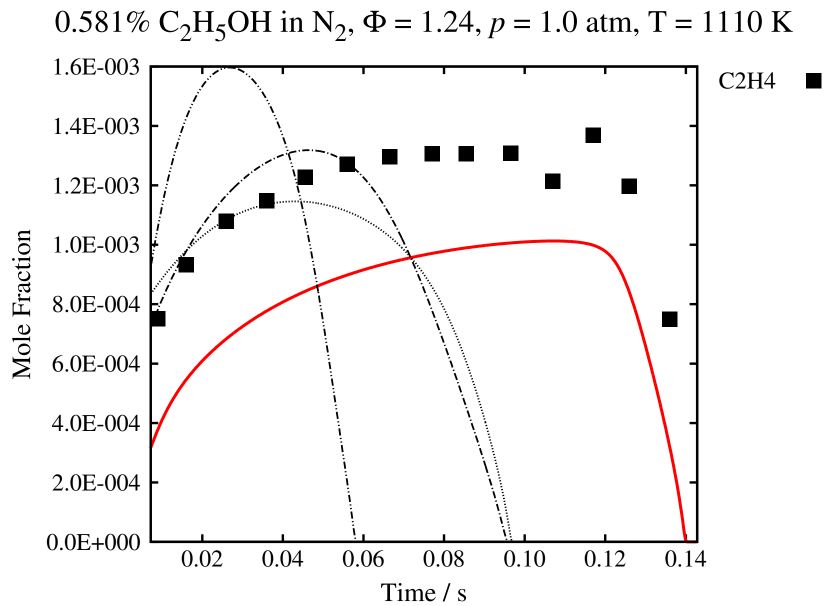
(c)


0.581% C2H5OH in N2, Φ = 1.24, p = 1.0 atm, T = 1110 K
C2H6
Mole Fraction
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

(d)

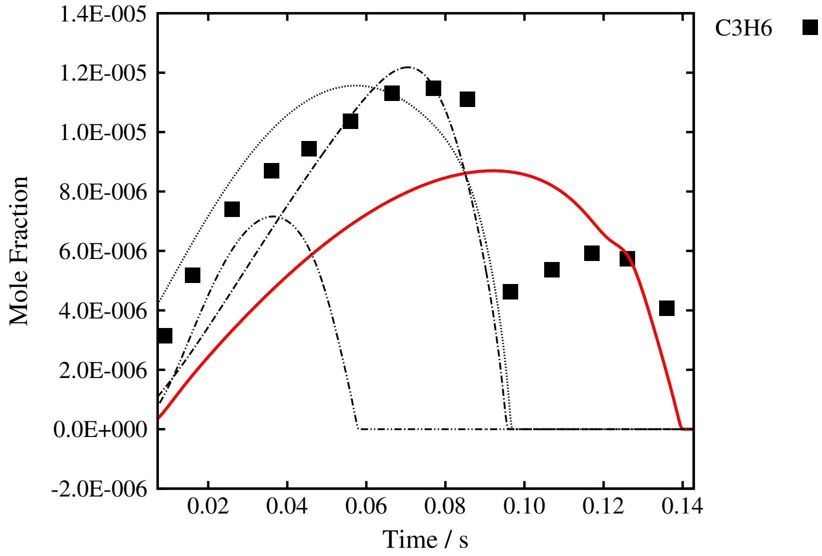

0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K
C2H2
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
Mole Fraction
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

(e)


0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K
C2H4
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
Mole Fraction
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

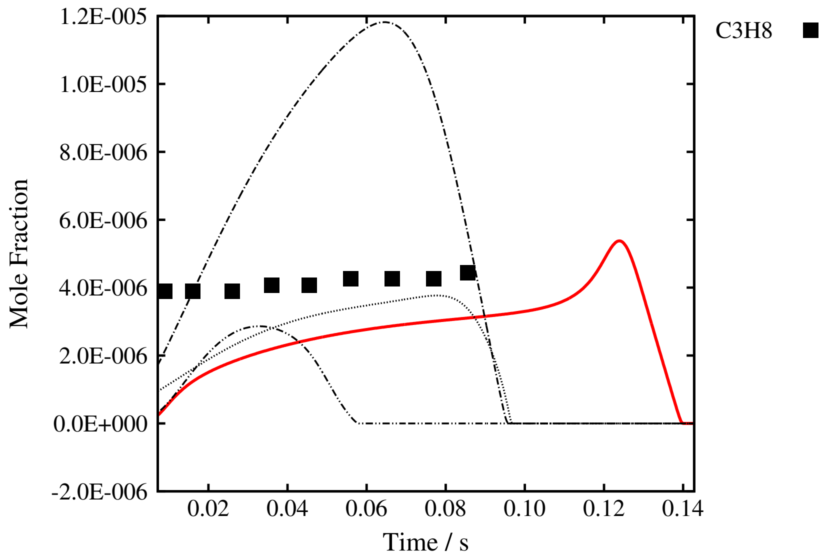
(f)

0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K

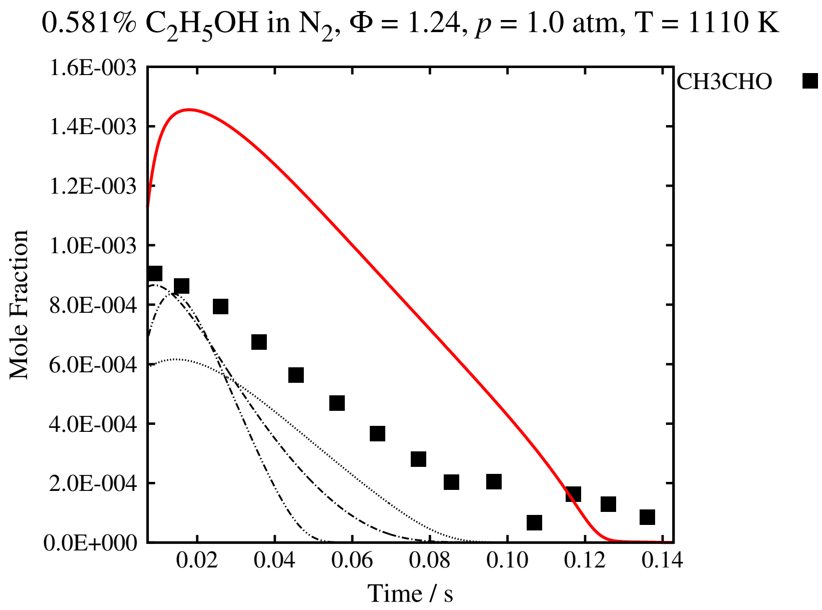


(g)

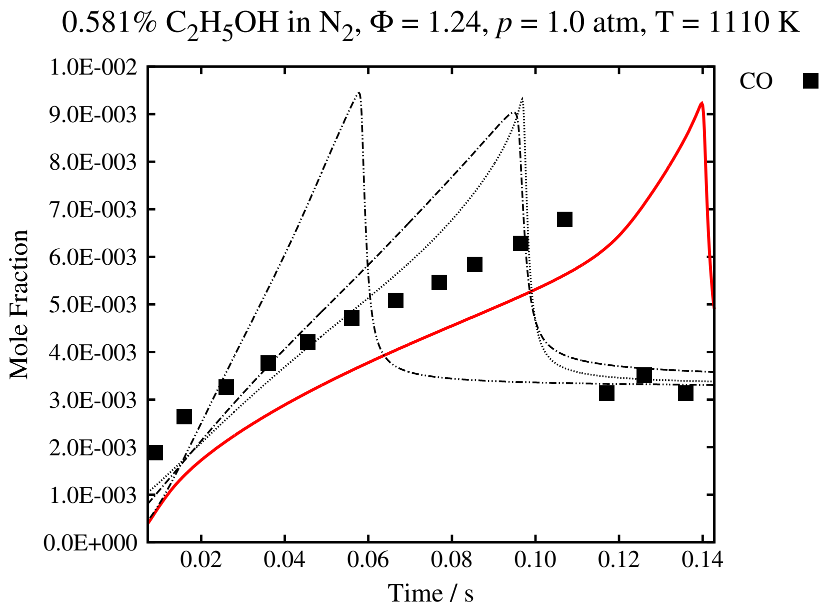
0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K



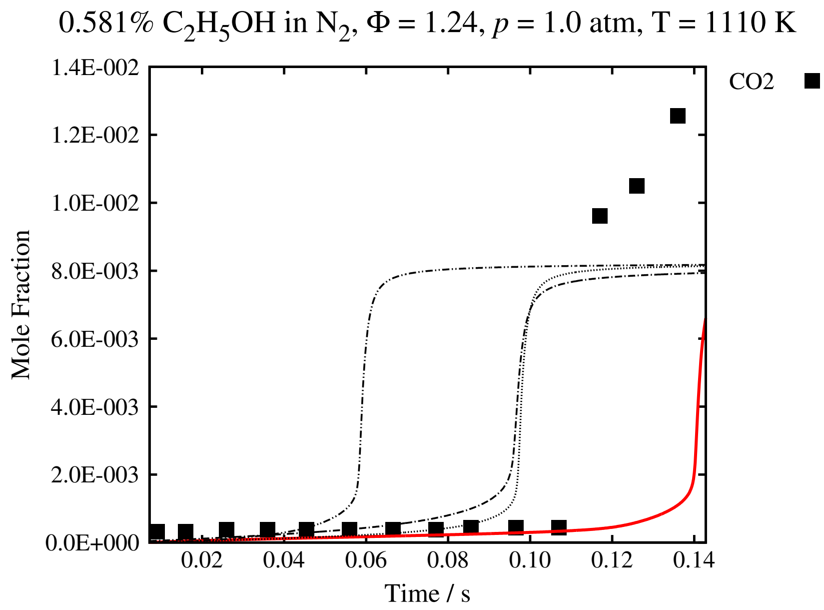
(h)


0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K
CH3CHO
Mole Fraction
Time / s
1.6E-003
1.4E-003
1.2E-003
1.0E-003
8.0E-004
6.0E-004
4.0E-004
2.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14

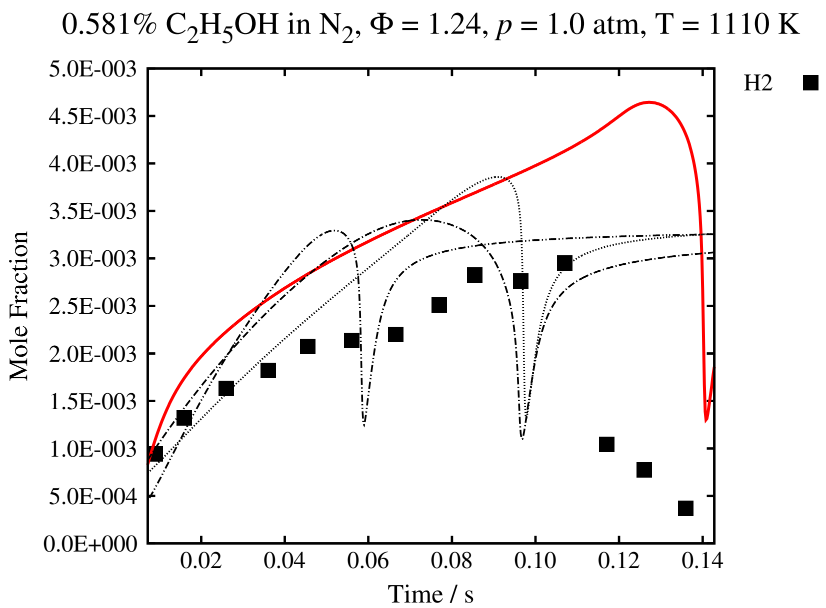
(i)


0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K
CO
Mole Fraction
Time / s
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14

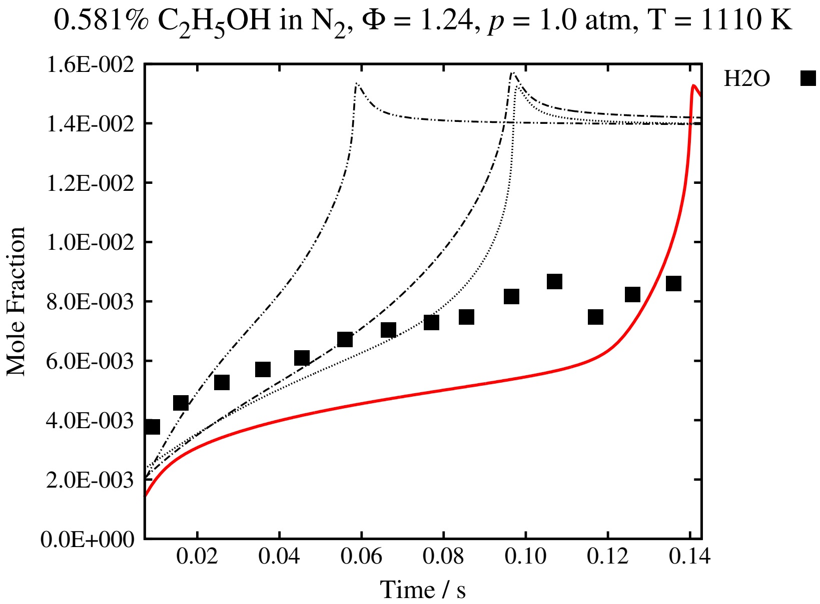
(j)


0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K
CO2
Mole Fraction
1.4E-002
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

(k)


0.581% C_2H_5OH in N_2, Φ = 1.24, p = 1.0 atm, T = 1110 K
H2
Mole Fraction
5.0E-003
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Time / s

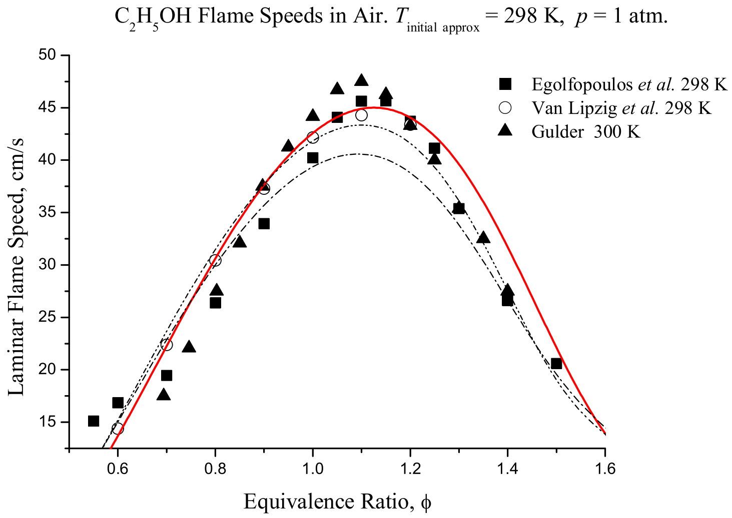
(l)

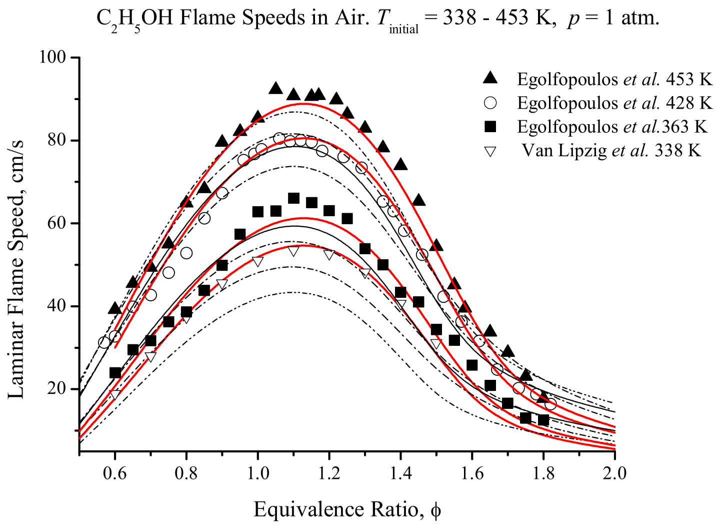


(m)

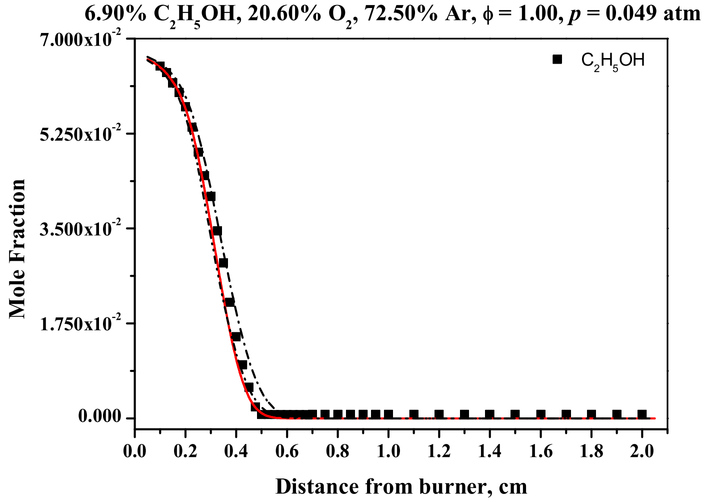
S91 Flow reactor species profiles of ethanol/oxygen/nitrogen mixtures. Symbols are experimental data [57] lines are model predictions. Model predictions are shifted in order to match 50% fuel consumed. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

2.8.4. Flame Speed

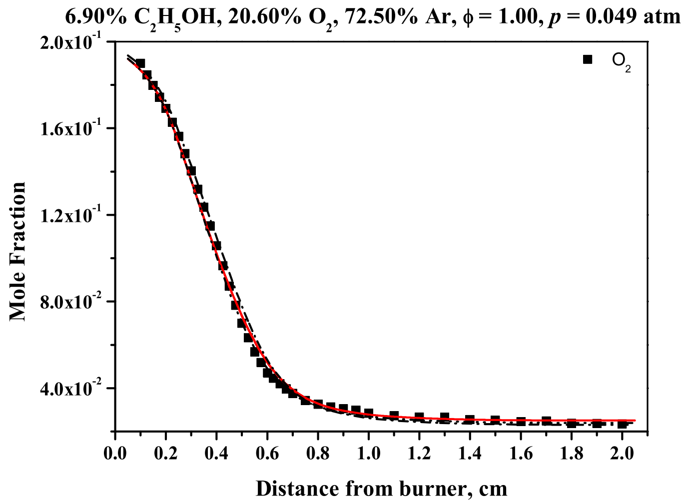




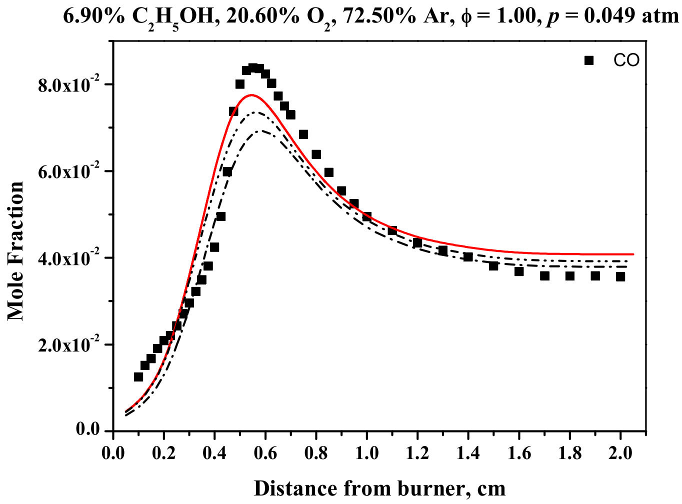
S92 Laminar flame speed measurements ethanol/air mixtures. Symbols are experimental data [59–61] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


6.90% C_2H_5OH, 20.60% O_2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
C_2H_5OH
Mole Fraction
Distance from burner, cm
7.000x10^{-2}
5.250x10^{-2}
3.500x10^{-2}
1.750x10^{-2}
0.000
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

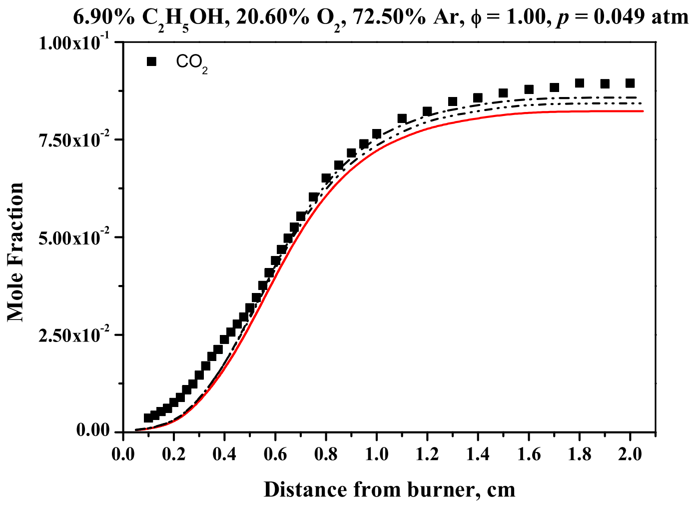
(a)


6.90% C_2H_5OH, 20.60% O_2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
O_2
Mole Fraction
Distance from burner, cm
2.0x10^{-1}
1.6x10^{-1}
1.2x10^{-1}
8.0x10^{-2}
4.0x10^{-2}
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

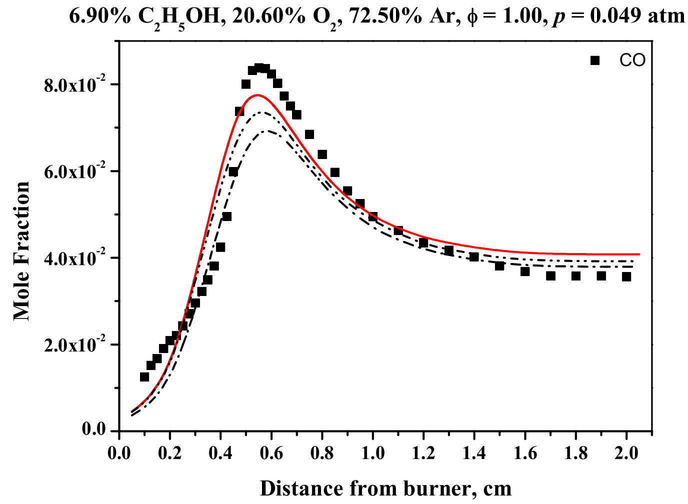
(b)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
CO
Mole Fraction
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

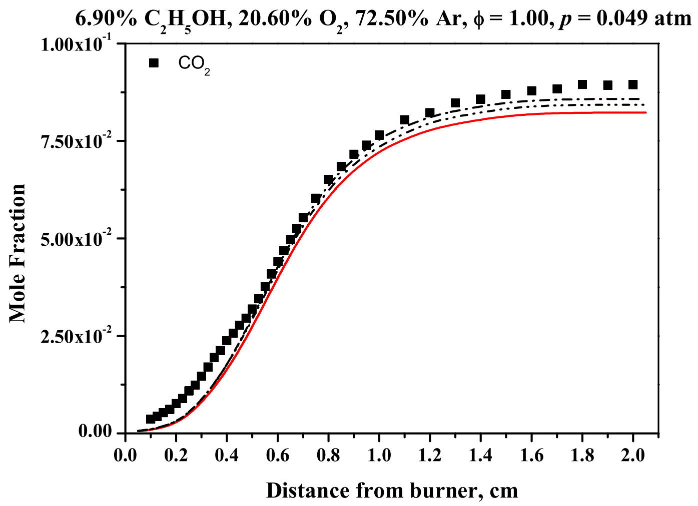
(c)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
CO2
Mole Fraction
1.00x10-1
7.50x10-2
5.00x10-2
2.50x10-2
0.00
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

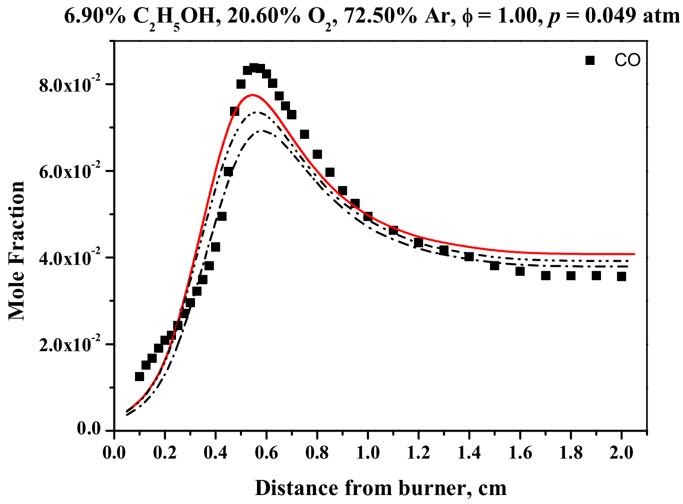
(d)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
CO
Mole Fraction
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

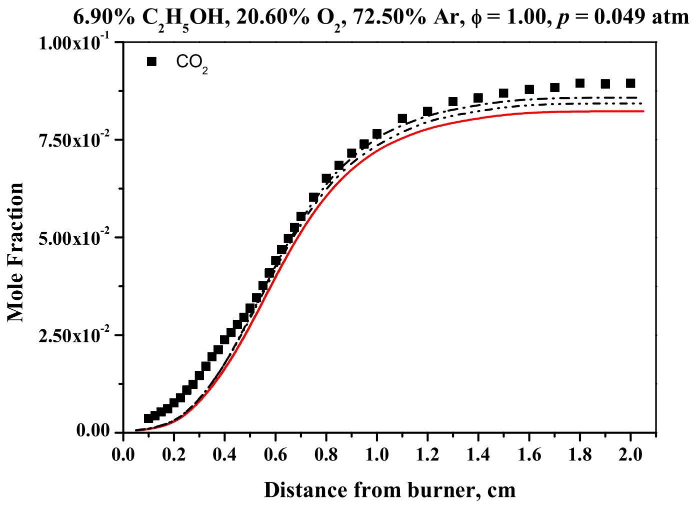
(e)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
CO2
Mole Fraction
1.00x10-1
7.50x10-2
5.00x10-2
2.50x10-2
0.00
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

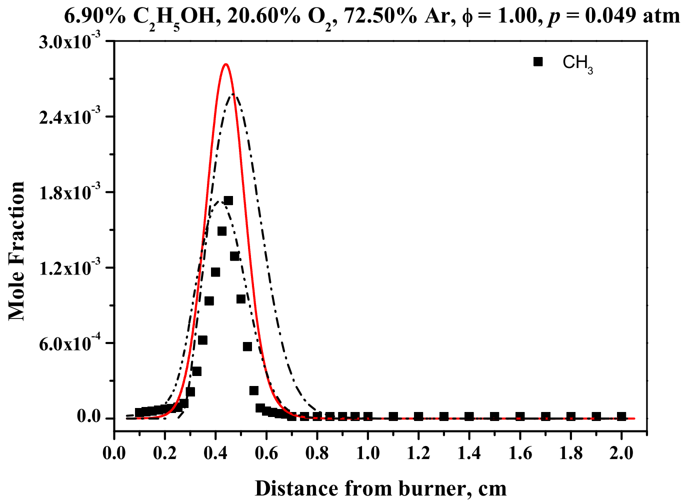
(f)


6.90% C_2H_5OH, 20.60% O_2, 72.50% Ar, ϕ = 1.00, *p* = 0.049 atm
CO
Mole Fraction
8.0x10^{-2}
6.0x10^{-2}
4.0x10^{-2}
2.0x10^{-2}
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

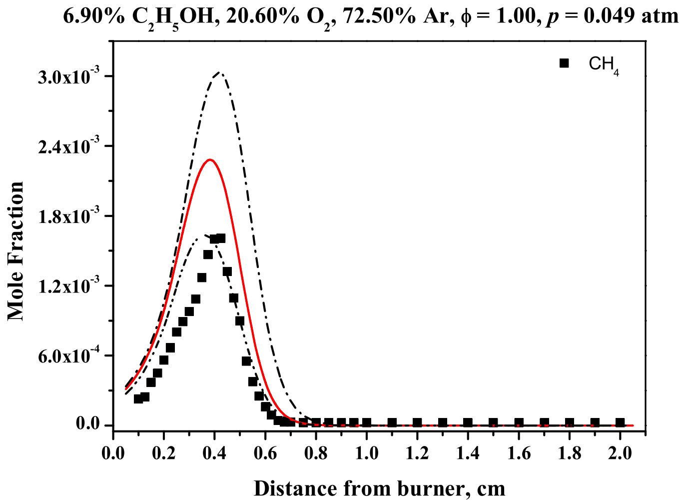
(g)


6.90% C_2H_5OH, 20.60% O_2, 72.50% Ar, ϕ = 1.00, *p* = 0.049 atm
CO_2
Mole Fraction
1.00x10^{-1}
7.50x10^{-2}
5.00x10^{-2}
2.50x10^{-2}
0.00
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

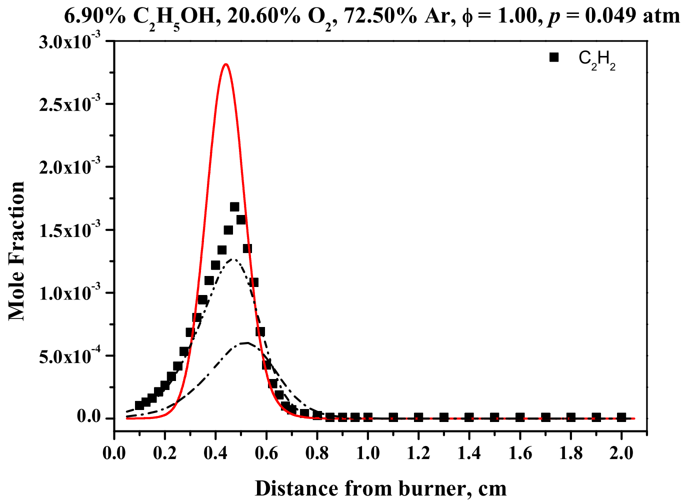
(h)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
CH3
Mole Fraction
3.0x10-3
2.4x10-3
1.8x10-3
1.2x10-3
6.0x10-4
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

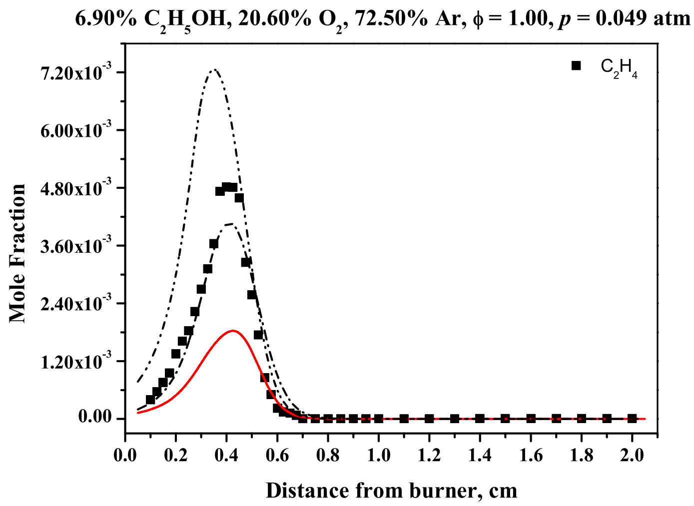
(i)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
CH4
Mole Fraction
3.0x10-3
2.4x10-3
1.8x10-3
1.2x10-3
6.0x10-4
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

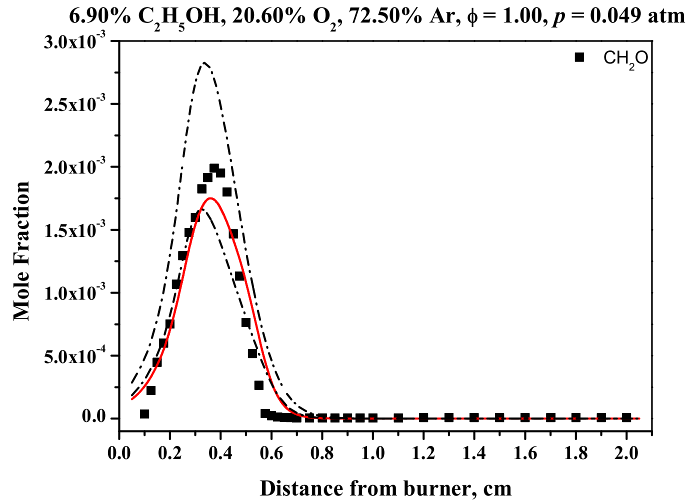
(j)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
C2H2
Mole Fraction
3.0x10-3
2.5x10-3
2.0x10-3
1.5x10-3
1.0x10-3
5.0x10-4
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

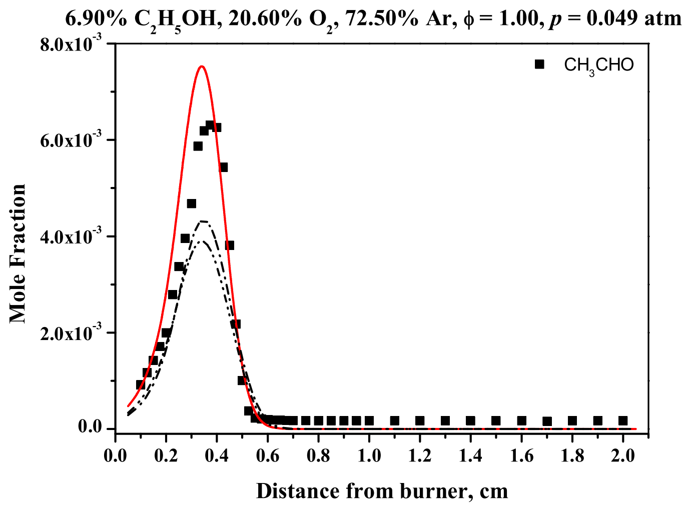
(k)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, ϕ = 1.00, p = 0.049 atm
C2H4
Mole Fraction
7.20x10-3
6.00x10-3
4.80x10-3
3.60x10-3
2.40x10-3
1.20x10-3
0.00
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

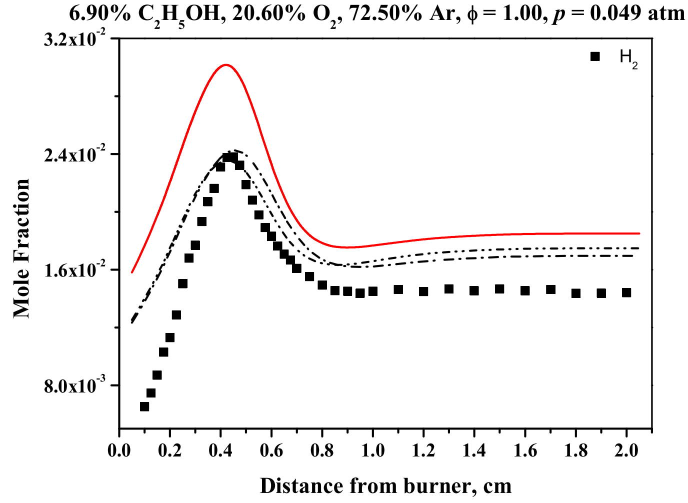
(l)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, φ = 1.00, p = 0.049 atm
CH2O
Mole Fraction
Distance from burner, cm

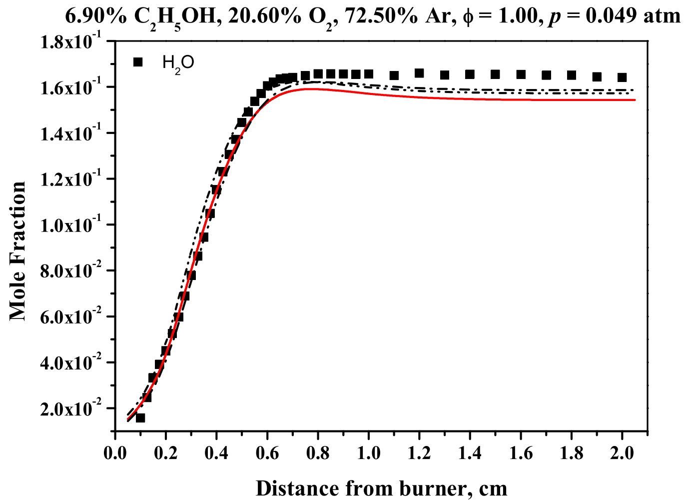
(m)


6.90% C2H5OH, 20.60% O2, 72.50% Ar, φ = 1.00, p = 0.049 atm
CH3CHO
Mole Fraction
Distance from burner, cm

(n)

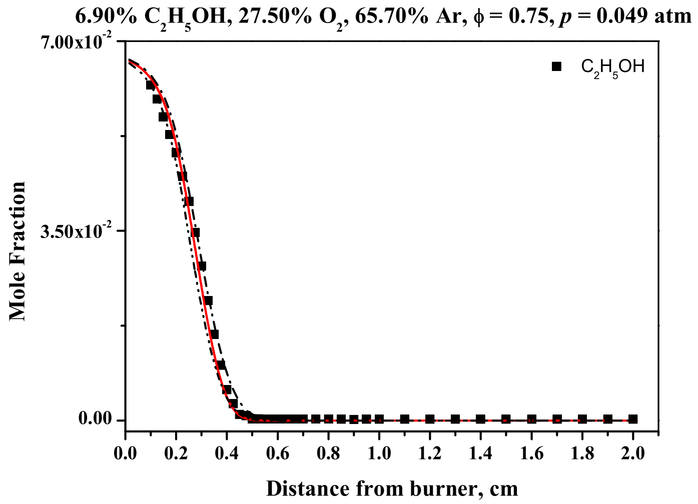


(o)

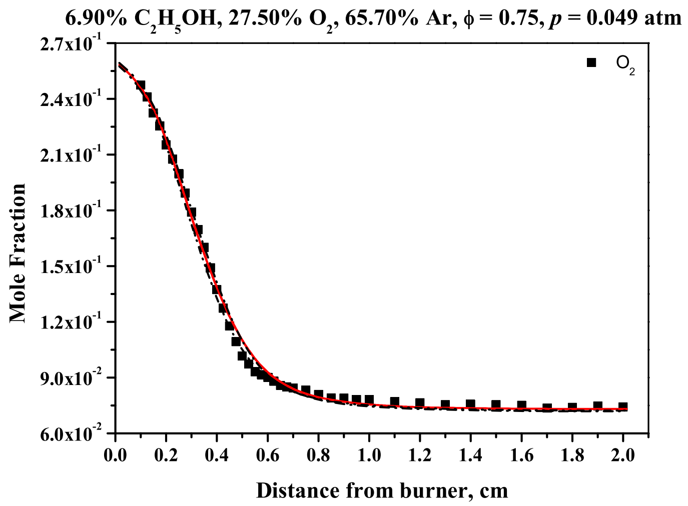


(p)

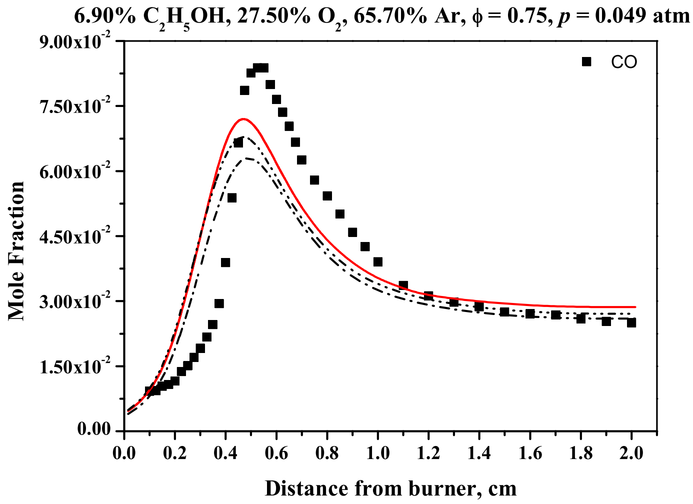
S93 Flame species profiles of ethanol/oxygen/argon mixtures. Experimental data has been shifted by 0.05 cm which is within experimental uncertainty. Symbols are experimental data [62] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


6.90% C_2H_5OH, 27.50% O_2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
7.00x10^{-2}
3.50x10^{-2}
0.00
Mole Fraction
C_2H_5OH
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Distance from burner, cm

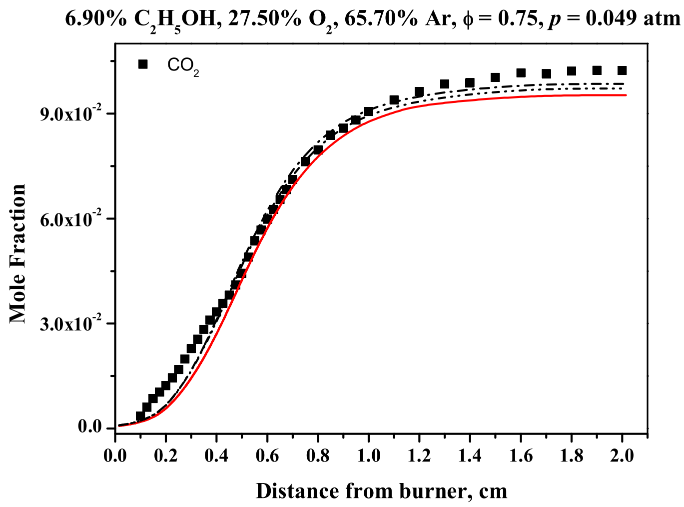
(a)


6.90% C_2H_5OH, 27.50% O_2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
2.7x10^{-1}
2.4x10^{-1}
2.1x10^{-1}
1.8x10^{-1}
1.5x10^{-1}
1.2x10^{-1}
9.0x10^{-2}
6.0x10^{-2}
Mole Fraction
O_2
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Distance from burner, cm

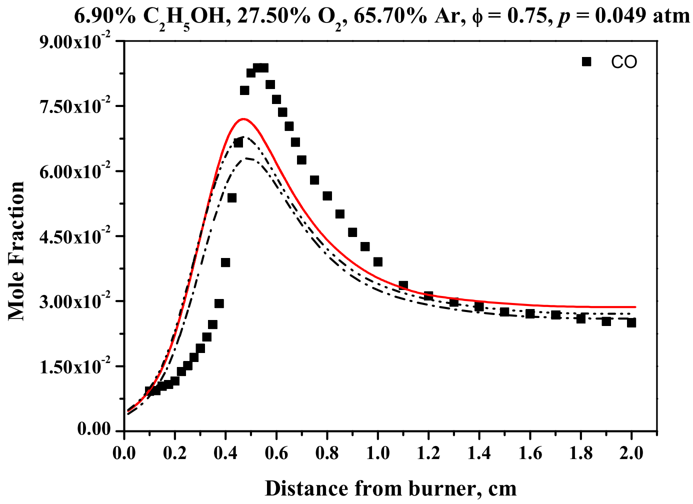
(b)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CO
Mole Fraction
9.00x10-2
7.50x10-2
6.00x10-2
4.50x10-2
3.00x10-2
1.50x10-2
0.00
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

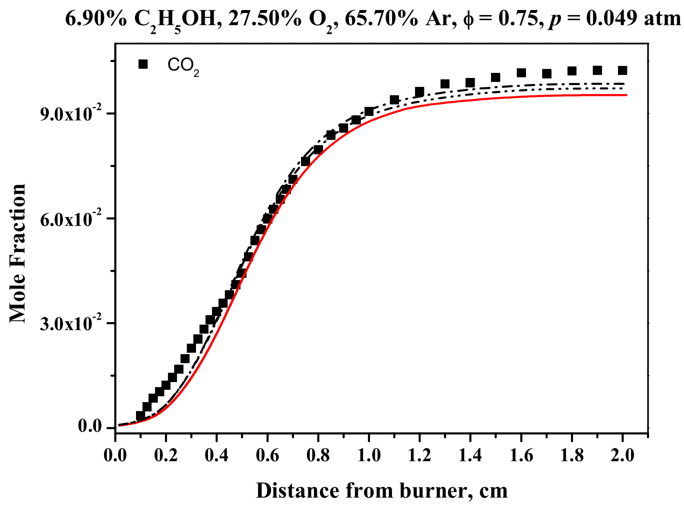
(c)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CO2
Mole Fraction
9.0x10-2
6.0x10-2
3.0x10-2
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

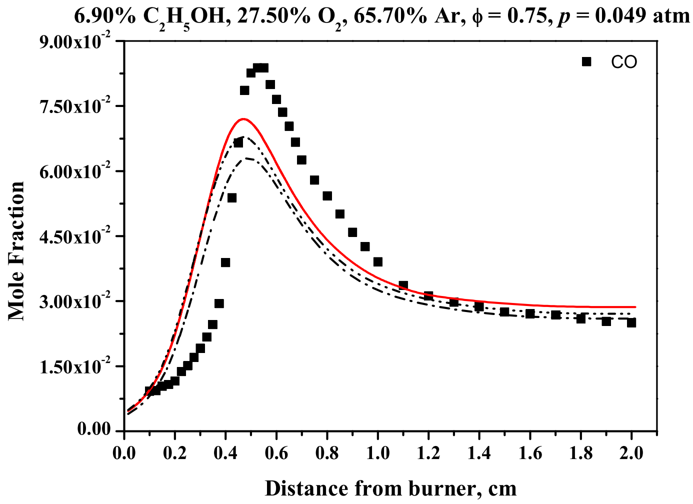
(d)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CO
Mole Fraction
9.00x10-2
7.50x10-2
6.00x10-2
4.50x10-2
3.00x10-2
1.50x10-2
0.00
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

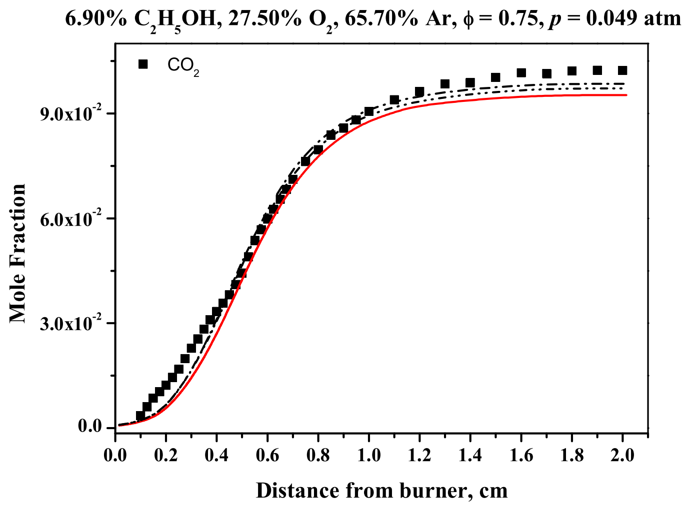
(e)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CO2
Mole Fraction
9.0x10-2
6.0x10-2
3.0x10-2
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

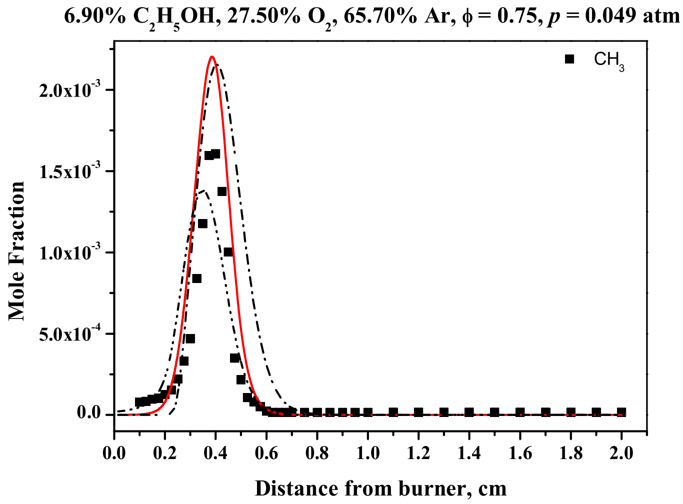
(f)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CO
9.00x10-2
7.50x10-2
6.00x10-2
4.50x10-2
3.00x10-2
1.50x10-2
0.00
Mole Fraction
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

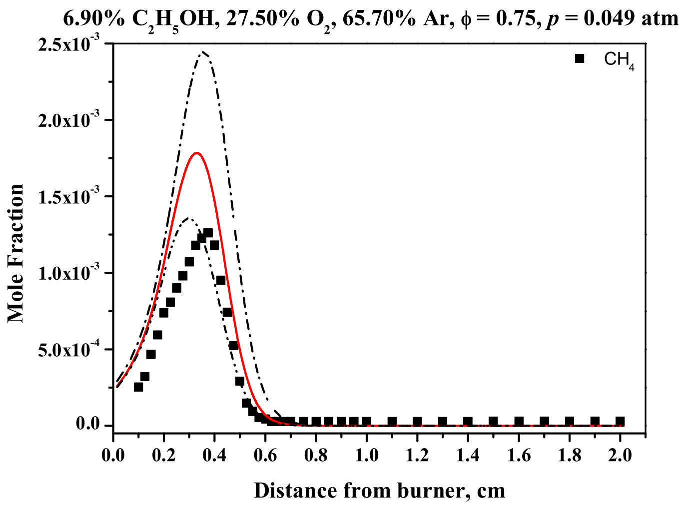
(g)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CO2
9.0x10-2
6.0x10-2
3.0x10-2
0.0
Mole Fraction
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

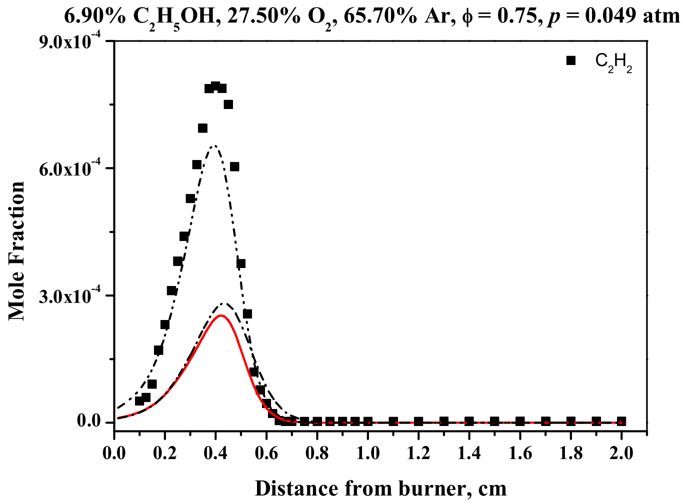
(h)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CH3
Mole Fraction
Distance from burner, cm

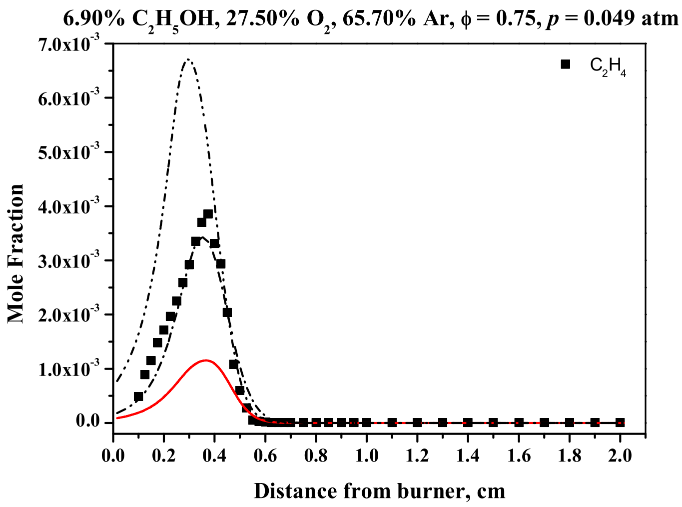
(i)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CH4
Mole Fraction
Distance from burner, cm

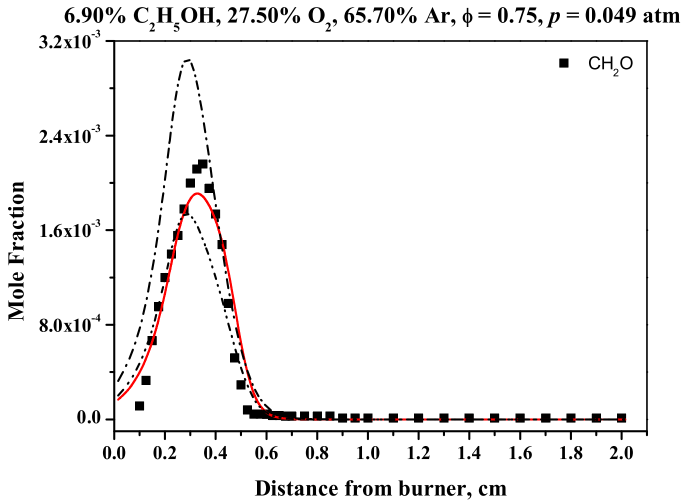
(j)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
C2H2
Mole Fraction
Distance from burner, cm
9.0x10-4
6.0x10-4
3.0x10-4
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0

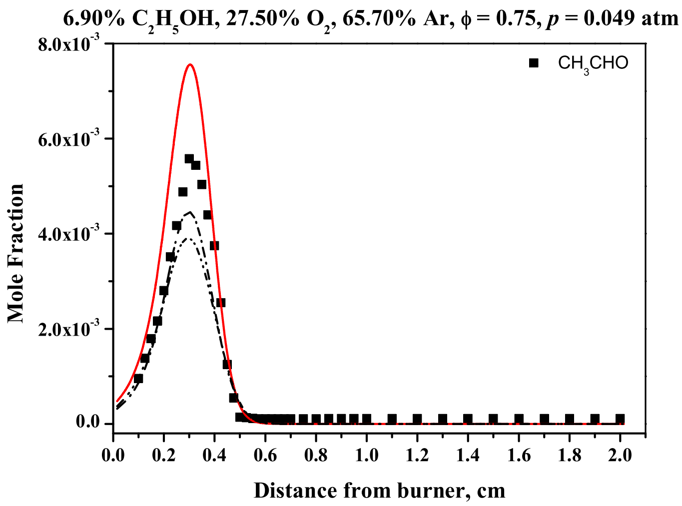
(k)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
C2H4
Mole Fraction
Distance from burner, cm
7.0x10-3
6.0x10-3
5.0x10-3
4.0x10-3
3.0x10-3
2.0x10-3
1.0x10-3
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0

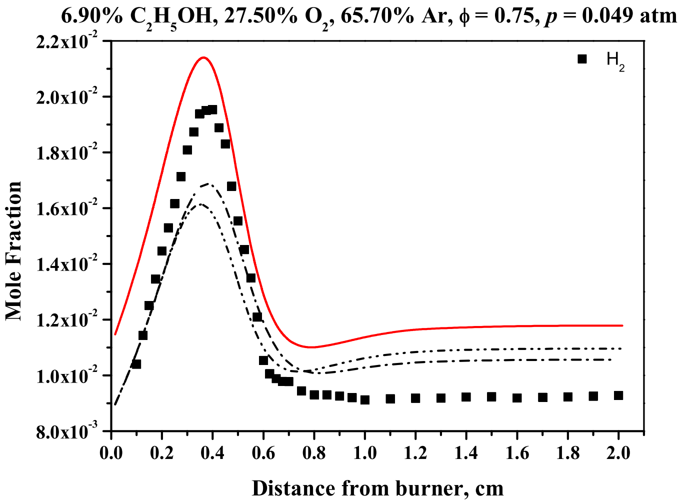
(l)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CH2O
Mole Fraction
3.2x10-3
2.4x10-3
1.6x10-3
8.0x10-4
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

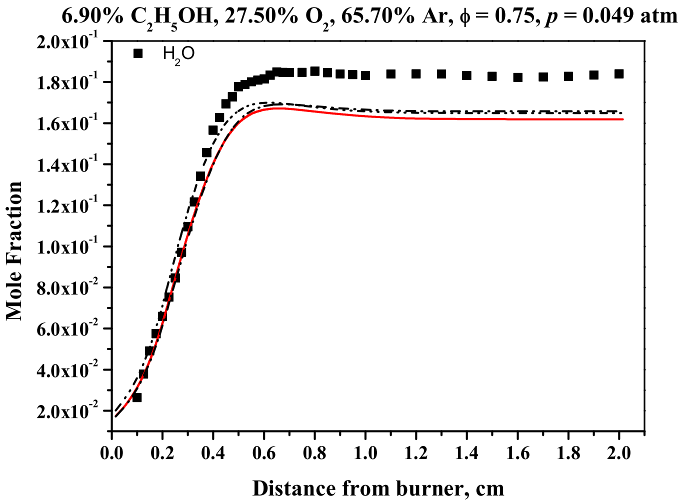
(m)


6.90% C2H5OH, 27.50% O2, 65.70% Ar, ϕ = 0.75, p = 0.049 atm
CH3CHO
Mole Fraction
8.0x10-3
6.0x10-3
4.0x10-3
2.0x10-3
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

(n)

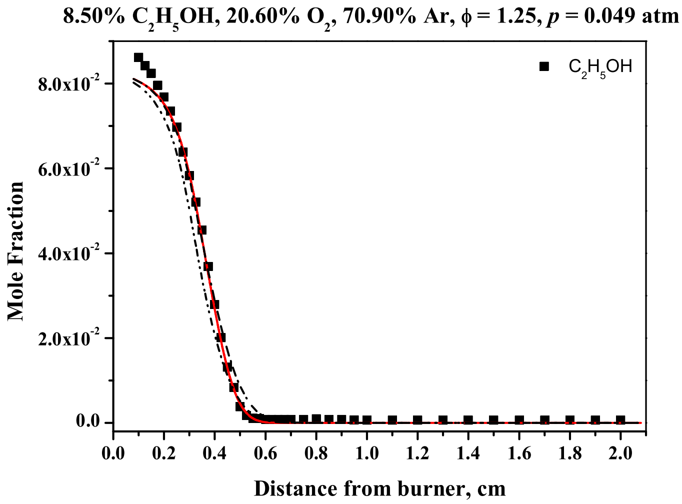


(o)

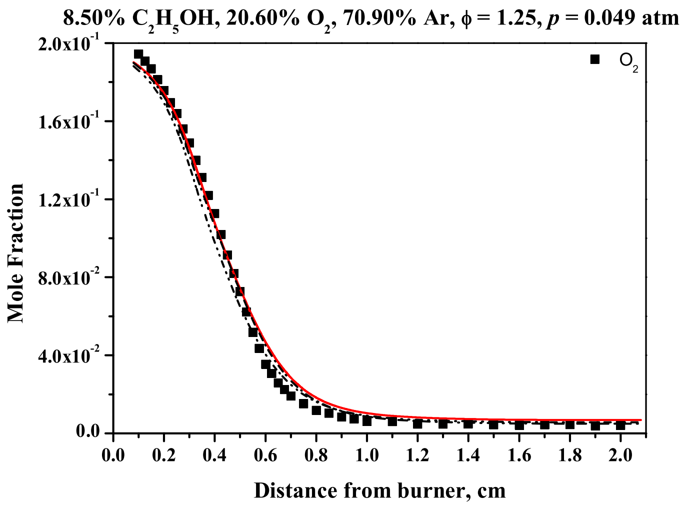


(p)

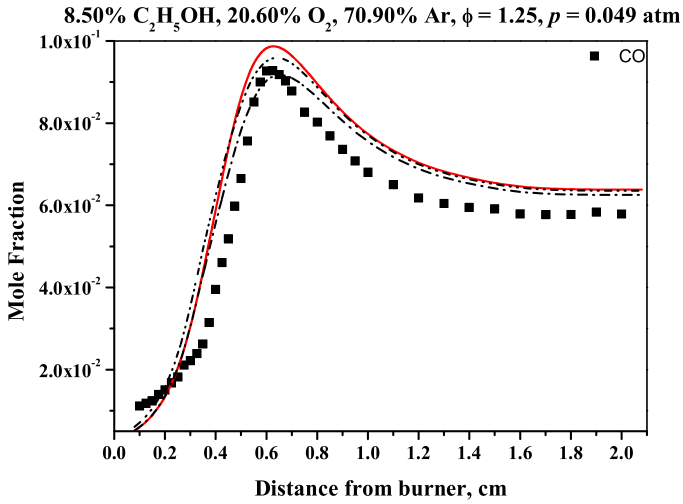
S94 Flame species profiles of ethanol/oxygen/argon mixtures. Experimental data has been shifted by 0.015 cm which is within experimental uncertainty. Symbols are experimental data [62] lines are model predictions. —— AramcoMech 1.3, —— GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, —— USC II.


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
C2H5OH
Mole Fraction
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Distance from burner, cm

(a)

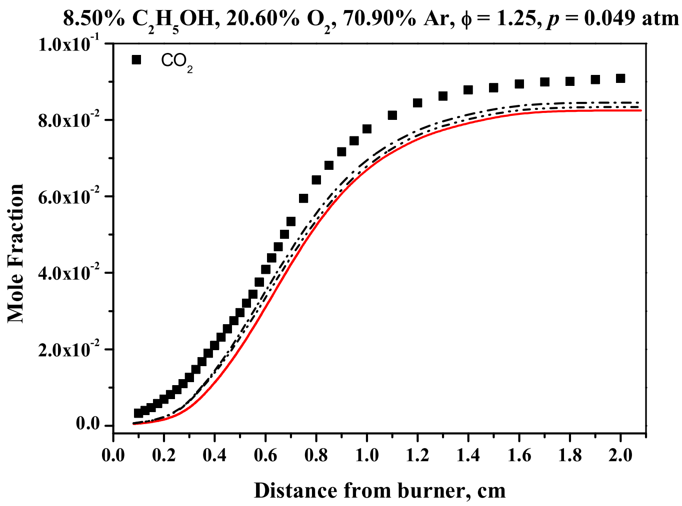

8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
O2
Mole Fraction
2.0x10-1
1.6x10-1
1.2x10-1
8.0x10-2
4.0x10-2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Distance from burner, cm

(b)



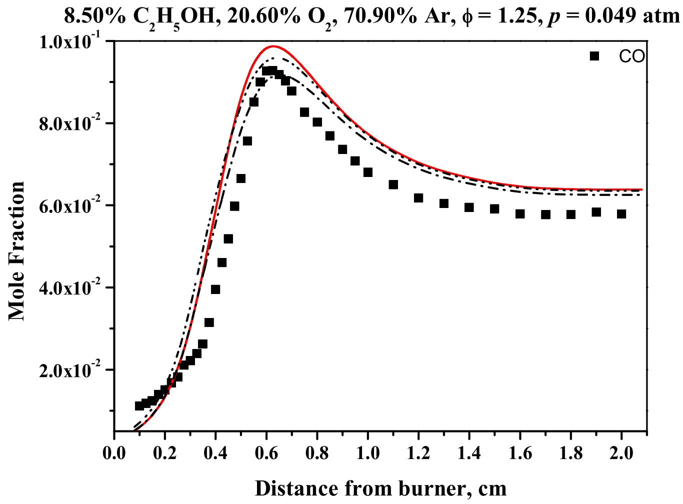
8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CO
Mole Fraction
Distance from burner, cm
1.0x10-1
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0

(c)

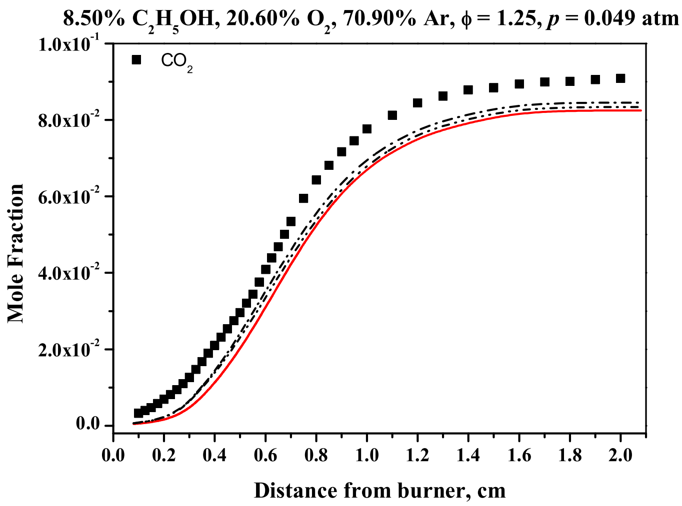


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CO2
Mole Fraction
Distance from burner, cm
1.0x10-1
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0

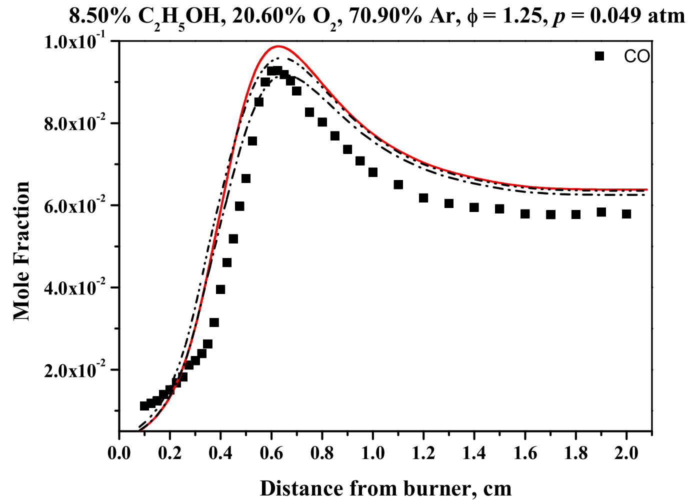
(d)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CO
Mole Fraction
1.0x10-1
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

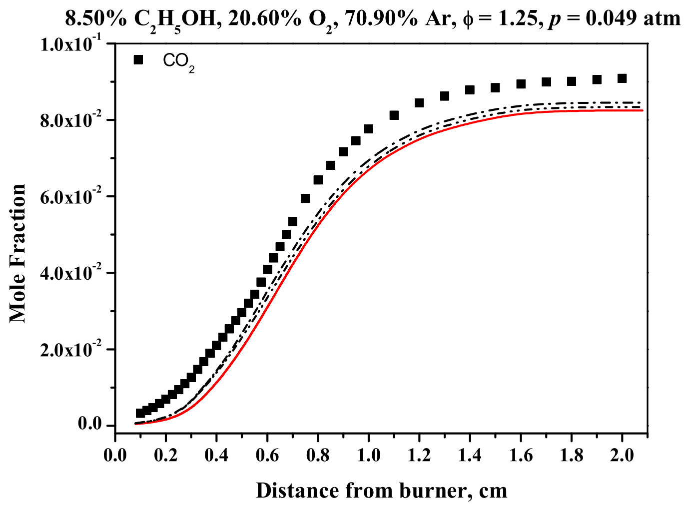
(e)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CO2
Mole Fraction
1.0x10-1
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

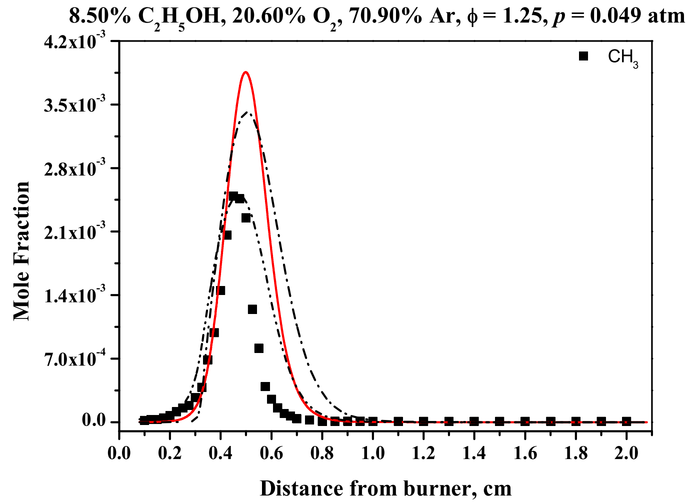
(f)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CO
Mole Fraction
1.0x10-1
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

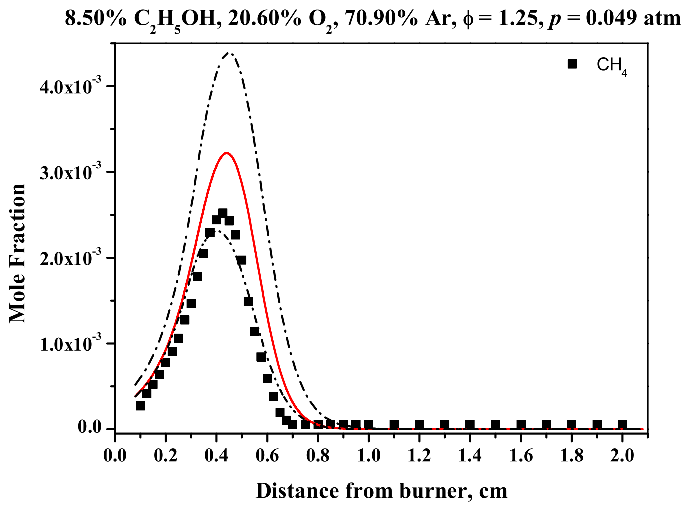
(g)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CO2
Mole Fraction
1.0x10-1
8.0x10-2
6.0x10-2
4.0x10-2
2.0x10-2
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

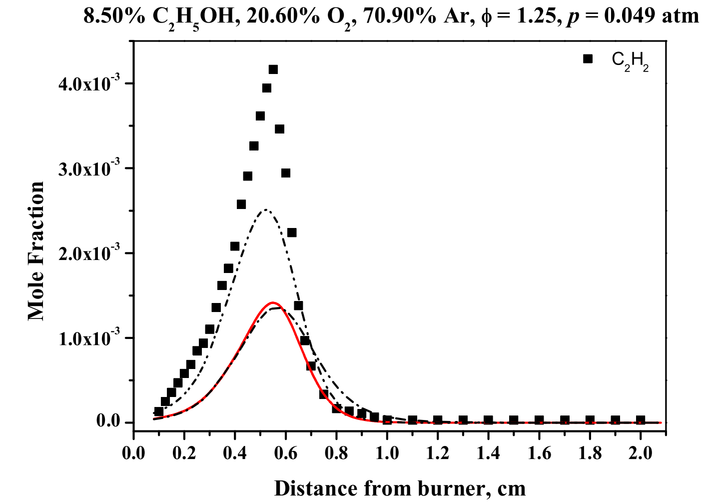
(h)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CH3
Mole Fraction
4.2x10-3
3.5x10-3
2.8x10-3
2.1x10-3
1.4x10-3
7.0x10-4
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

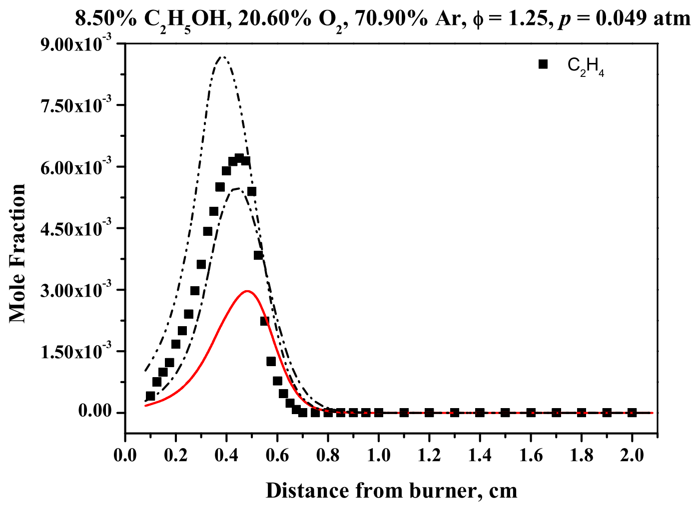
(i)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CH4
Mole Fraction
4.0x10-3
3.0x10-3
2.0x10-3
1.0x10-3
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

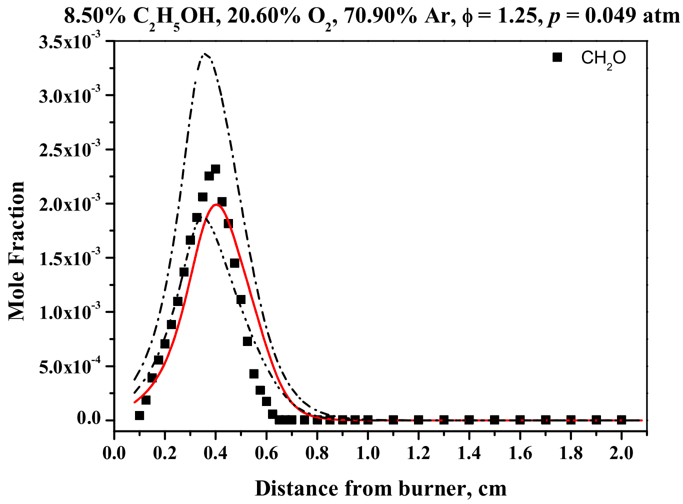
(j)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
C2H2
Mole Fraction
4.0x10-3
3.0x10-3
2.0x10-3
1.0x10-3
0.0
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

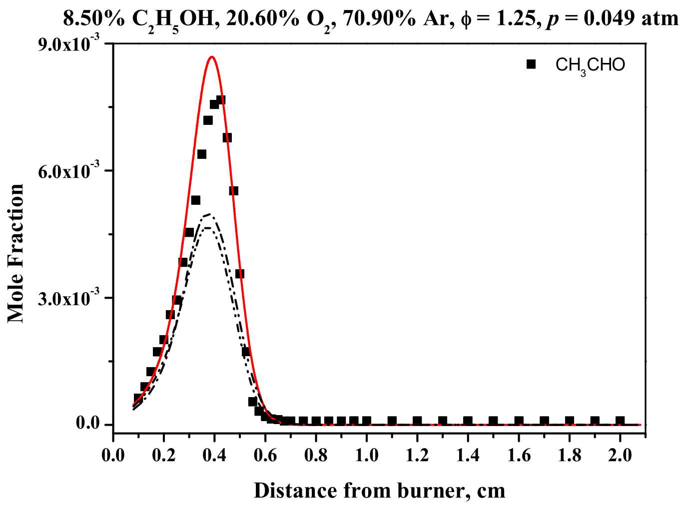
(k)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
C2H4
Mole Fraction
9.00x10-3
7.50x10-3
6.00x10-3
4.50x10-3
3.00x10-3
1.50x10-3
0.00
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Distance from burner, cm

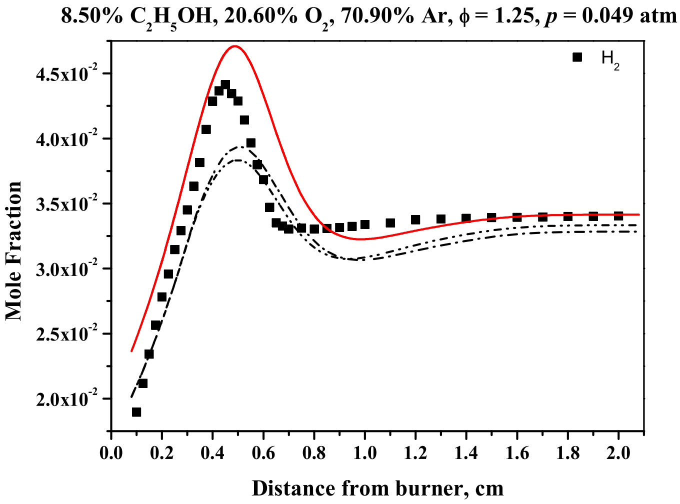
(l)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CH2O
Mole Fraction
3.5x10-3
3.0x10-3
2.5x10-3
2.0x10-3
1.5x10-3
1.0x10-3
5.0x10-4
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Distance from burner, cm

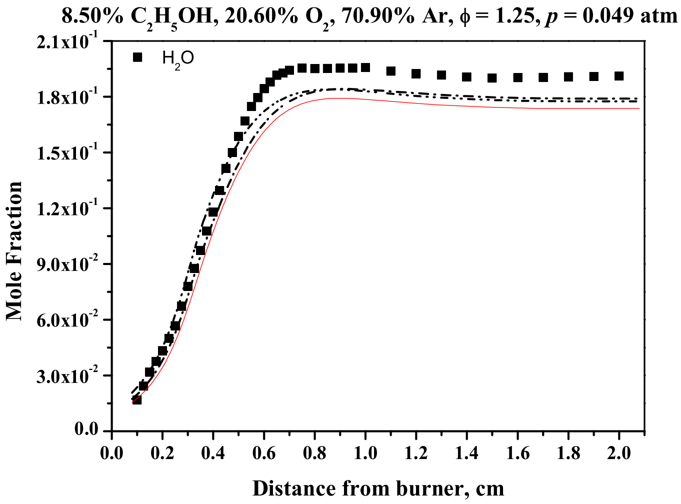
(m)


8.50% C2H5OH, 20.60% O2, 70.90% Ar, ϕ = 1.25, p = 0.049 atm
CH3CHO
Mole Fraction
9.0x10-3
6.0x10-3
3.0x10-3
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Distance from burner, cm

(n)



(o)

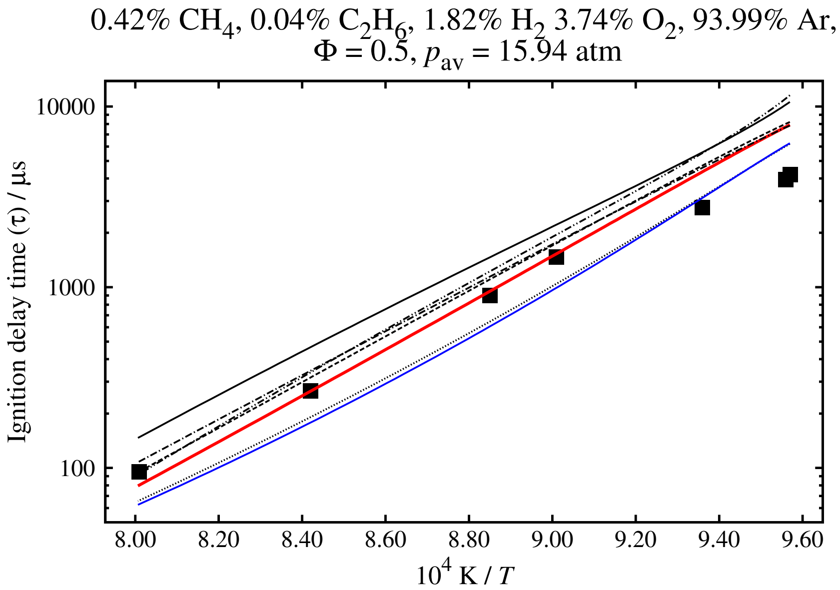


(p)

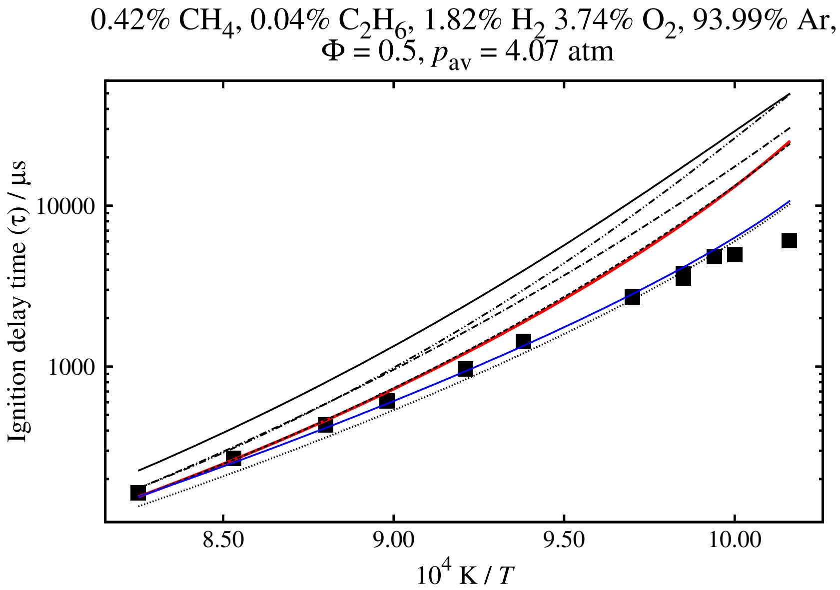
S95 Flame species profiles of ethanol/oxygen/argon mixtures. Experimental data has been shifted by 0.08 cm which is within experimental uncertainty. Symbols are experimental data [62] lines are model predictions. —— AramcoMech 1.3, —— GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, —— USC II.

2.9. Methane/Ethane

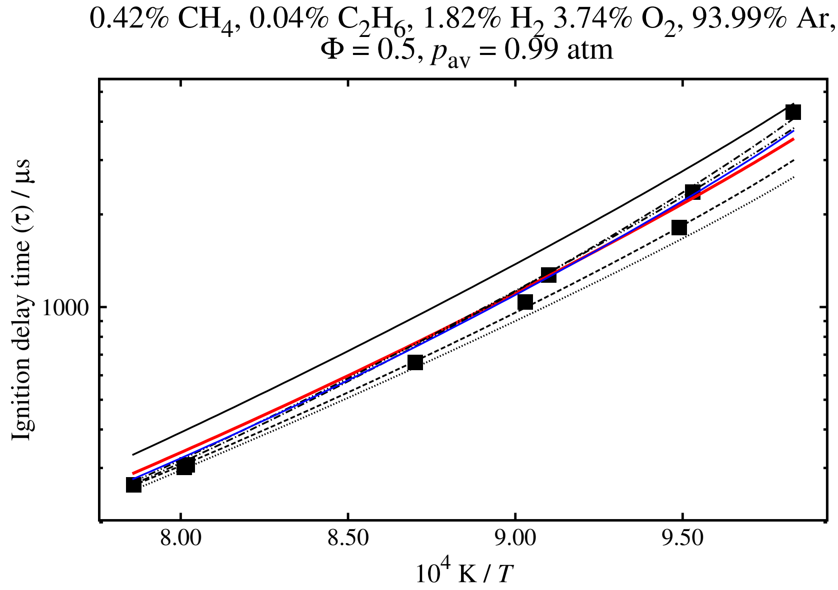
2.9.1. Shock Tube



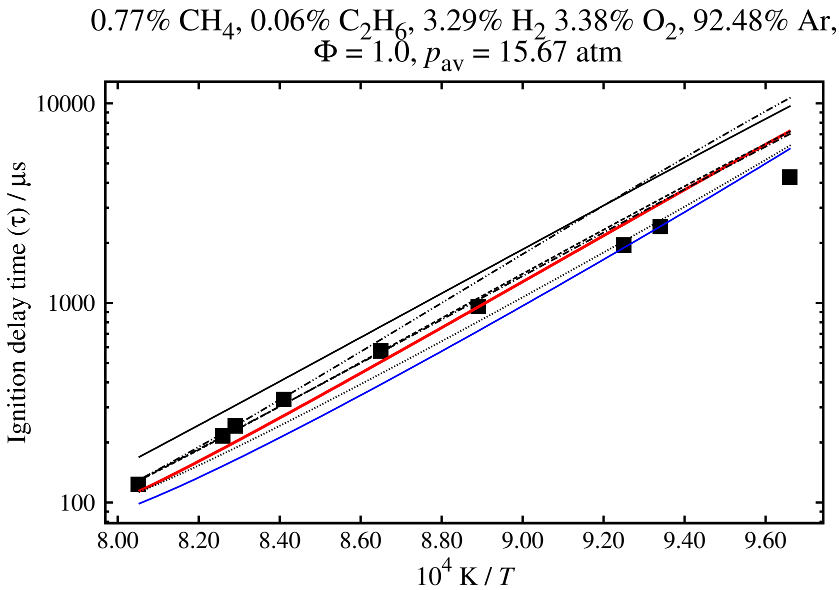
(a)



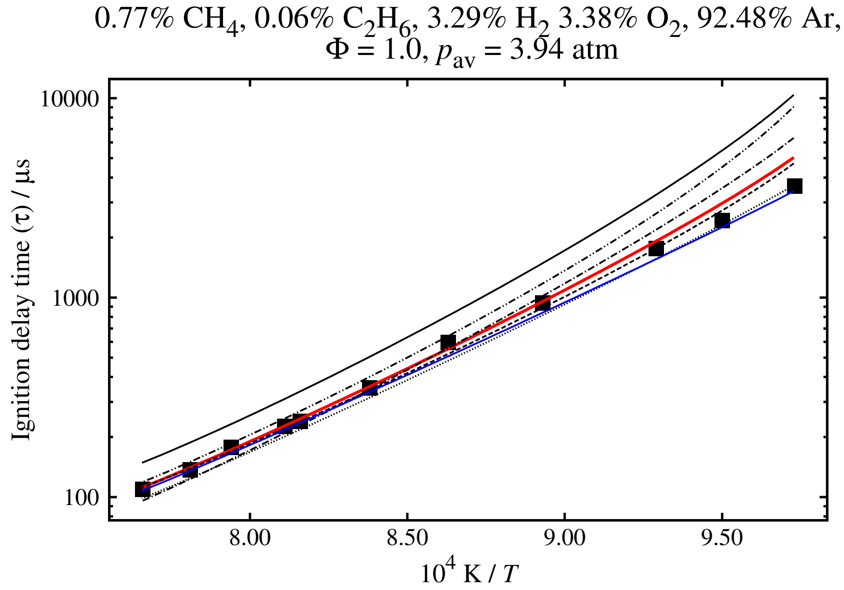
(b)


0.42% CH4, 0.04% C2H6, 1.82% H2 3.74% O2, 93.99% Ar,
Φ = 0.5, pav = 0.99 atm
Ignition delay time (τ) / μs
1000
8.00
8.50
9.00
9.50
10^4 K / T

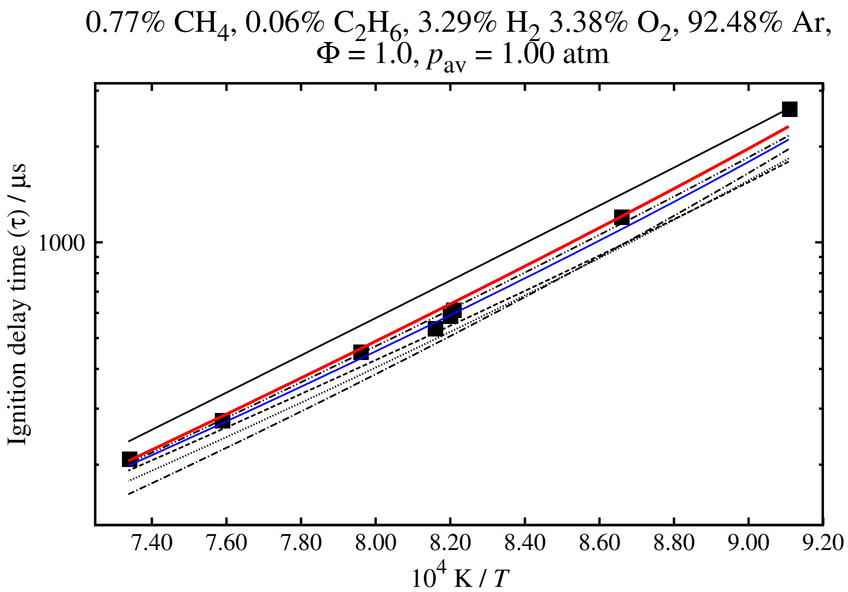
(c)


0.77% CH4, 0.06% C2H6, 3.29% H2 3.38% O2, 92.48% Ar,
Φ = 1.0, pav = 15.67 atm
Ignition delay time (τ) / μs
10000
1000
100
8.00
8.20
8.40
8.60
8.80
9.00
9.20
9.40
9.60
10^4 K / T

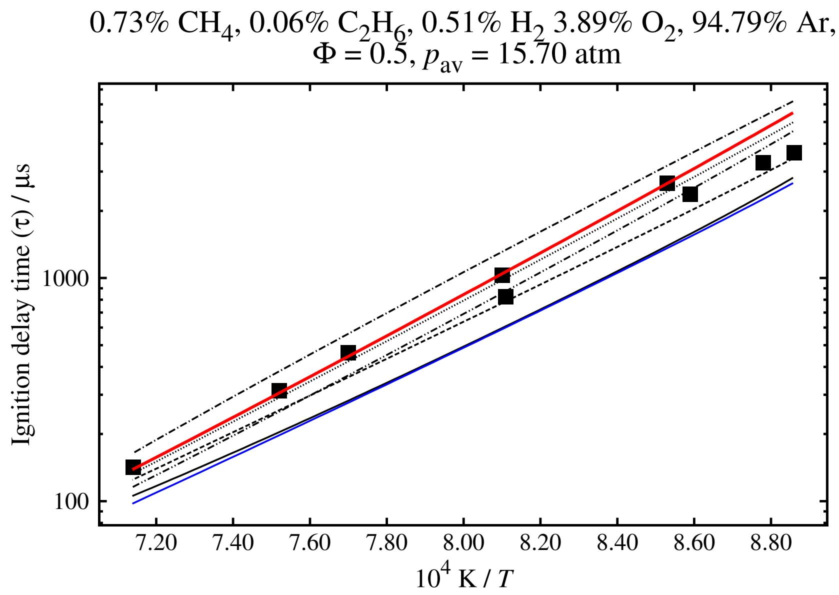
(d)


0.77% CH_4, 0.06% C_2H_6, 3.29% H_2 3.38% O_2, 92.48% Ar,
Φ = 1.0, p_{av} = 3.94 atm
Ignition delay time (τ) / µs
10000
1000
100
8.00
8.50
9.00
9.50
10^4 K / T

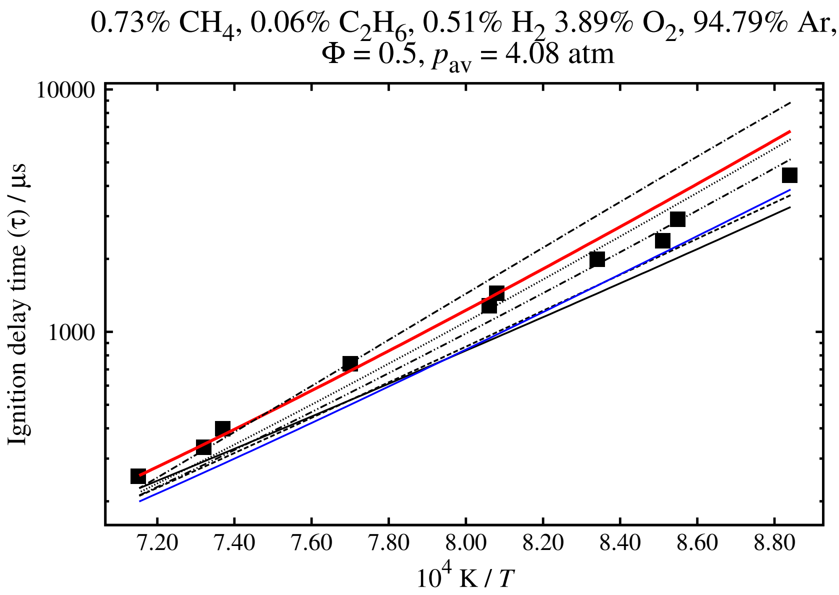
(e)


0.77% CH_4, 0.06% C_2H_6, 3.29% H_2 3.38% O_2, 92.48% Ar,
Φ = 1.0, p_{av} = 1.00 atm
Ignition delay time (τ) / µs
1000
7.40
7.60
7.80
8.00
8.20
8.40
8.60
8.80
9.00
9.20
10^4 K / T

(f)

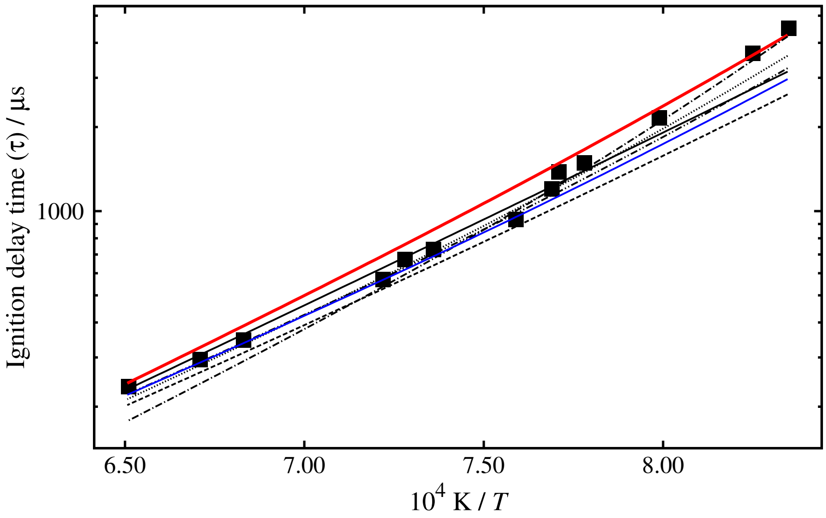

0.73% CH4, 0.06% C2H6, 0.51% H2 3.89% O2, 94.79% Ar,
Φ = 0.5, pav = 15.70 atm
Ignition delay time (τ) / µs
1000
100
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
8.80
10^4 K / T

(g)


0.73% CH4, 0.06% C2H6, 0.51% H2 3.89% O2, 94.79% Ar,
Φ = 0.5, pav = 4.08 atm
Ignition delay time (τ) / µs
10000
1000
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
8.80
10^4 K / T

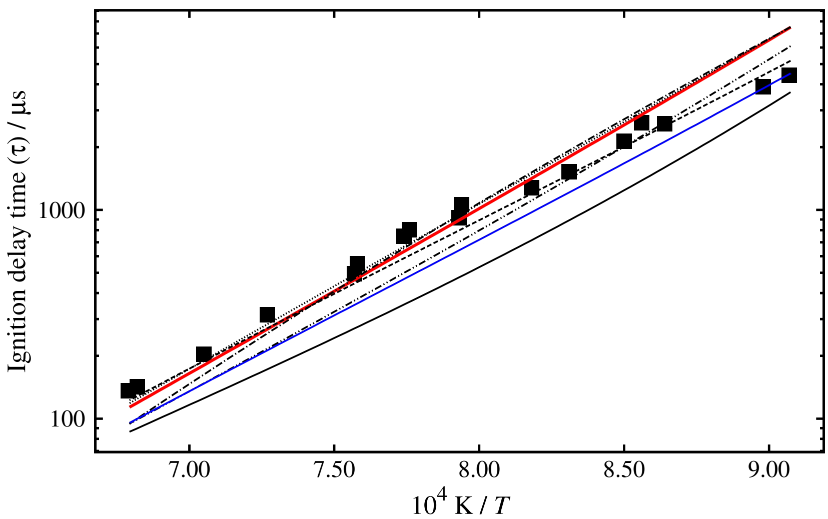
(h)

0.73% CH_4, 0.06% C_2H_6, 0.51% H_2 3.89% O_2, 94.79% Ar,
$\Phi = 0.5$, $p_{av} = 1.00$ atm

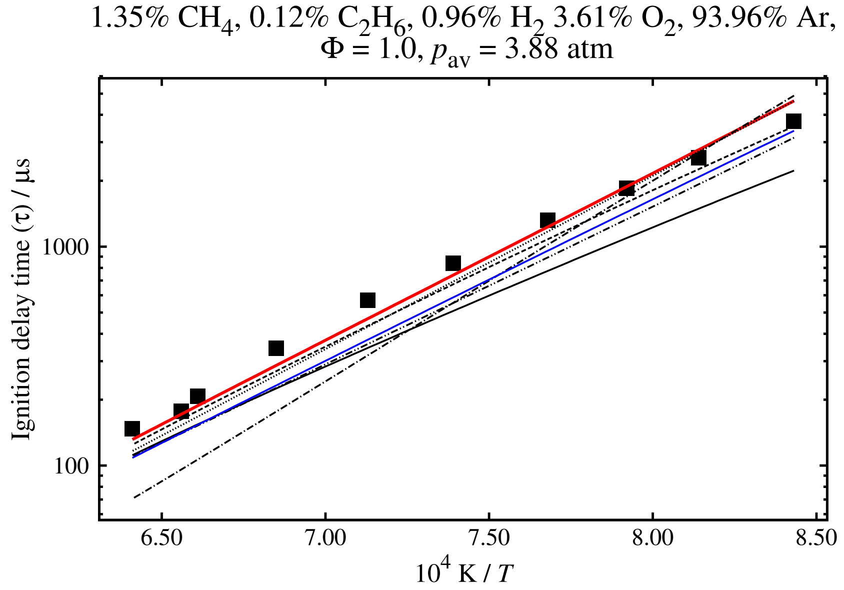


(i)

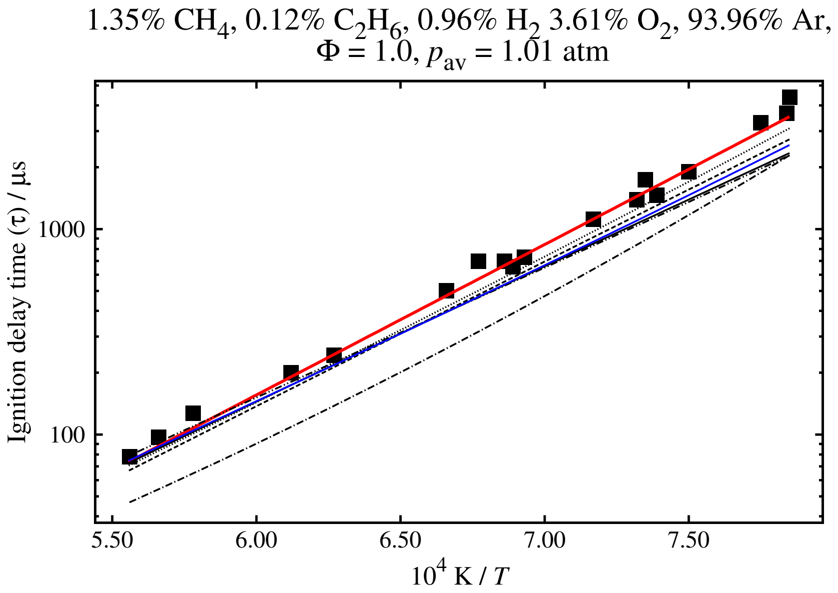
1.35% CH_4, 0.12% C_2H_6, 0.96% H_2 3.61% O_2, 93.96% Ar,
$\Phi = 0.5$, $p_{av} = 15.35$ atm



(j)

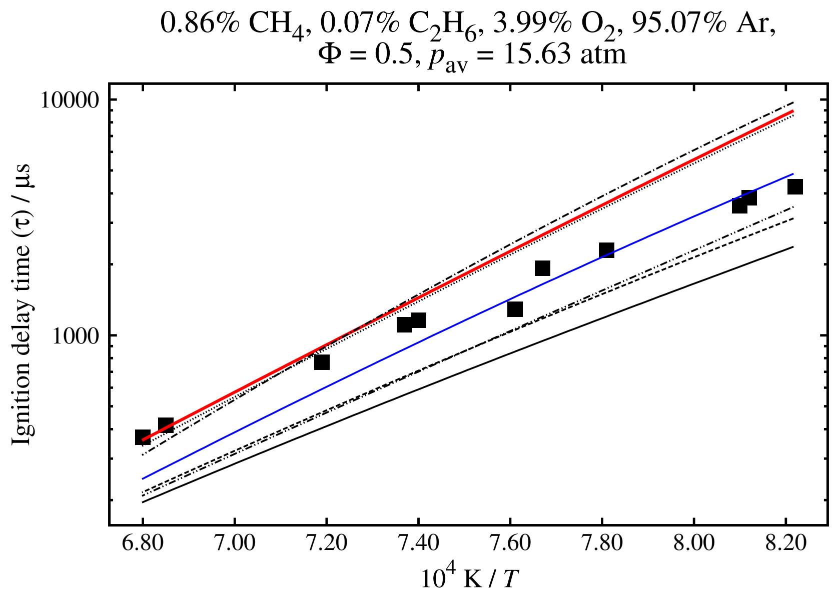


(k)

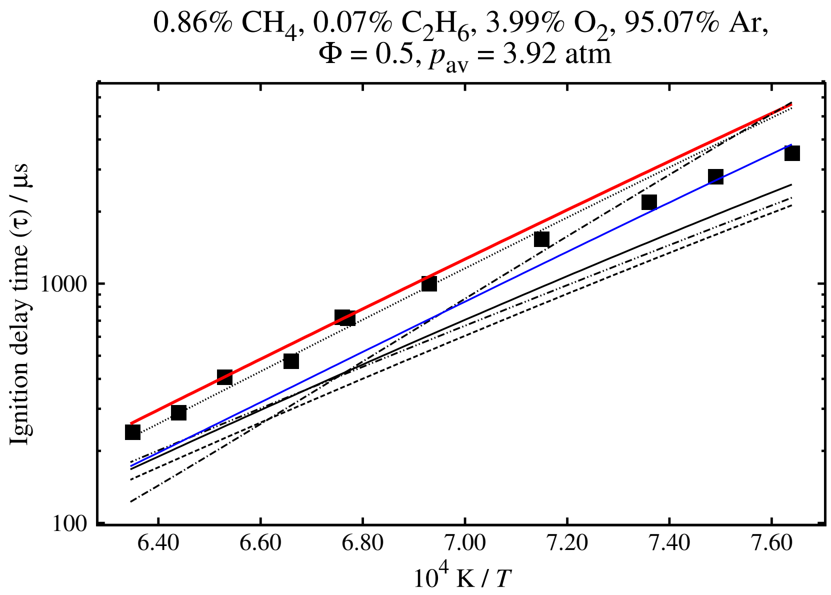


(l)

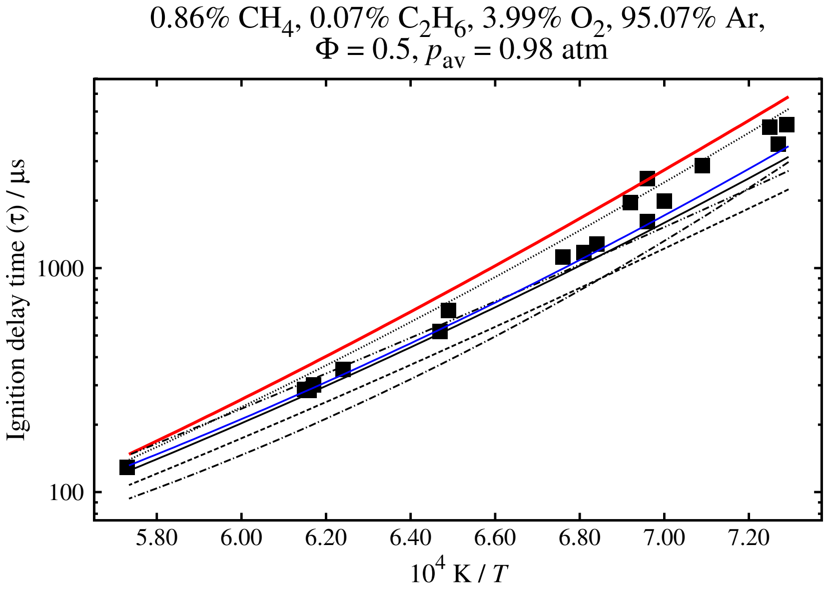
S96 Shock tube ignition delay times of methane/ethane/hydrogen/oxygen/argon mixtures. Symbols are experimental data [64] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.86% CH4, 0.07% C2H6, 3.99% O2, 95.07% Ar,
Φ = 0.5, pav = 15.63 atm
10000
1000
Ignition delay time (τ) / μs
6.80
7.00
7.20
7.40
7.60
7.80
8.00
8.20
10^4 K / T

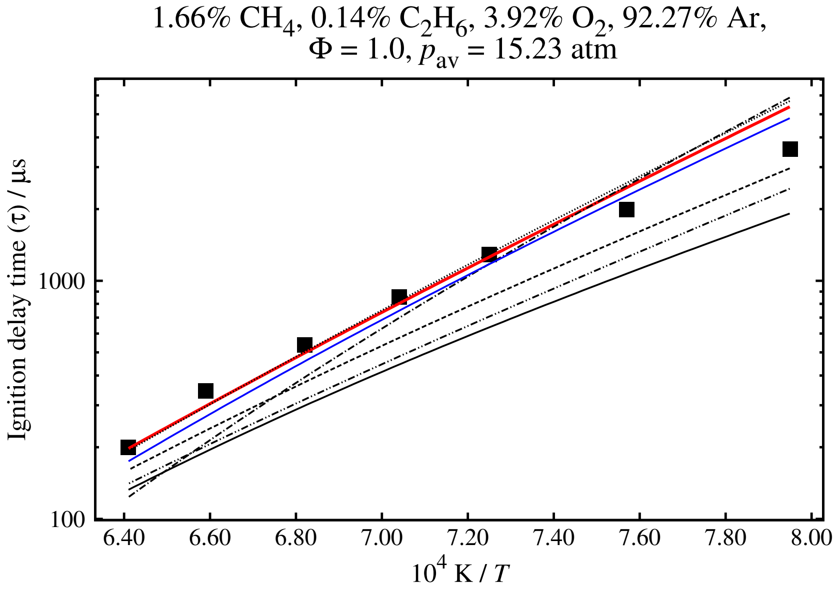
(a)


0.86% CH4, 0.07% C2H6, 3.99% O2, 95.07% Ar,
Φ = 0.5, pav = 3.92 atm
1000
100
Ignition delay time (τ) / μs
6.40
6.60
6.80
7.00
7.20
7.40
7.60
10^4 K / T

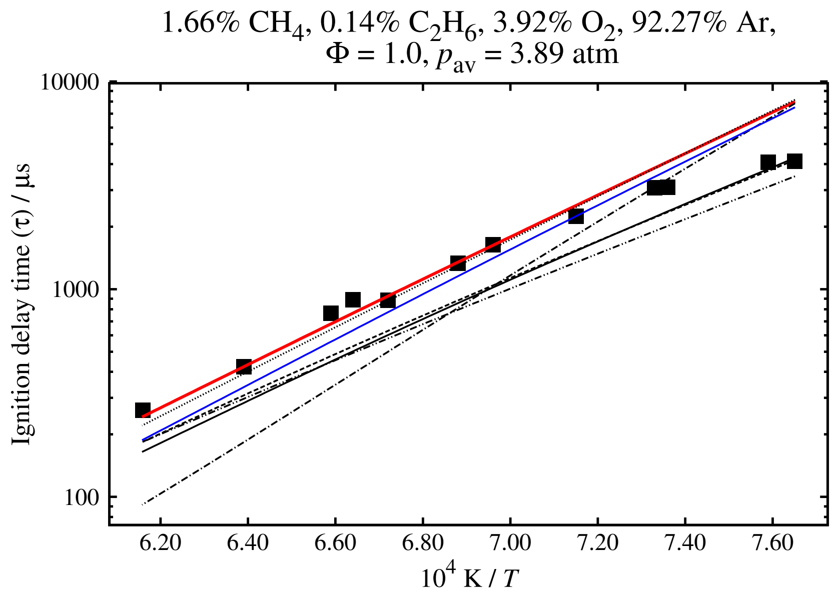
(b)


0.86% CH4, 0.07% C2H6, 3.99% O2, 95.07% Ar,
Φ = 0.5, pav = 0.98 atm
Ignition delay time (τ) / µs
1000
100
5.80
6.00
6.20
6.40
6.60
6.80
7.00
7.20
10^4 K / T

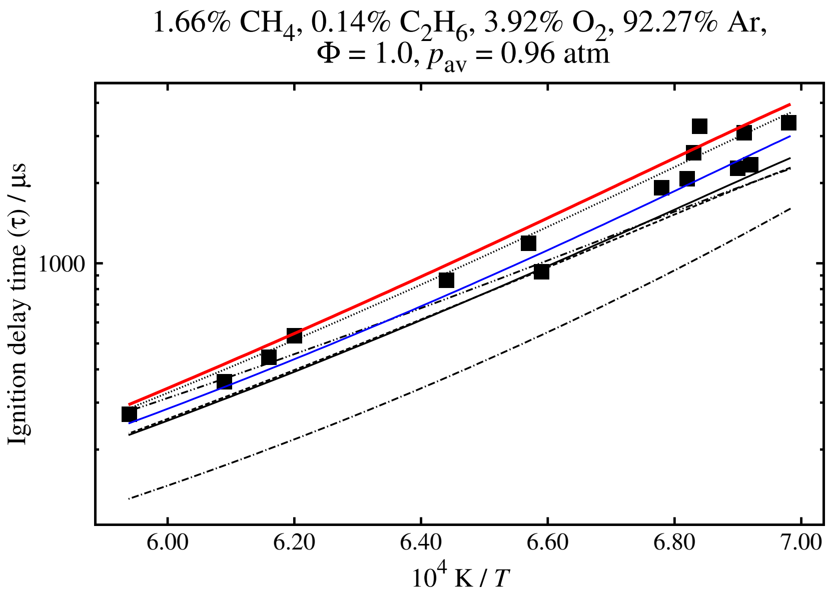
(c)


1.66% CH4, 0.14% C2H6, 3.92% O2, 92.27% Ar,
Φ = 1.0, pav = 15.23 atm
Ignition delay time (τ) / µs
1000
100
6.40
6.60
6.80
7.00
7.20
7.40
7.60
7.80
8.00
10^4 K / T

(d)



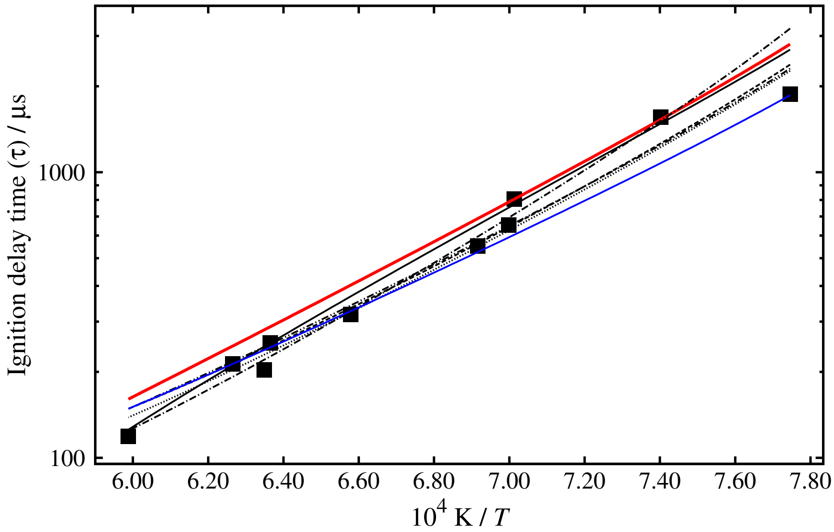
(e)



(f)

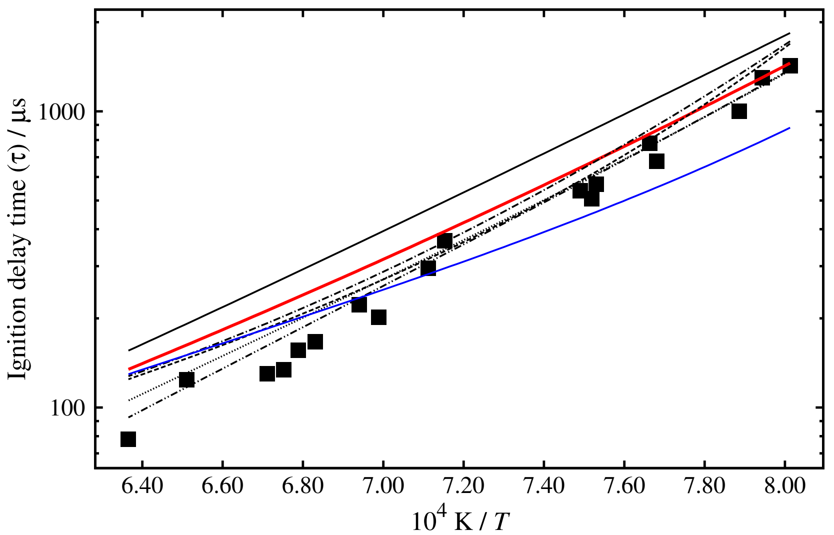
S97 Shock tube ignition delay times of methane/ethane/oxygen/argon mixtures. Symbols are experimental data [63] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

0.26% CH_4, 0.09% C_2H_6, 1.65% O_2, 98.0% Ar, Φ = 0.5, p = 1.0 atm



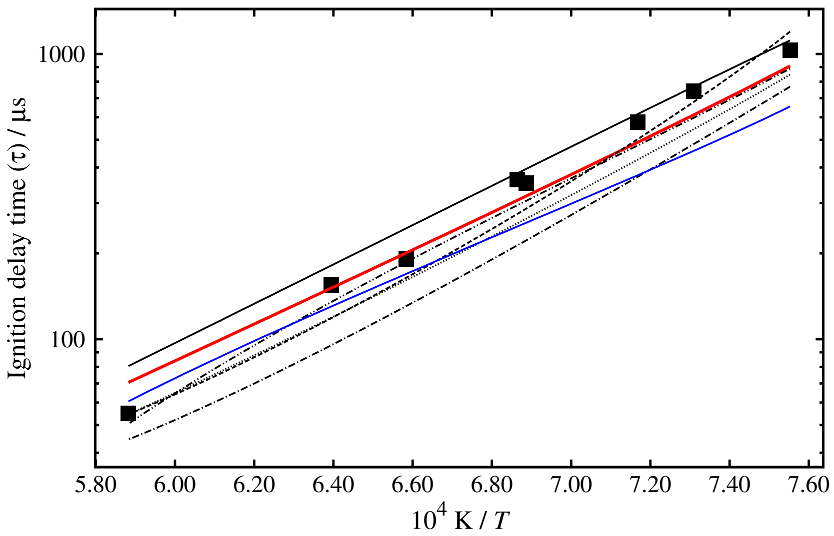
(a)

0.15% CH_4, 0.15% C_2H_6, 1.69% O_2, 98.0% Ar, Φ = 0.5, p = 1.0 atm



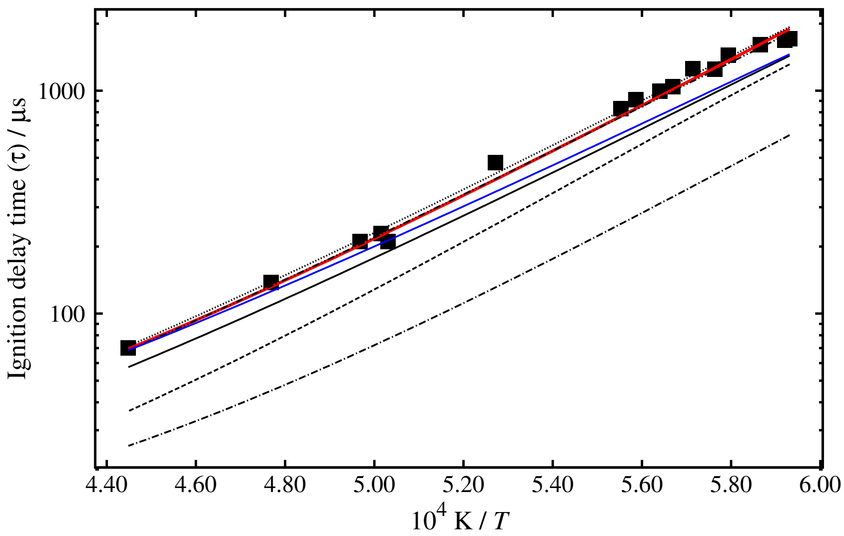
(b)

0.12% CH_4, 0.36% C_2H_6, 1.52% O_2, 98.0% Ar, Φ = 1.0, p = 1.0 atm



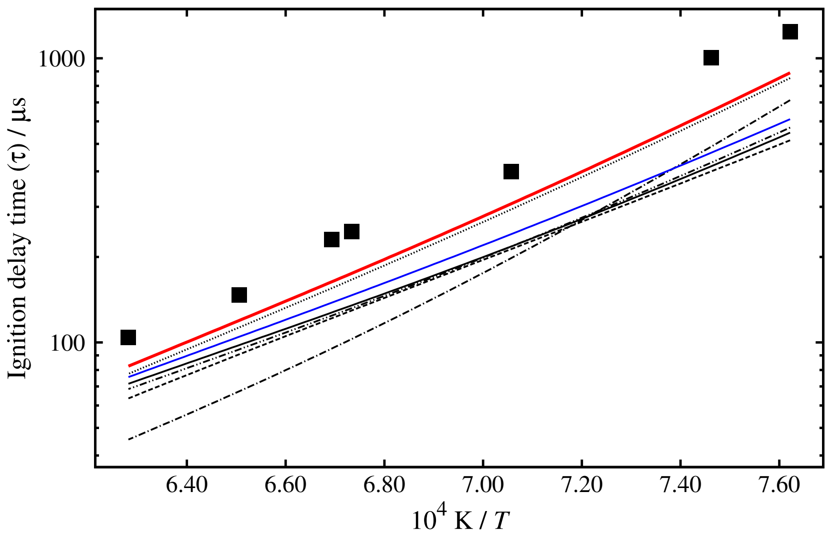
(c)

0.67% CH_4, 1.33% O_2, 98.0% Ar, Φ = 1.0, p = 1.0 atm



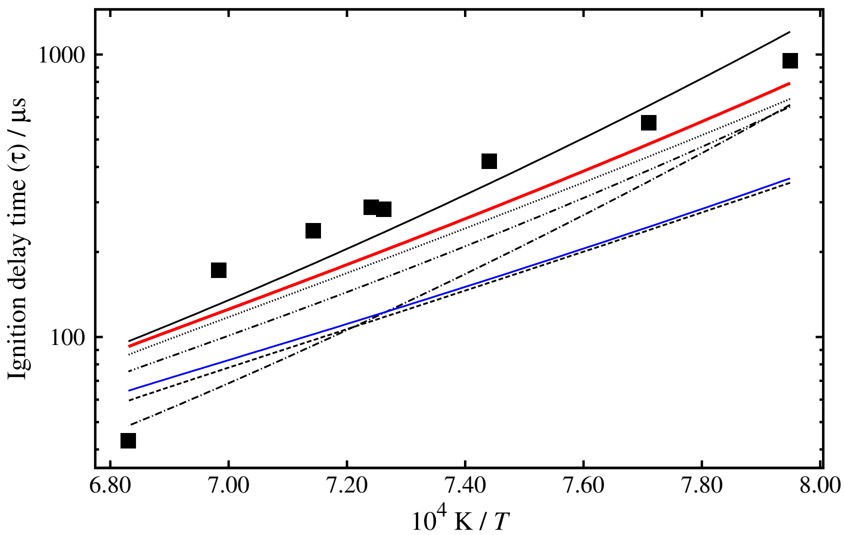
(d)

5.56% CH_4, 1.85% C_2H_6, 17.59% O_2, 75.0% Ar, Φ = 1.0, p = 1.0 atm

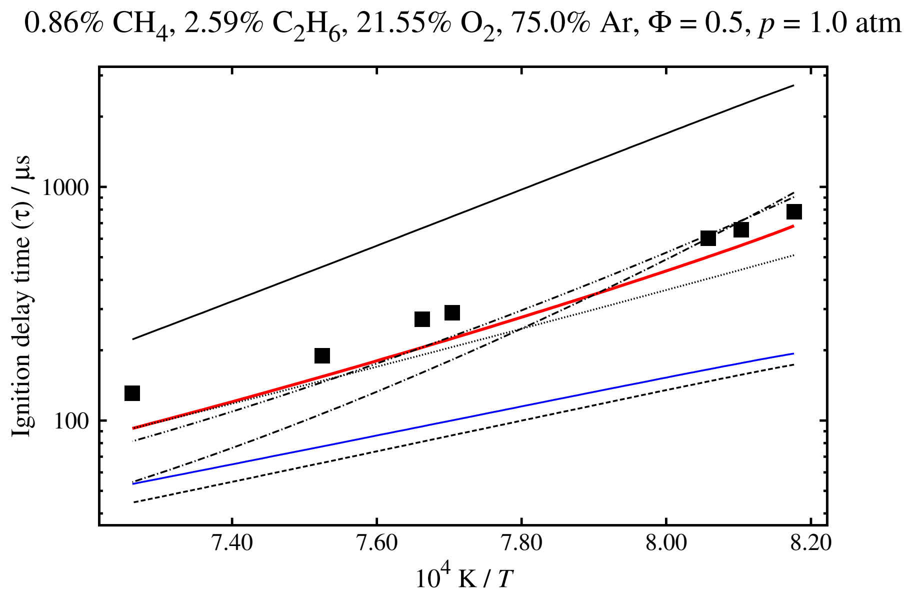


(e)

3.33% CH_4, 3.33% C_2H_6, 18.33% O_2, 75.0% Ar, Φ = 1.0, p = 1.0 atm

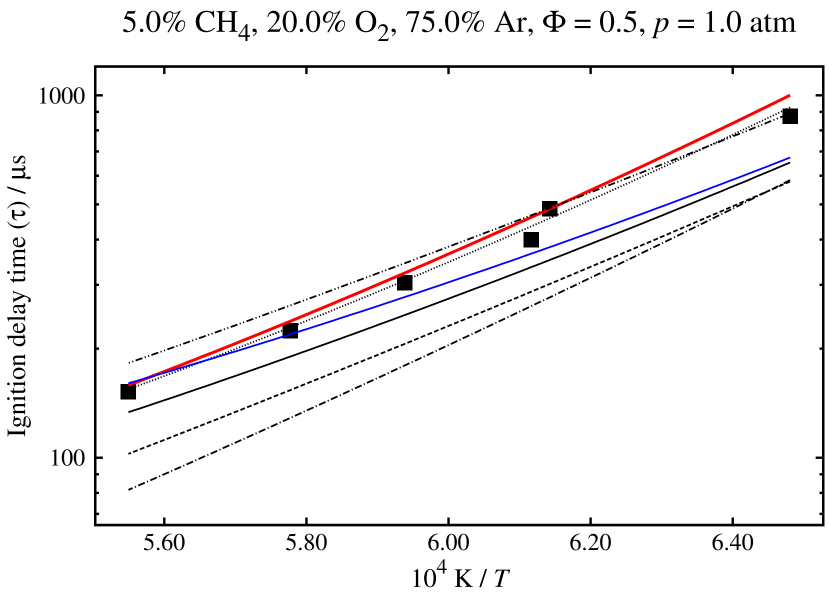


(f)



0.86% CH4, 2.59% C2H6, 21.55% O2, 75.0% Ar, Φ = 0.5, p = 1.0 atm
Ignition delay time (τ) / µs
1000
100
7.40
7.60
7.80
8.00
8.20
10^4 K / T

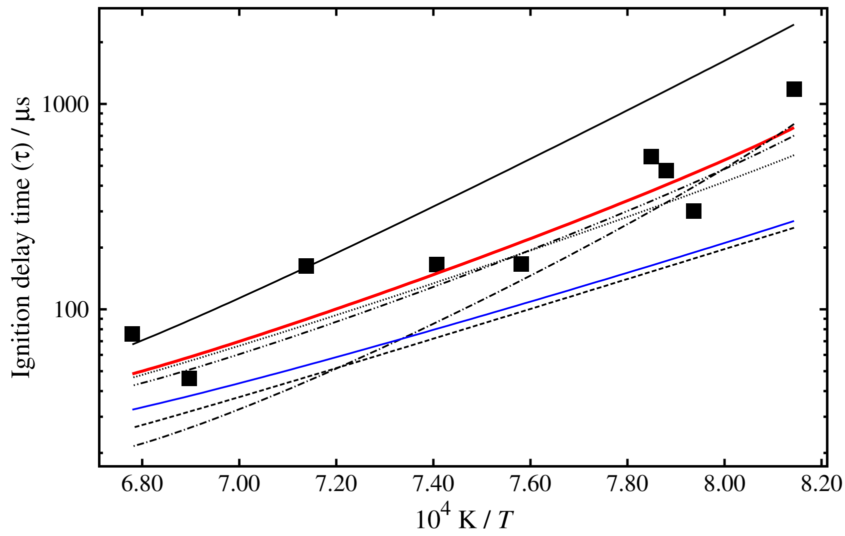
(g)



5.0% CH4, 20.0% O2, 75.0% Ar, Φ = 0.5, p = 1.0 atm
Ignition delay time (τ) / µs
1000
100
5.60
5.80
6.00
6.20
6.40
10^4 K / T

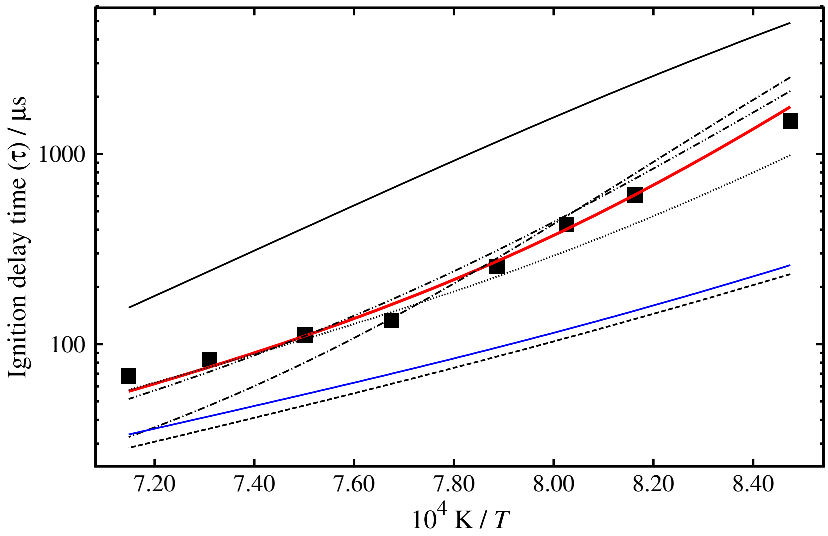
(h)

5.56% C_2H_6, 19.44% O_2, 75.0% Ar, Φ = 1.0, p = 1.0 atm

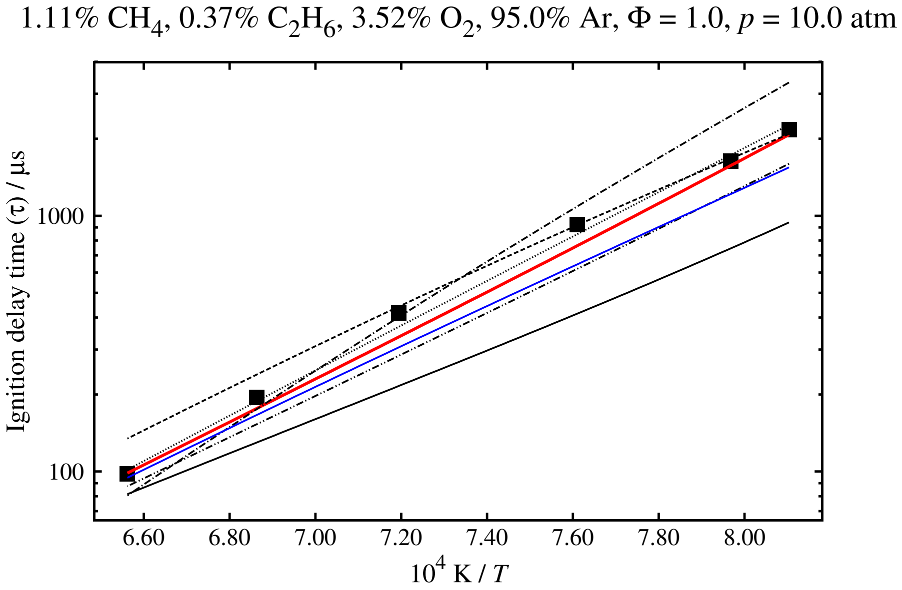


(i)

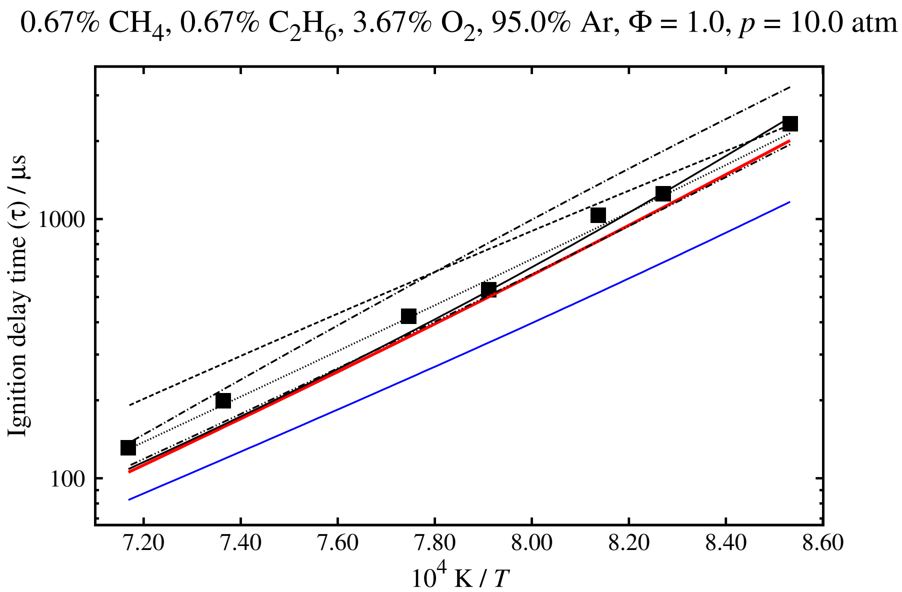
3.13% C_2H_6, 21.88% O_2, 75.0% Ar, Φ = 0.5, p = 1.0 atm



(j)

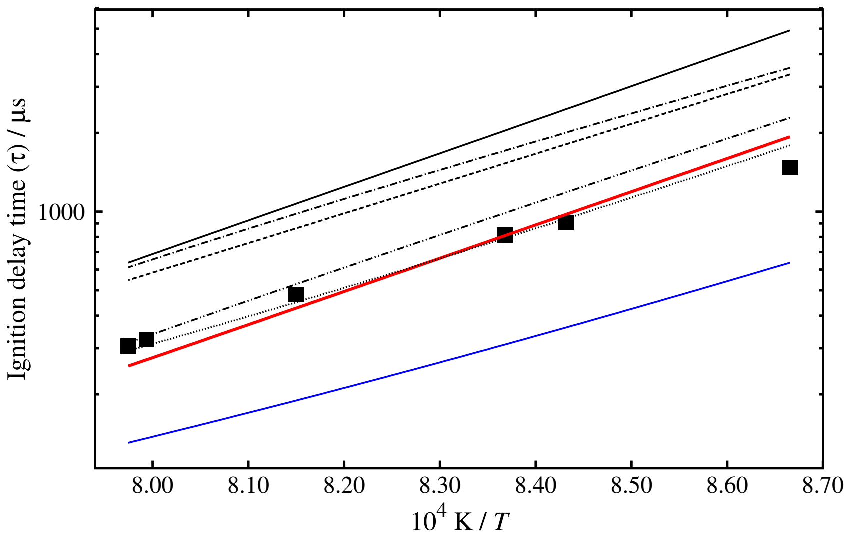

1.11% CH4, 0.37% C2H6, 3.52% O2, 95.0% Ar, Φ = 1.0, p = 10.0 atm
Ignition delay time (τ) / μs
1000
100
6.60
6.80
7.00
7.20
7.40
7.60
7.80
8.00
10^4 K / T

(k)


0.67% CH4, 0.67% C2H6, 3.67% O2, 95.0% Ar, Φ = 1.0, p = 10.0 atm
Ignition delay time (τ) / μs
1000
100
7.20
7.40
7.60
7.80
8.00
8.20
8.40
8.60
10^4 K / T

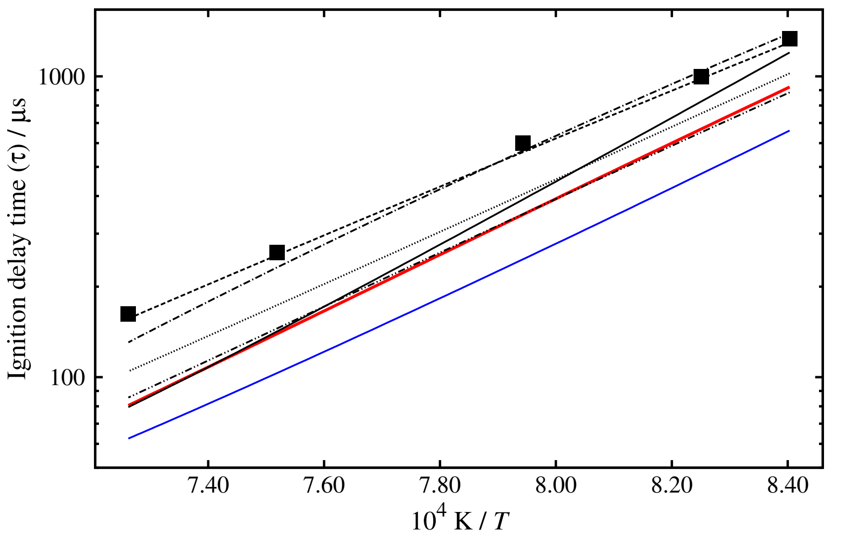
(l)

0.17% CH_4, 0.52% C_2H_6, 4.31% O_2, 95.0% Ar, Φ = 0.5, p = 10.0 atm



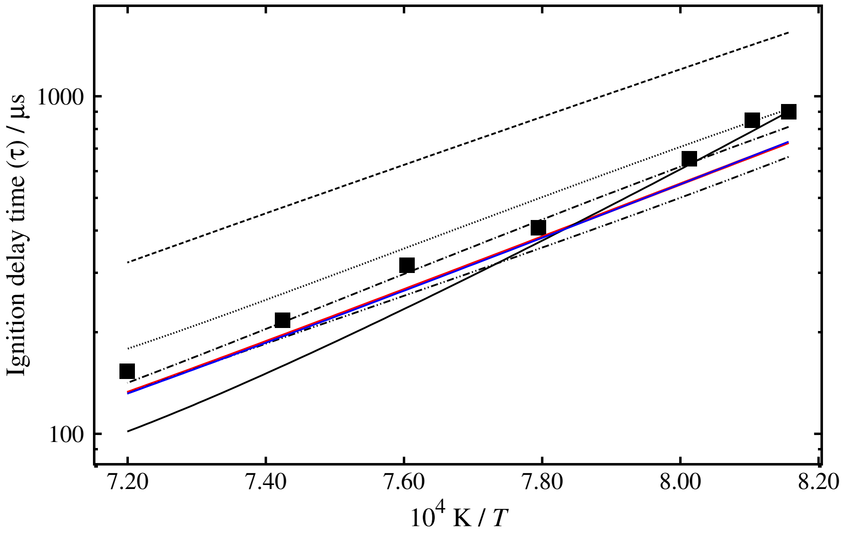
(m)

0.67% CH_4, 0.67% C_2H_6, 3.67% O_2, 95.0% Ar, Φ = 1.0, p = 30.0 atm



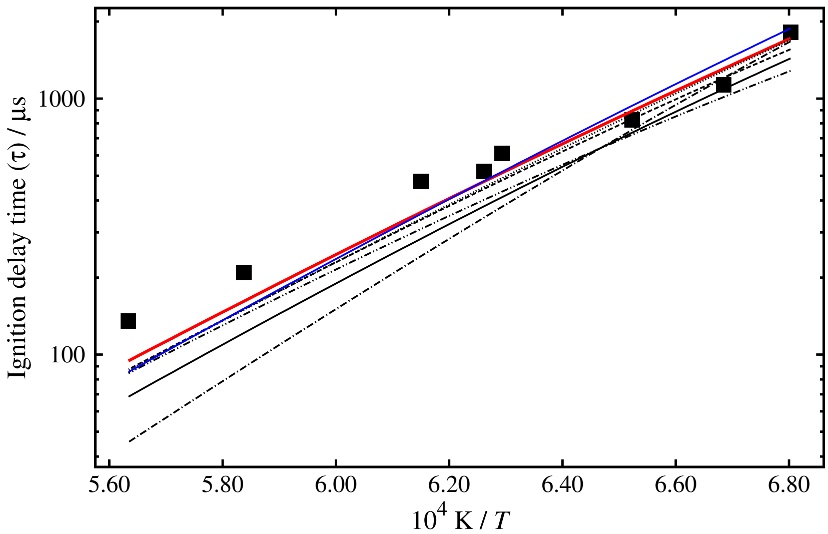
(n)

0.49% CH_4, 1.46% C_2H_6, 3.05% O_2, 95.0% Ar, Φ = 2.0, p = 10.0 atm



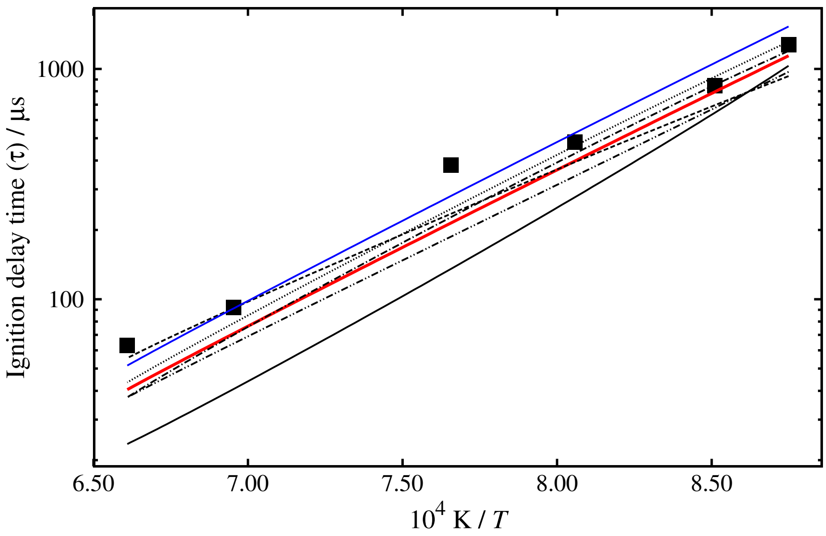
(o)

2.5% CH_4, 2.5% O_2, 95.0% Ar, Φ = 2.0, p = 30.0 atm



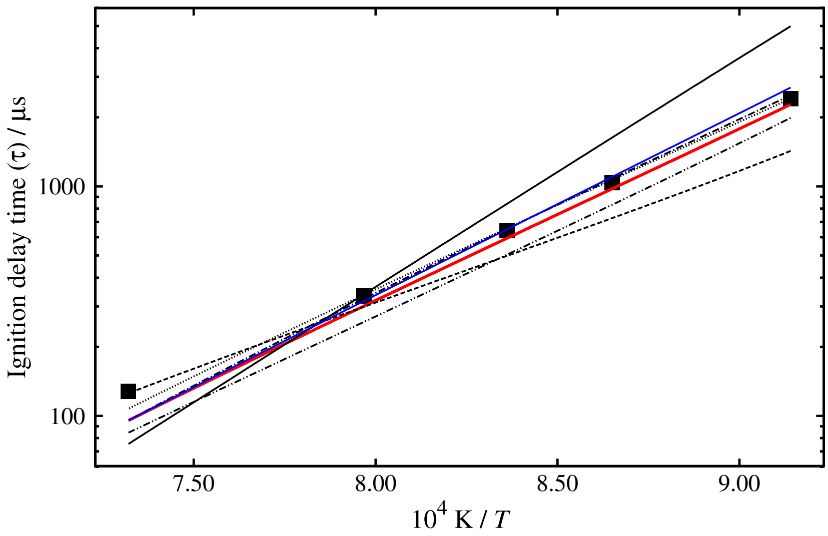
(p)

5.14% CH_4, 1.71% C_2H_6, 8.14% O_2, 85.0% Ar, Φ = 2.0, p = 30.0 atm



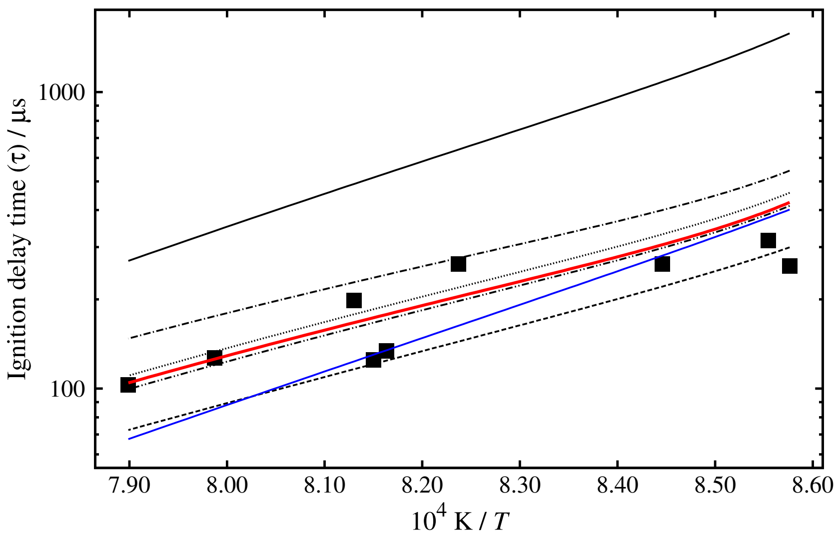
(q)

3.16% CH_4, 3.16% C_2H_6, 8.68% O_2, 85.0% Ar, Φ = 2.0, p = 10.0 atm



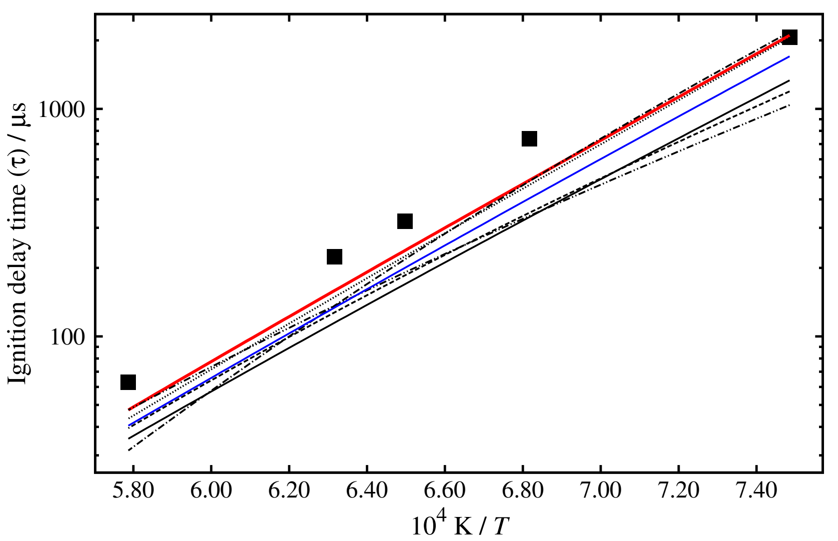
(r)

0.91% CH_4, 2.73% C_2H_6, 11.36% O_2, 85.0% Ar, $\Phi = 1.0$, $p = 30.0$ atm

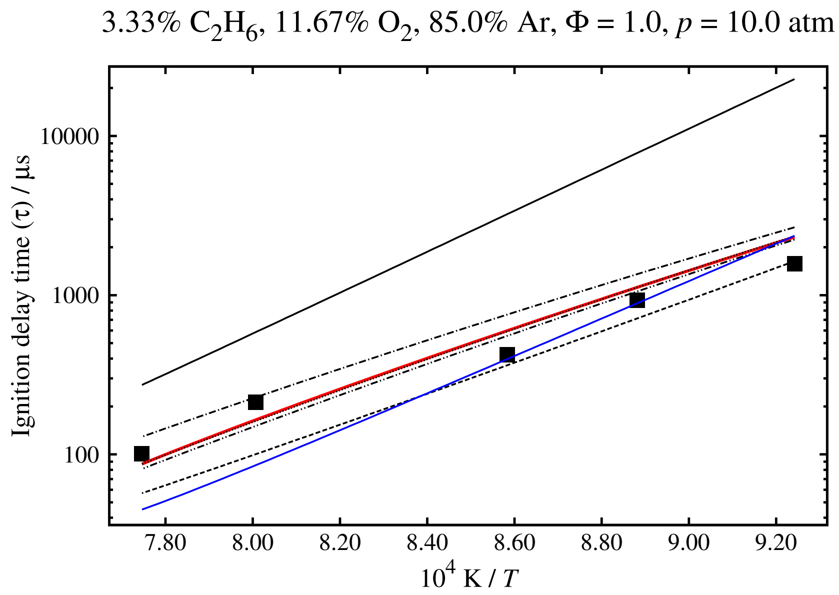


(s)

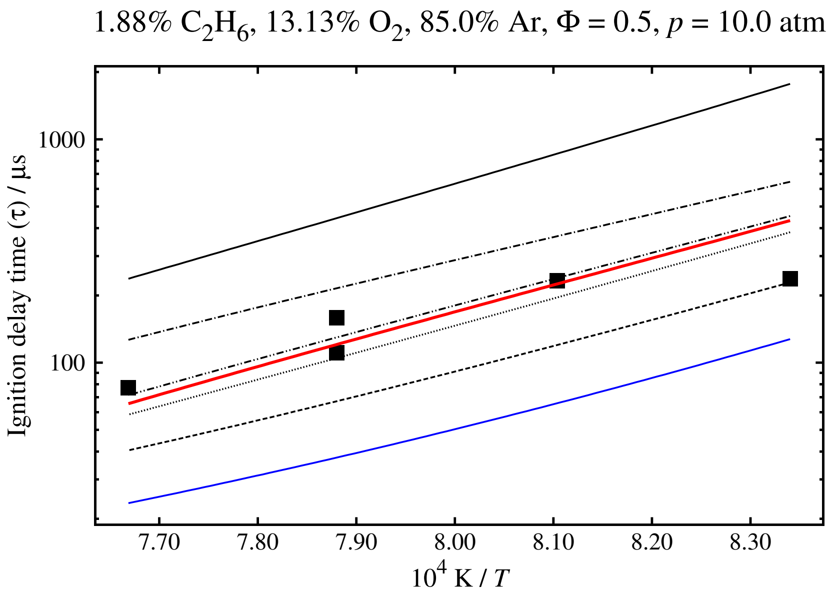
5.0% CH_4, 10.0% O_2, 85.0% Ar, $\Phi = 1.0$, $p = 10.0$ atm



(t)

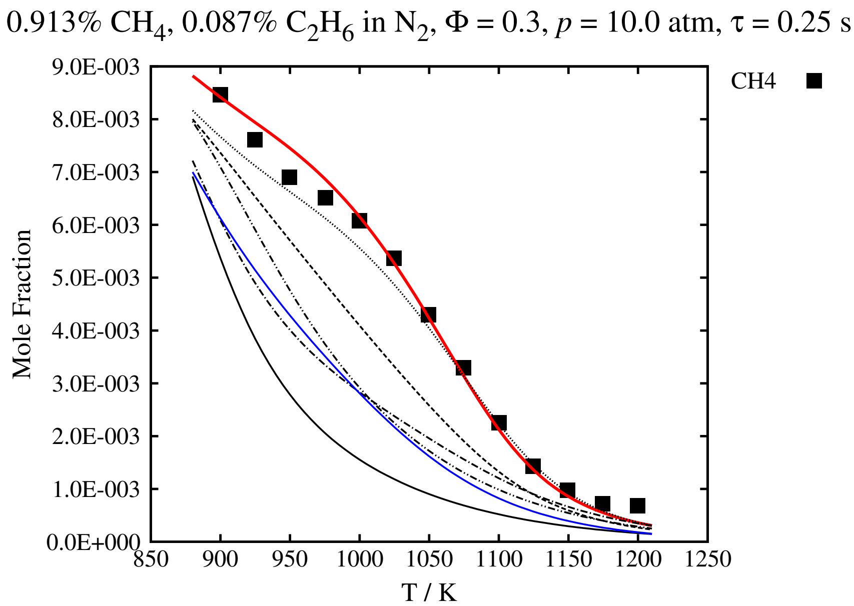


(u)

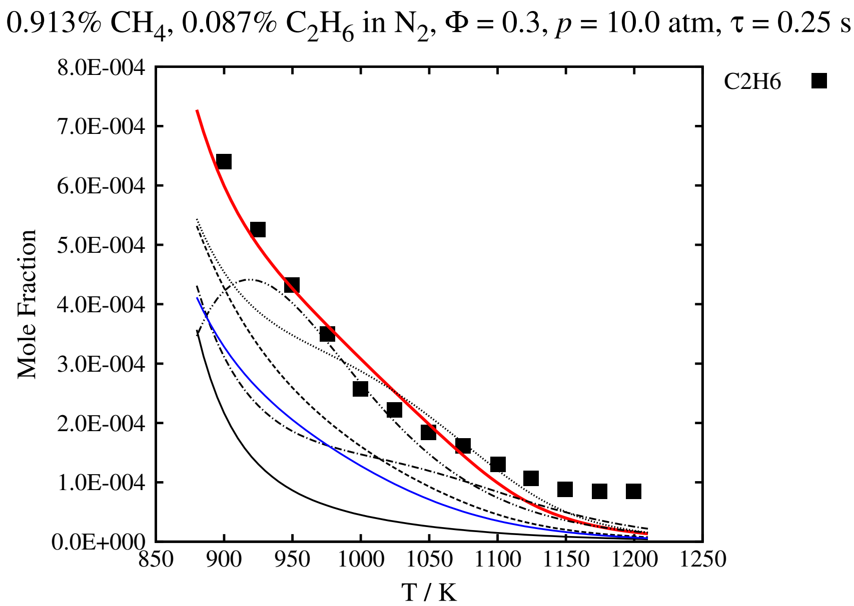


(v)

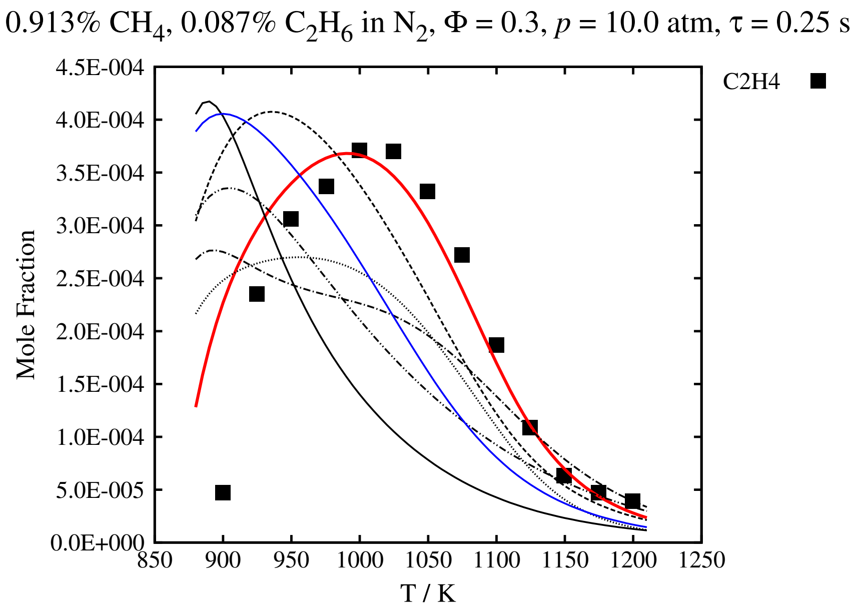
S98 Shock tube ignition delay times of methane/ethane/oxygen/argon mixtures. Symbols are experimental data [64] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

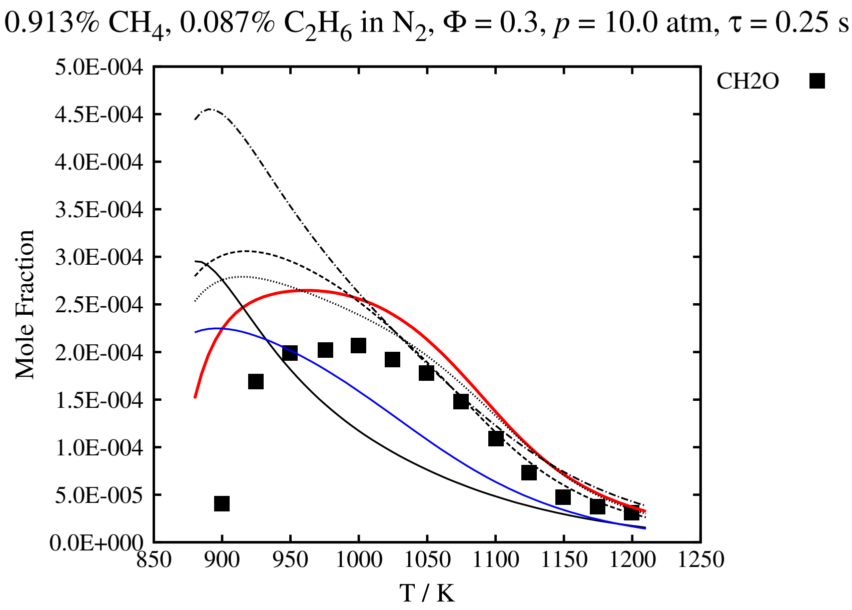
(a)


0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
C2H6
Mole Fraction
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

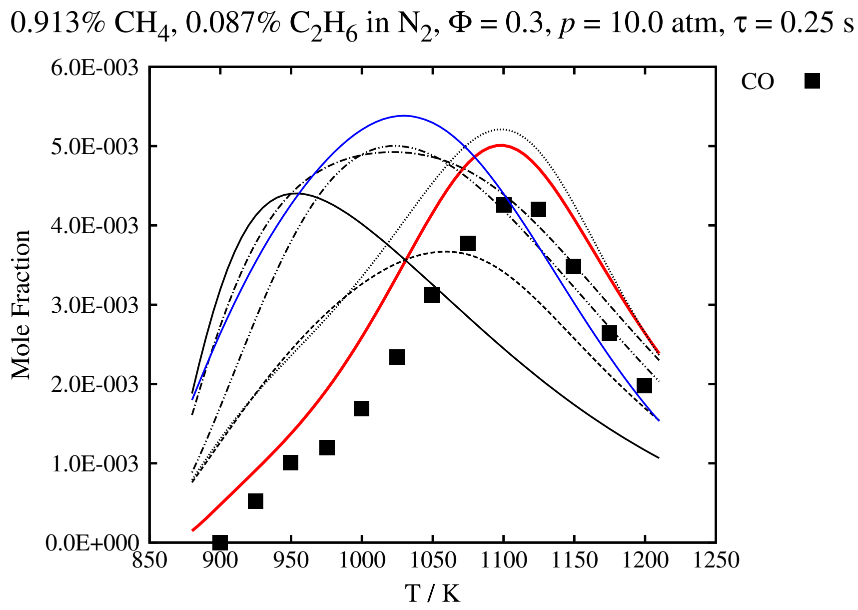
(b)


0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
C2H4
Mole Fraction
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

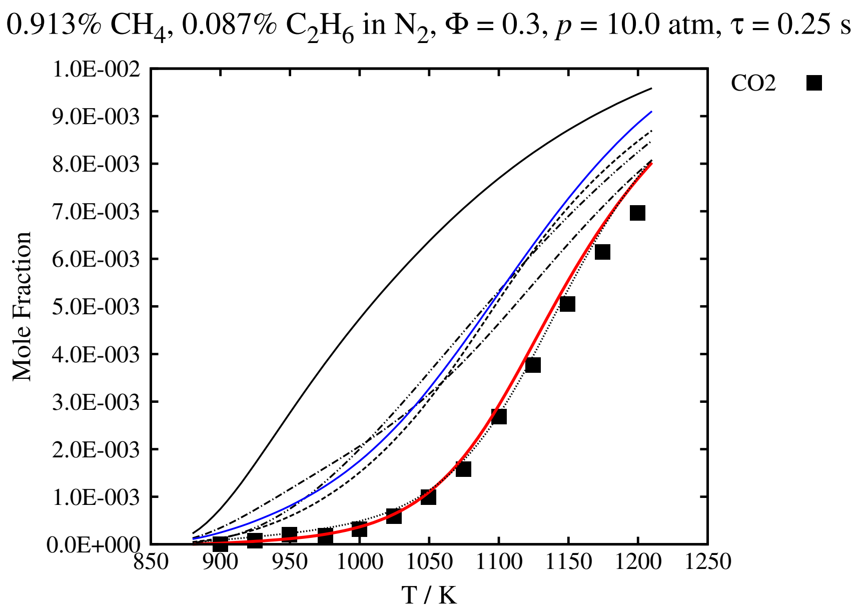
(c)


0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
5.0E-004
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

(d)

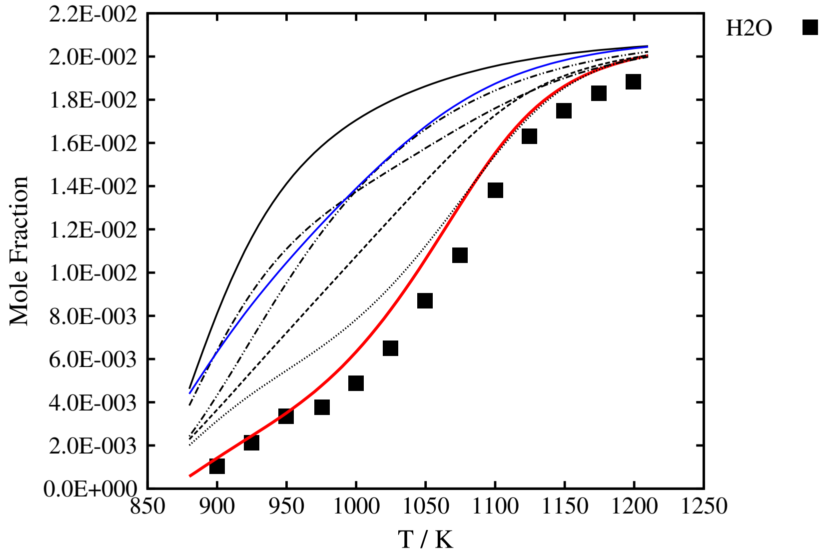

0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

(e)


0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CO2
Mole Fraction
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

(f)

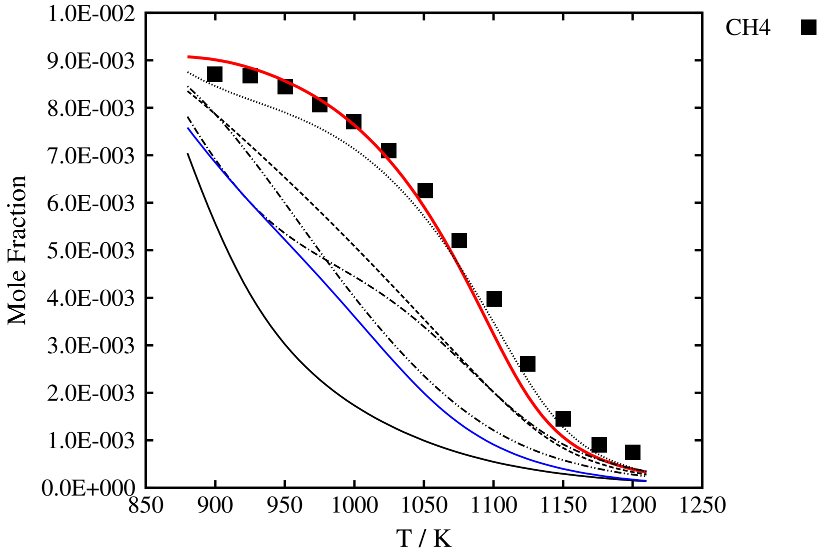
0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.3, p = 10.0 atm, τ = 0.25 s



(g)

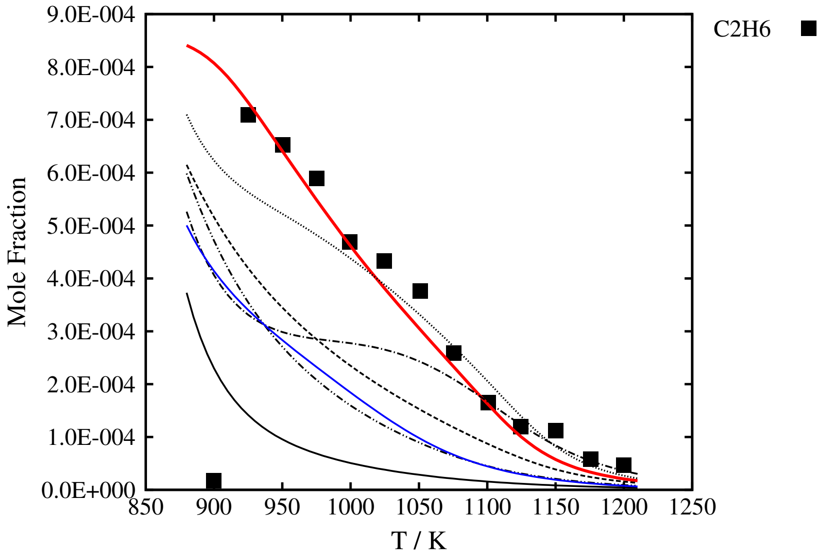
S99 Jet-stirred reactor species profiles of methane/ethane/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. —— AramcoMech 1.3, —— GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, —— USC II.

0.913% CH_4, 0.087% C_2H_6 in N_2, $\Phi = 0.6$, $p = 10.0$ atm, $\tau = 0.25$ s

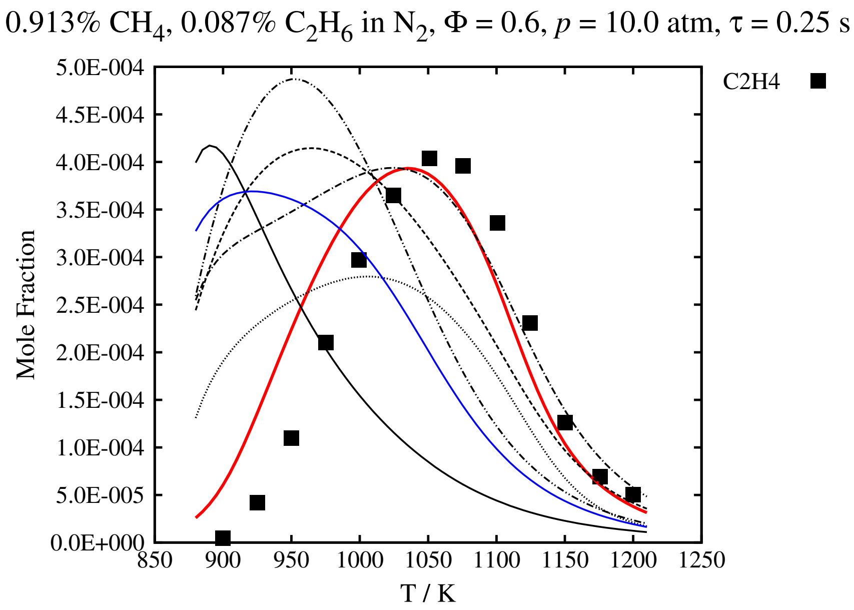


(a)

0.913% CH_4, 0.087% C_2H_6 in N_2, $\Phi = 0.6$, $p = 10.0$ atm, $\tau = 0.25$ s

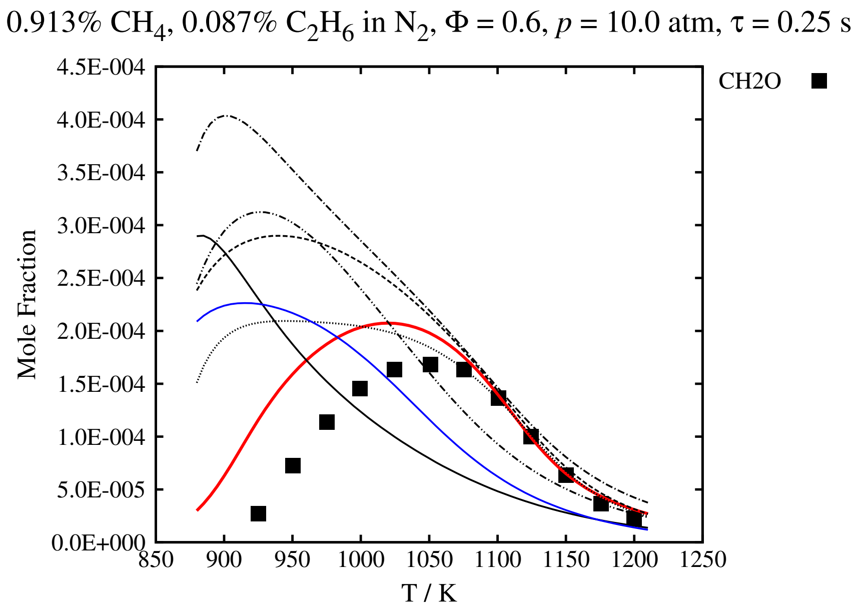


(b)



0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.25 s
C2H4
Mole Fraction
T / K

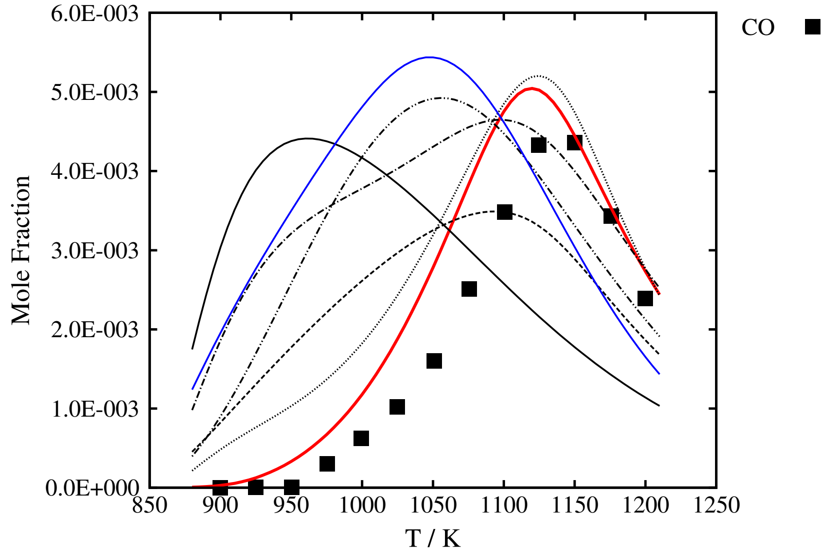
(c)



0.913% CH_4, 0.087% C_2H_6 in N_2, Φ = 0.6, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
T / K

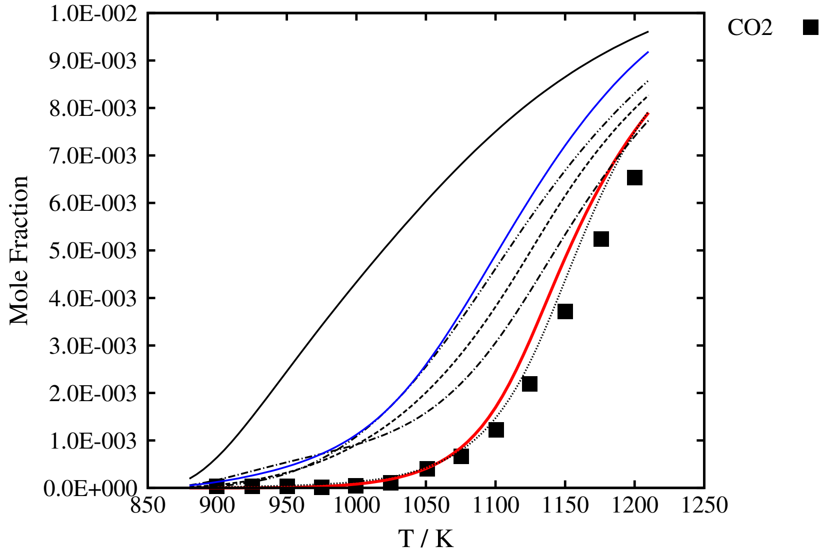
(d)

0.913% CH_4, 0.087% C_2H_6 in N_2, $\Phi = 0.6$, $p = 10.0$ atm, $\tau = 0.25$ s

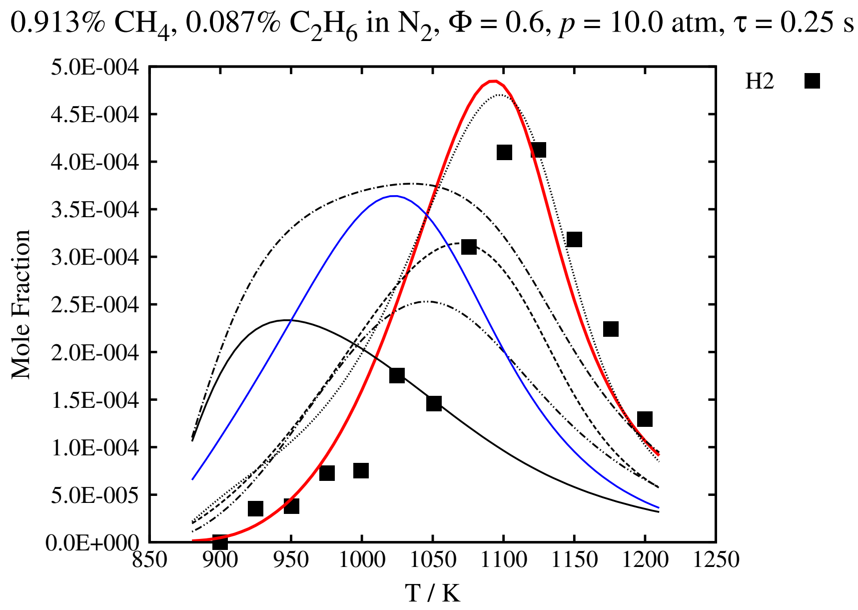


(e)

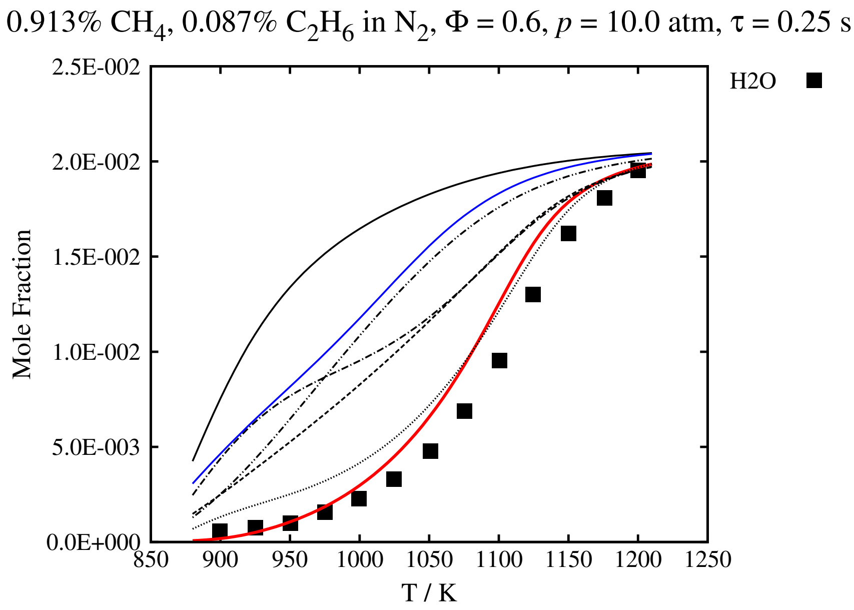
0.913% CH_4, 0.087% C_2H_6 in N_2, $\Phi = 0.6$, $p = 10.0$ atm, $\tau = 0.25$ s



(f)

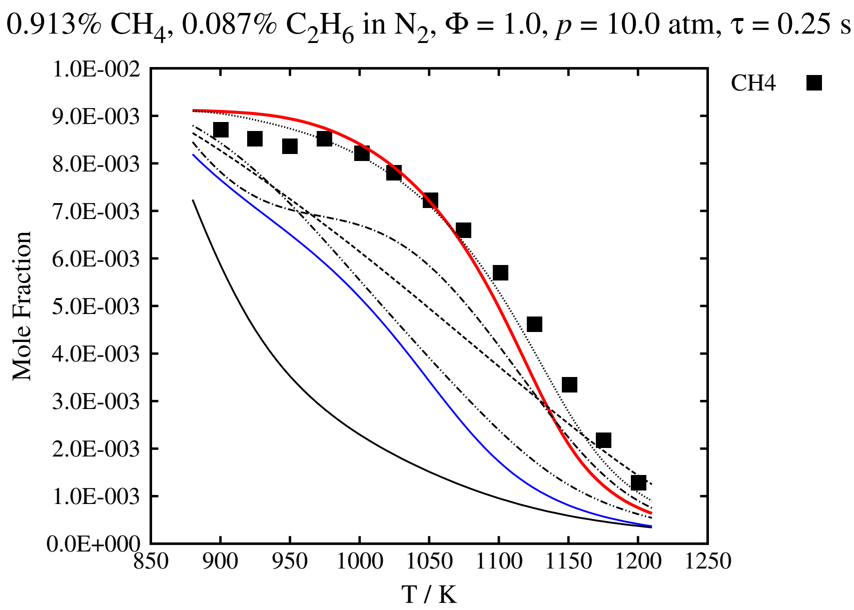


(g)

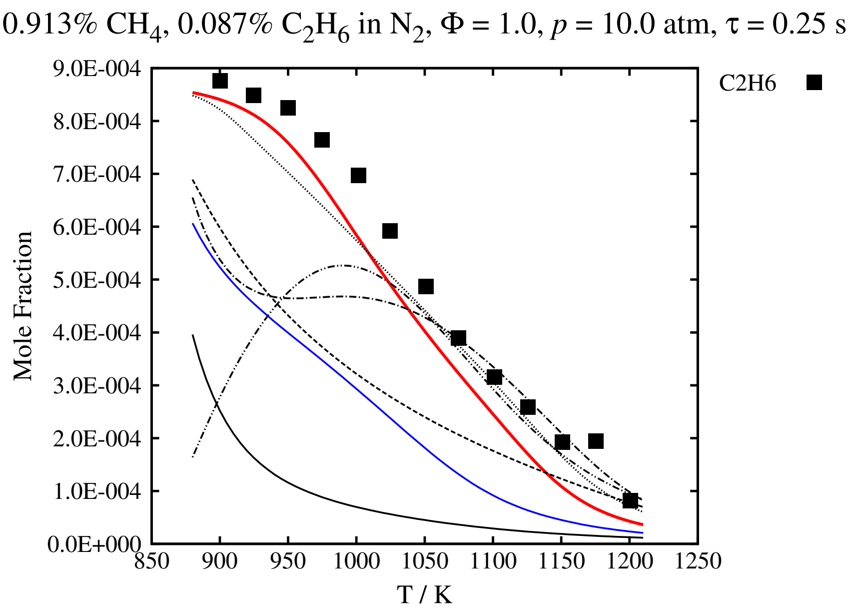


(h)

S100 Jet-stirred reactor species profiles of methane/ethane/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

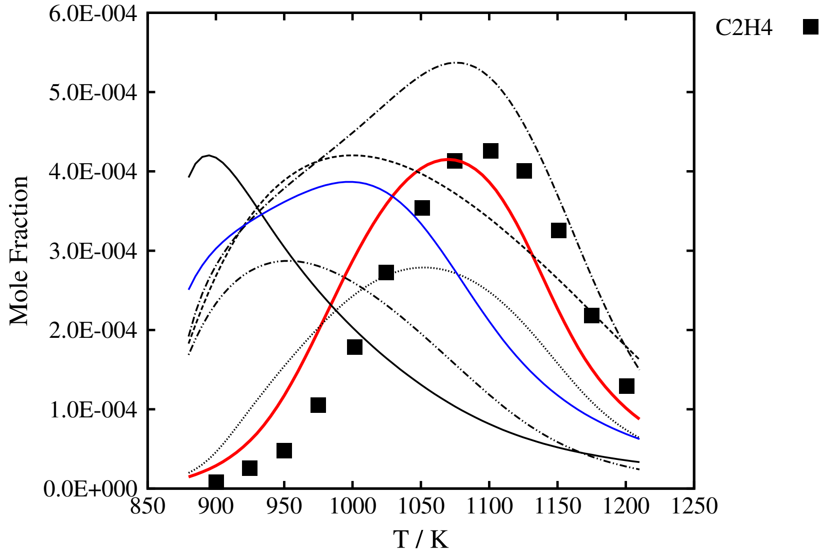

0.913% CH4, 0.087% C2H6 in N2, Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
1.0E-002
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K

(a)


0.913% CH4, 0.087% C2H6 in N2, Φ = 1.0, p = 10.0 atm, τ = 0.25 s
C2H6
Mole Fraction
9.0E-004
8.0E-004
7.0E-004
6.0E-004
5.0E-004
4.0E-004
3.0E-004
2.0E-004
1.0E-004
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K

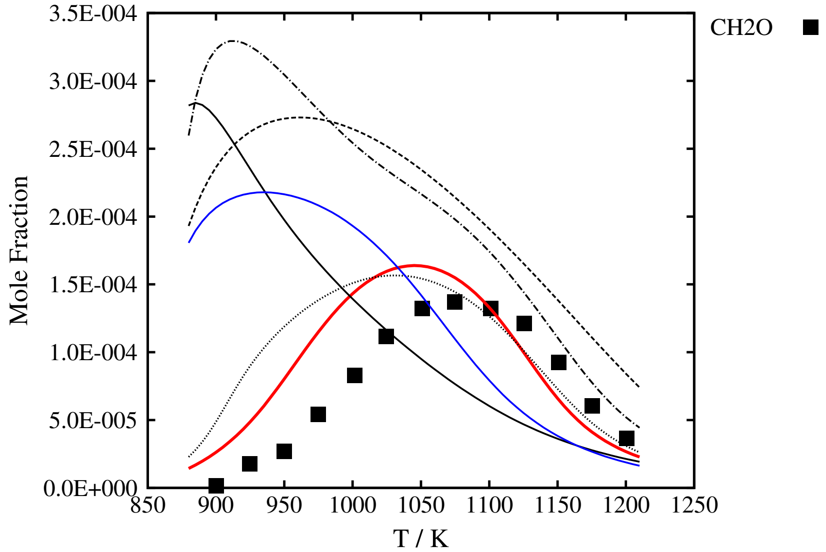
(b)

0.913% CH_4, 0.087% C_2H_6 in N_2, $\Phi = 1.0$, $p = 10.0$ atm, $\tau = 0.25$ s

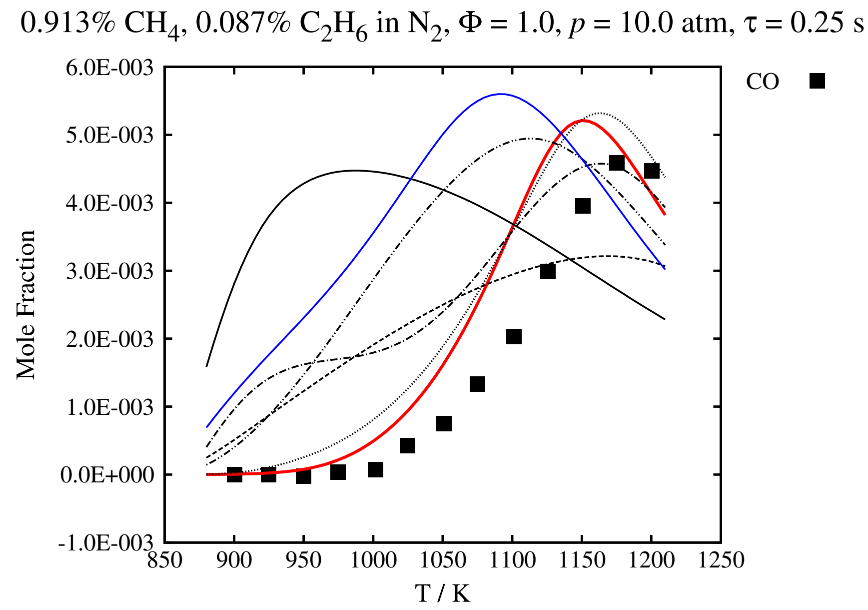


(c)

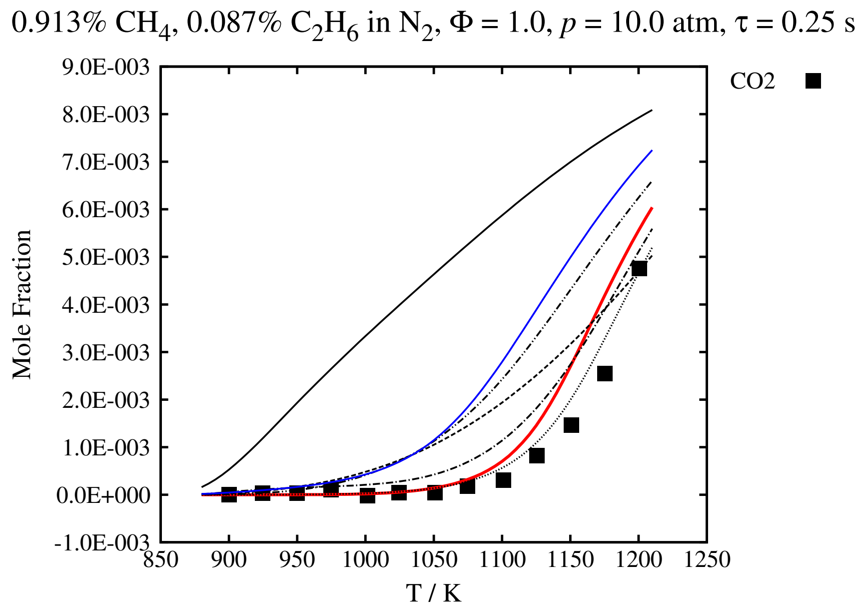
0.913% CH_4, 0.087% C_2H_6 in N_2, $\Phi = 1.0$, $p = 10.0$ atm, $\tau = 0.25$ s



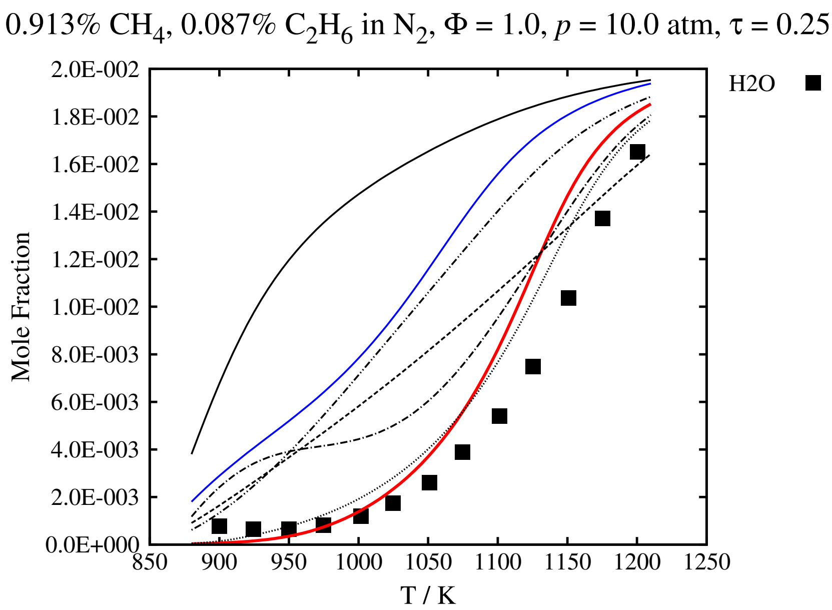
(d)


0.913% CH4, 0.087% C2H6 in N2, Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
-1.0E-003
850 900 950 1000 1050 1100 1150 1200 1250
T / K

(e)

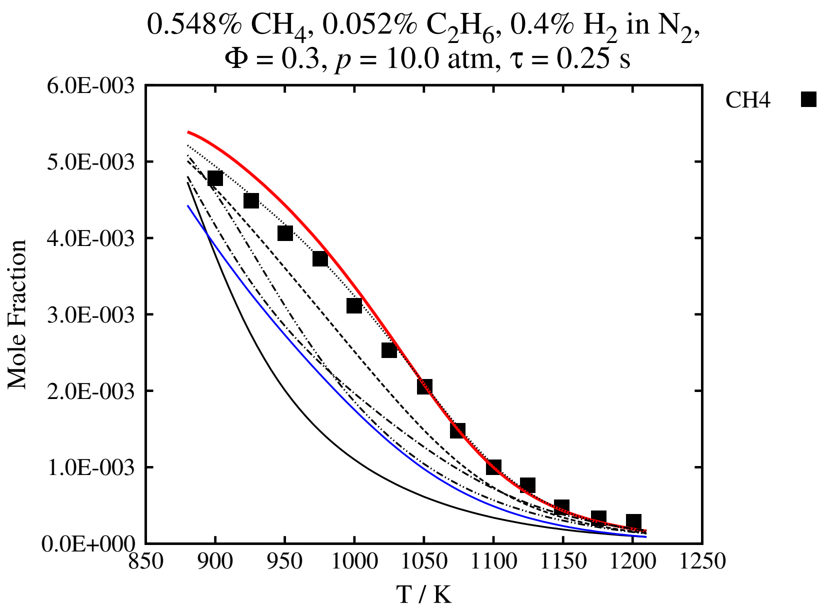

0.913% CH4, 0.087% C2H6 in N2, Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CO2
Mole Fraction
9.0E-003
8.0E-003
7.0E-003
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
-1.0E-003
850 900 950 1000 1050 1100 1150 1200 1250
T / K

(f)

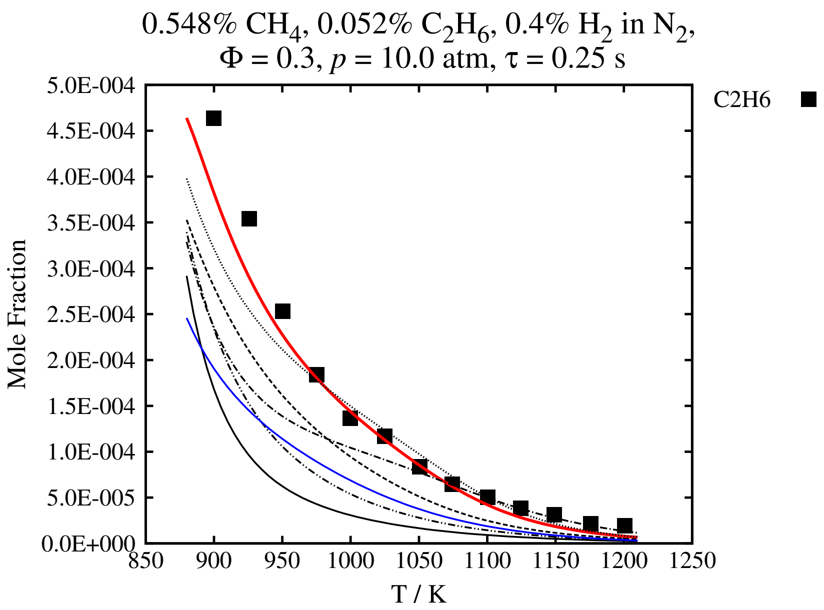


(g)

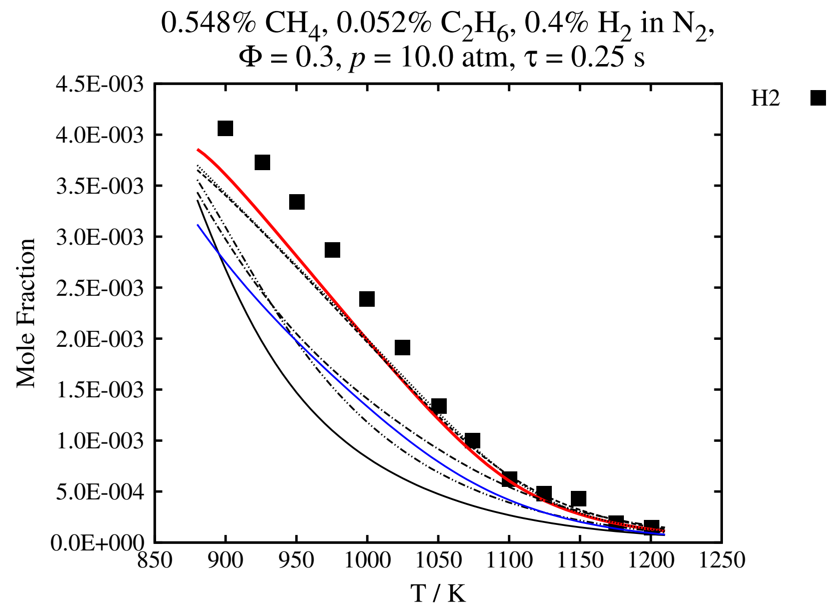
S101 Jet-stirred reactor species profiles of methane/ethane/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.548% CH4, 0.052% C2H6, 0.4% H2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
T / K
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

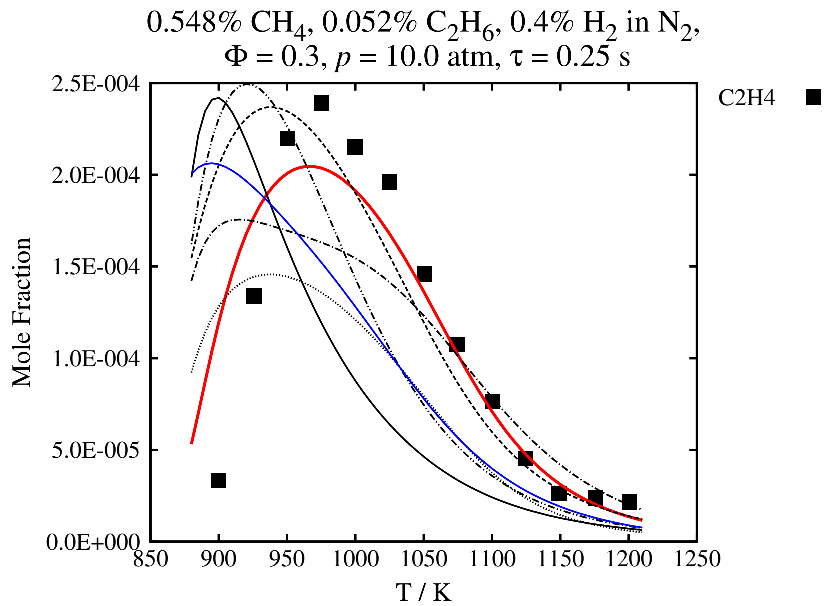
(a)


0.548% CH4, 0.052% C2H6, 0.4% H2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
C2H6
Mole Fraction
T / K
5.0E-004
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

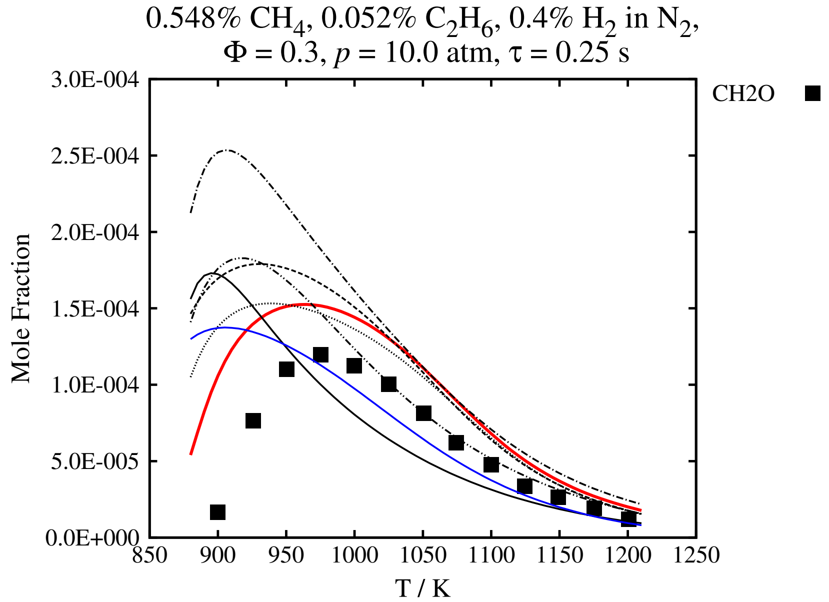
(b)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
$\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s
H2
Mole Fraction
T / K

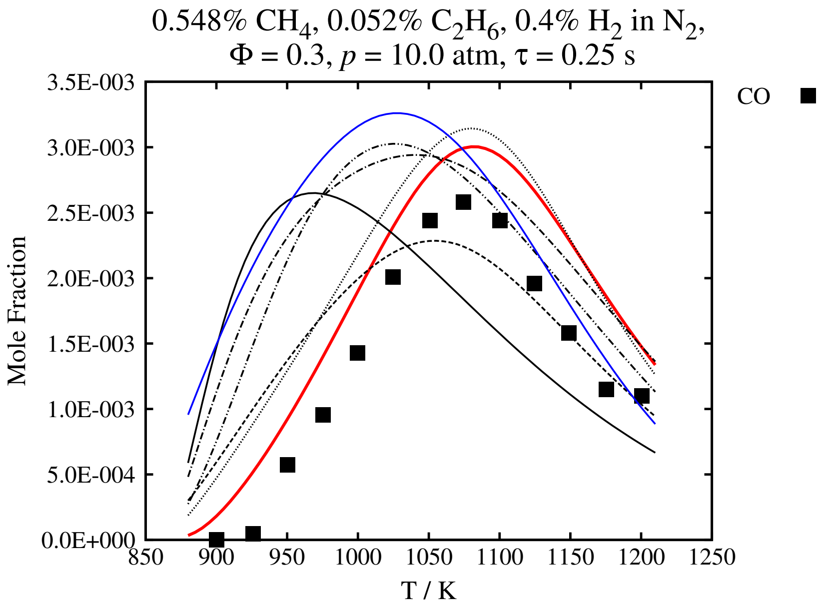
(c)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
$\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s
C2H4
Mole Fraction
T / K

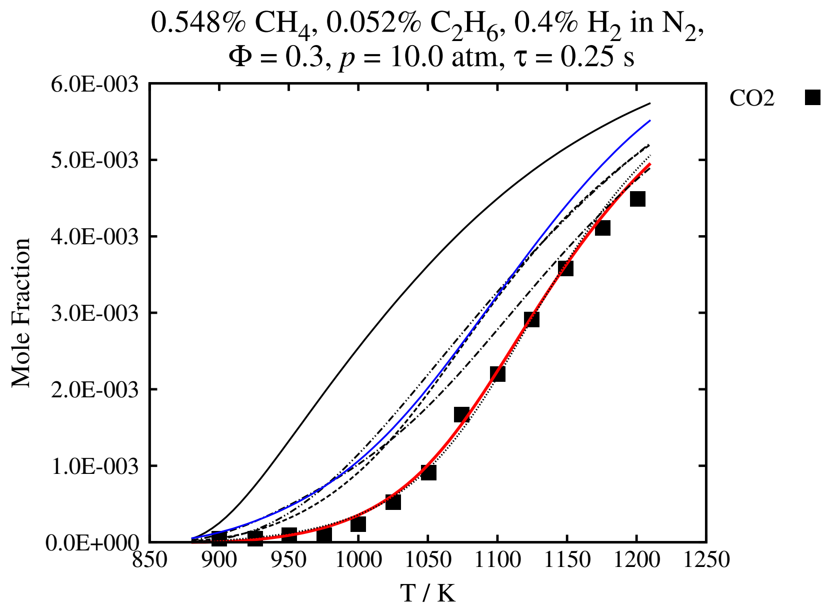
(d)


0.548% CH4, 0.052% C2H6, 0.4% H2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

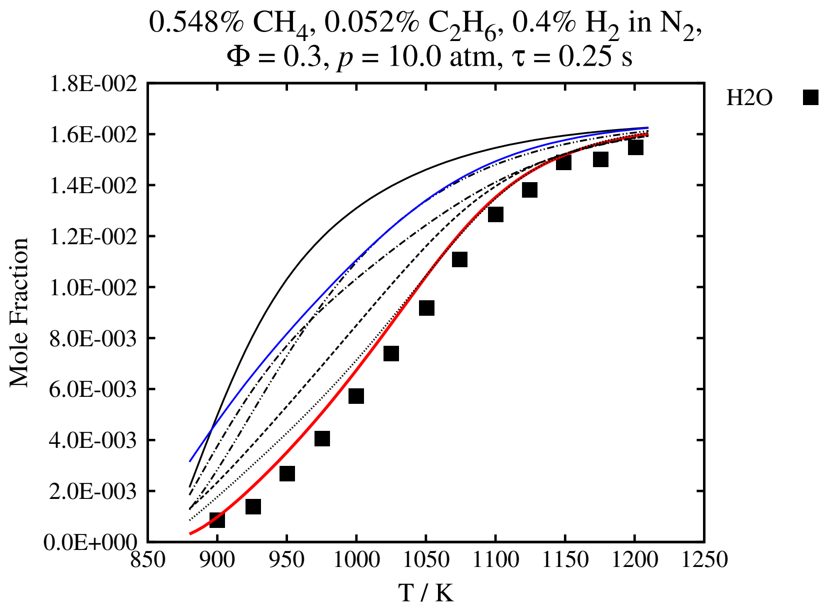
(e)


0.548% CH4, 0.052% C2H6, 0.4% H2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

(f)

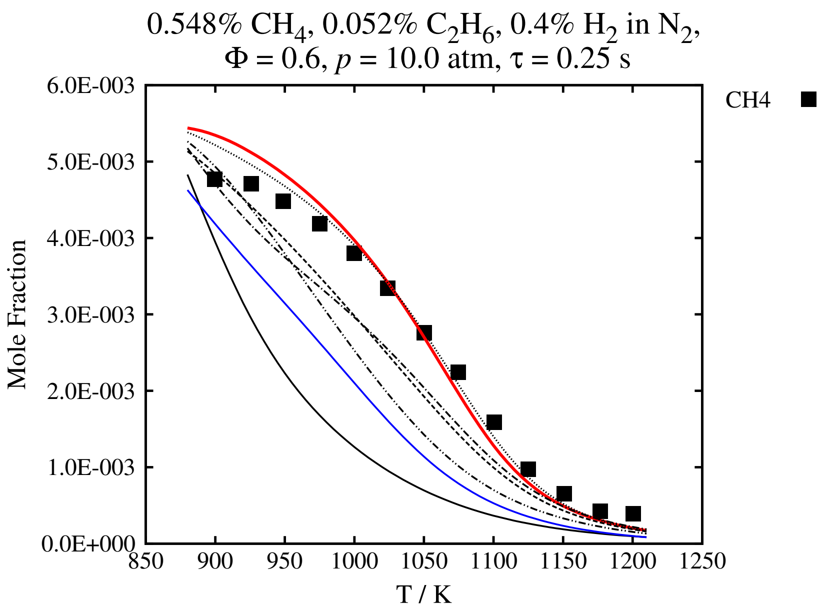


(g)

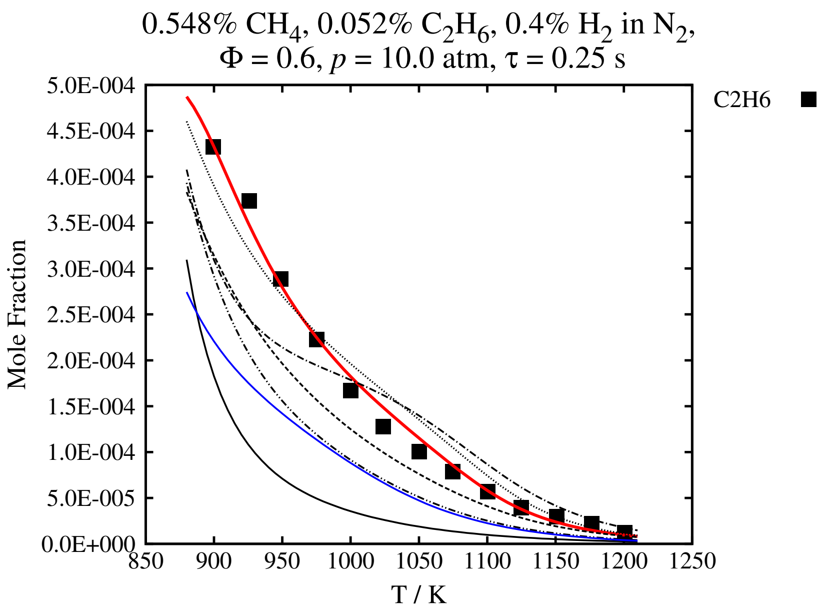


(h)

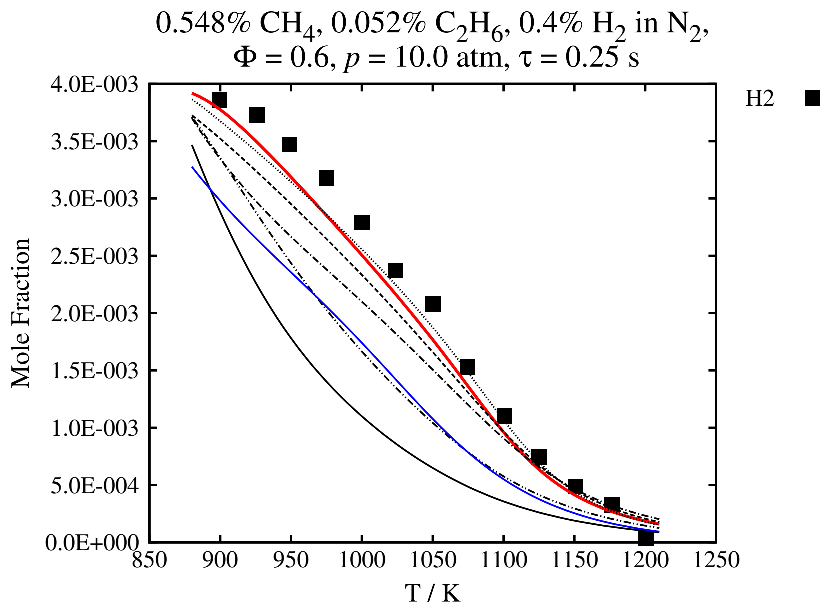
S102 Jet-stirred reactor species profiles of methane/ethane/hydrogen/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, ··· MFC, – · – Ranzi, – · · San Diego Mech, — USC II.


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
T / K
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

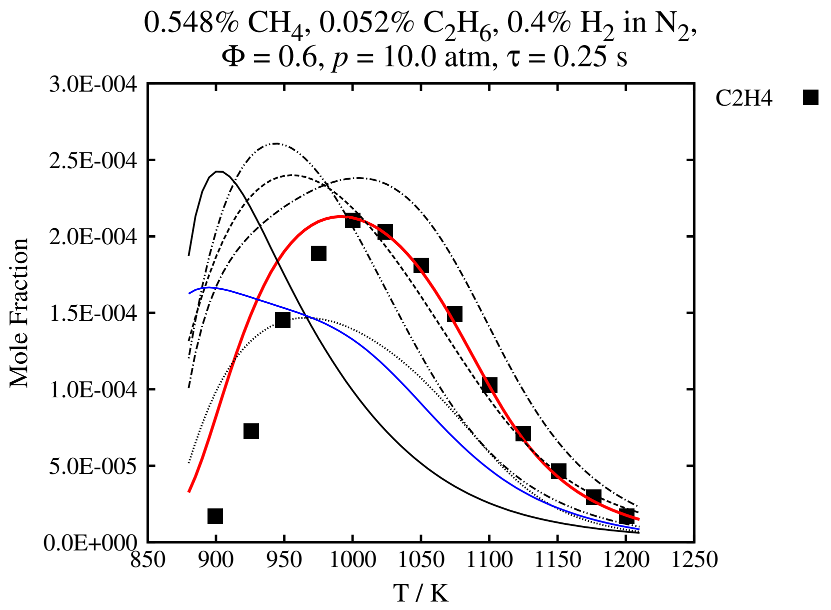
(a)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
C2H6
Mole Fraction
T / K
5.0E-004
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

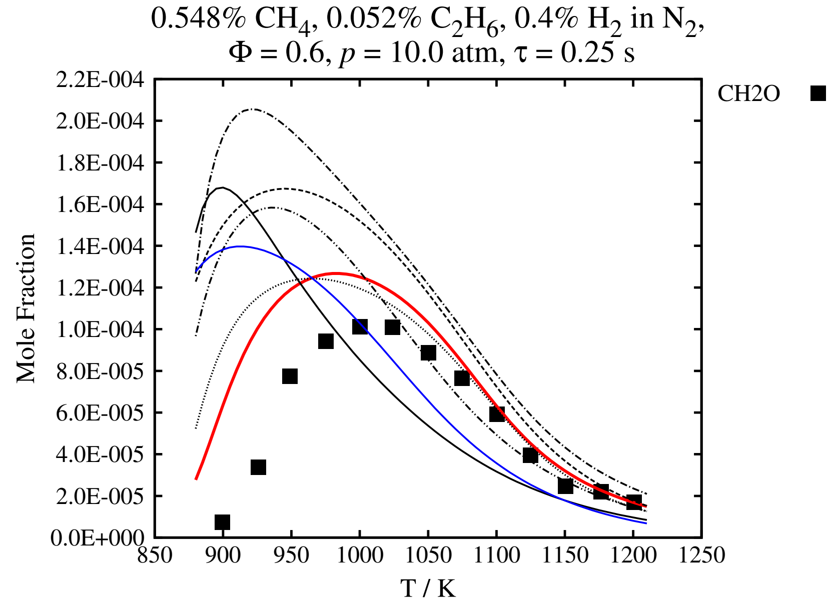
(b)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
H2
Mole Fraction
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

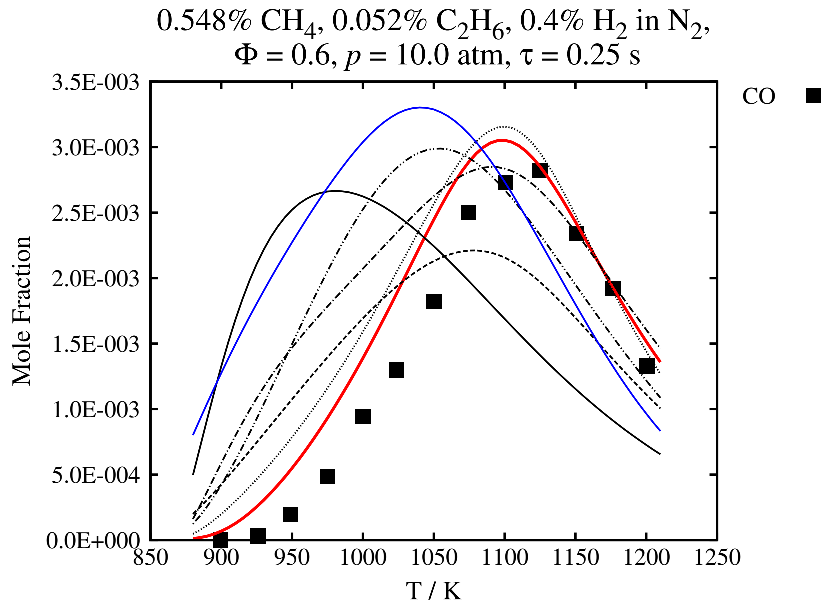
(c)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
C2H4
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

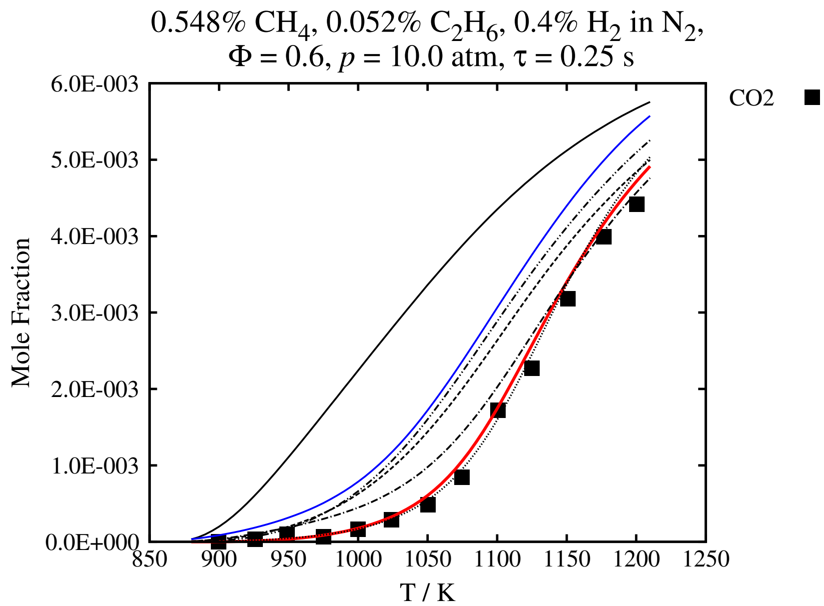
(d)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
T / K
2.2E-004
2.0E-004
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

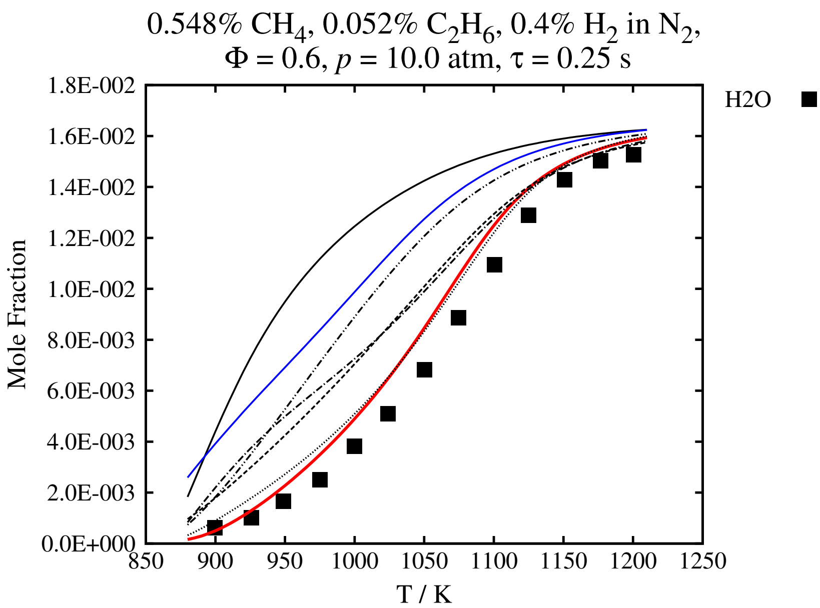
(e)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
T / K
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

(f)

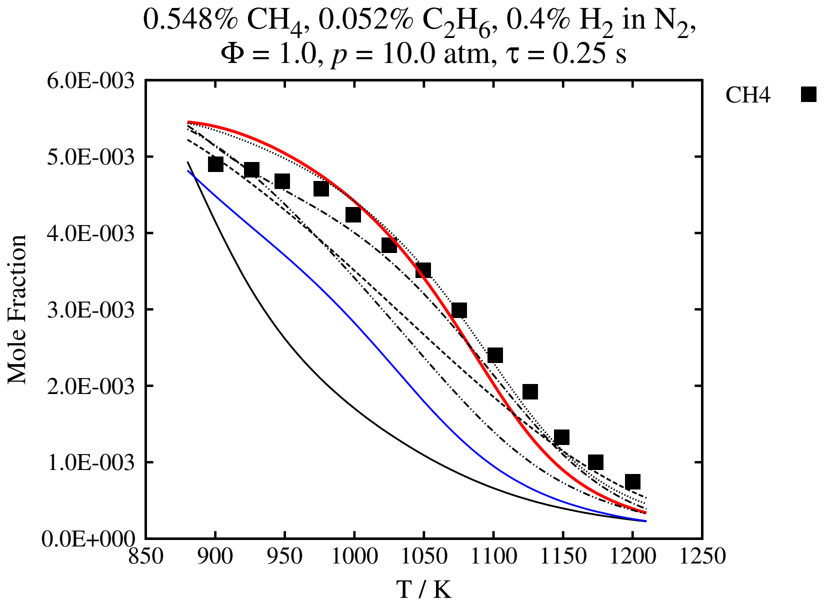


(g)



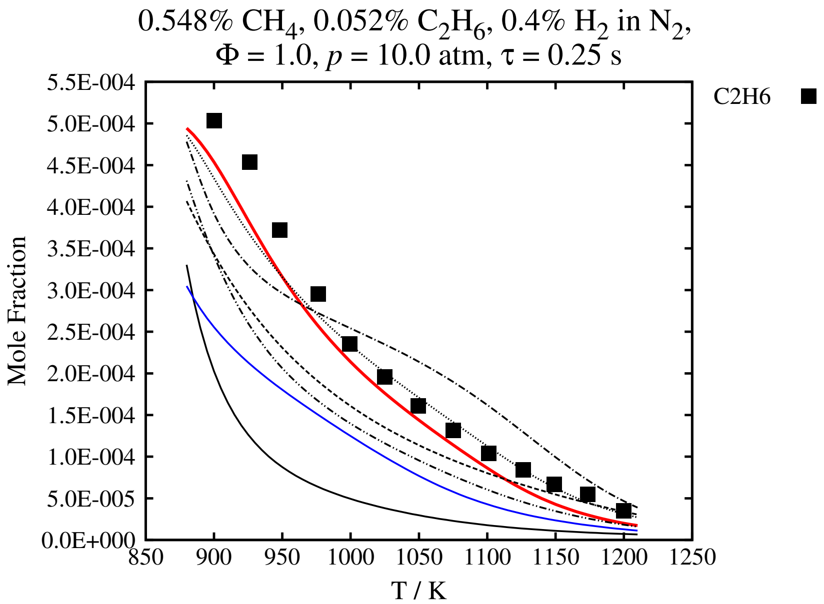
(h)

S103 Jet-stirred reactor species profiles of methane/ethane/hydrogen/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



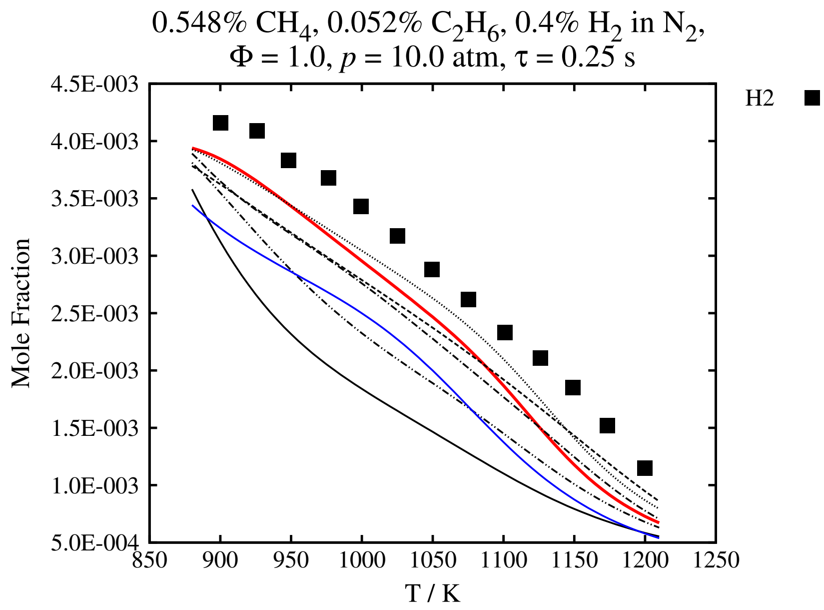
0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
T / K
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

(a)

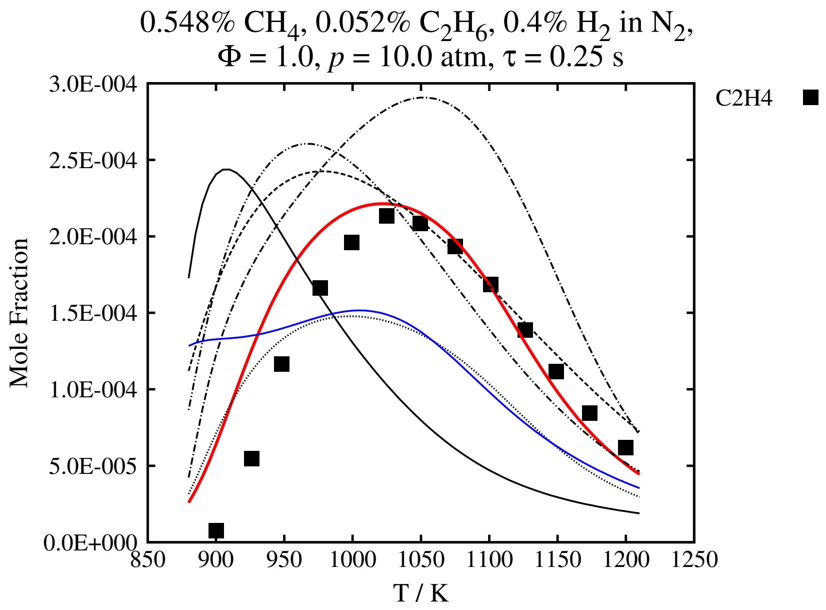


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
C2H6
Mole Fraction
T / K
5.5E-004
5.0E-004
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

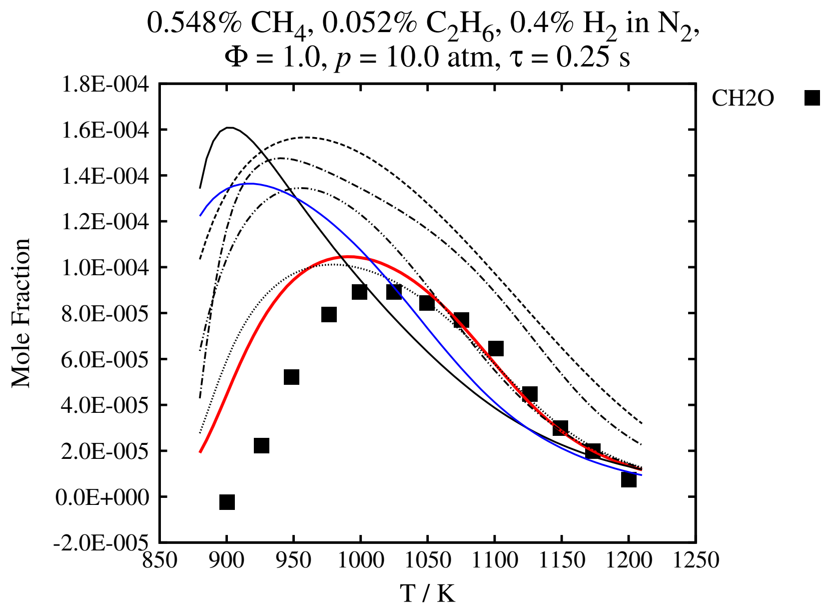
(b)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
H2
Mole Fraction
4.5E-003
4.0E-003
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
850
900
950
1000
1050
1100
1150
1200
1250
T / K

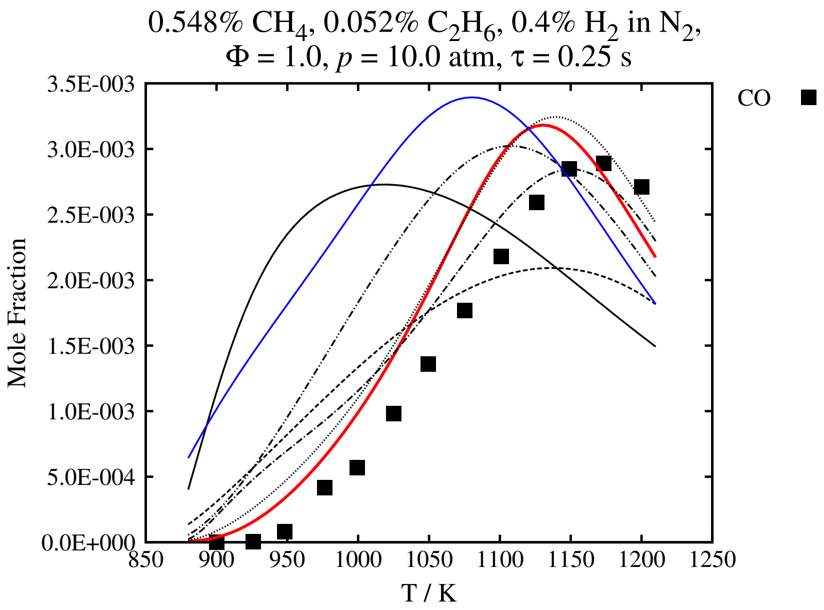
(c)


0.548% CH_4, 0.052% C_2H_6, 0.4% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
C2H4
Mole Fraction
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250
T / K

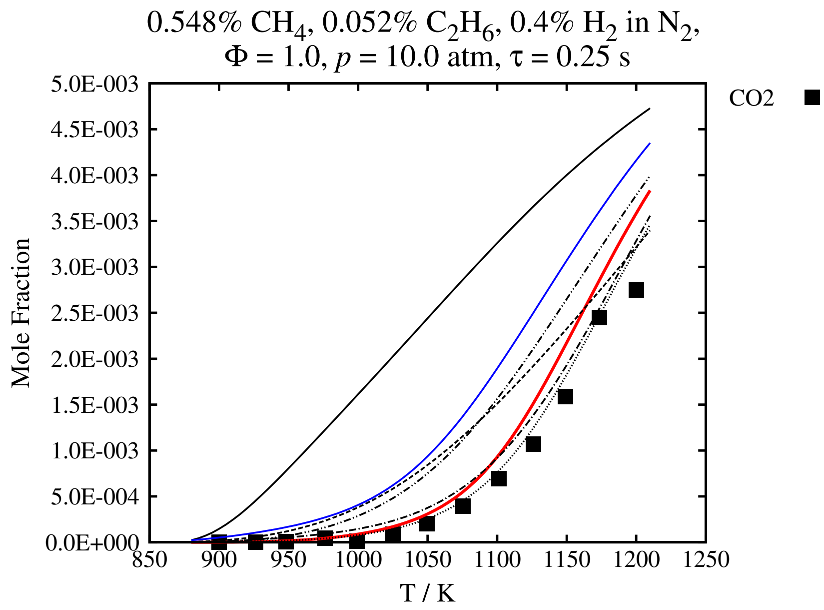
(d)


0.548% CH4, 0.052% C2H6, 0.4% H2 in N2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
T / K

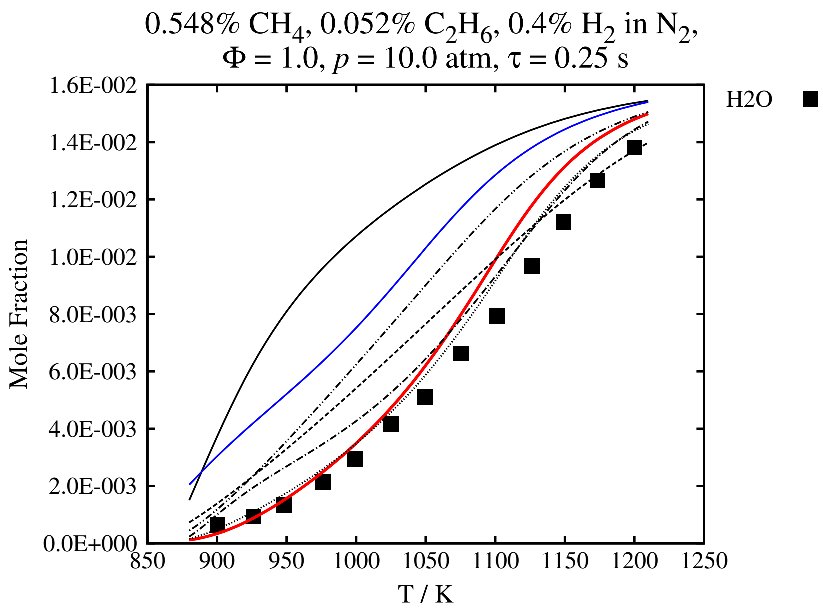
(e)


0.548% CH4, 0.052% C2H6, 0.4% H2 in N2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
T / K

(f)

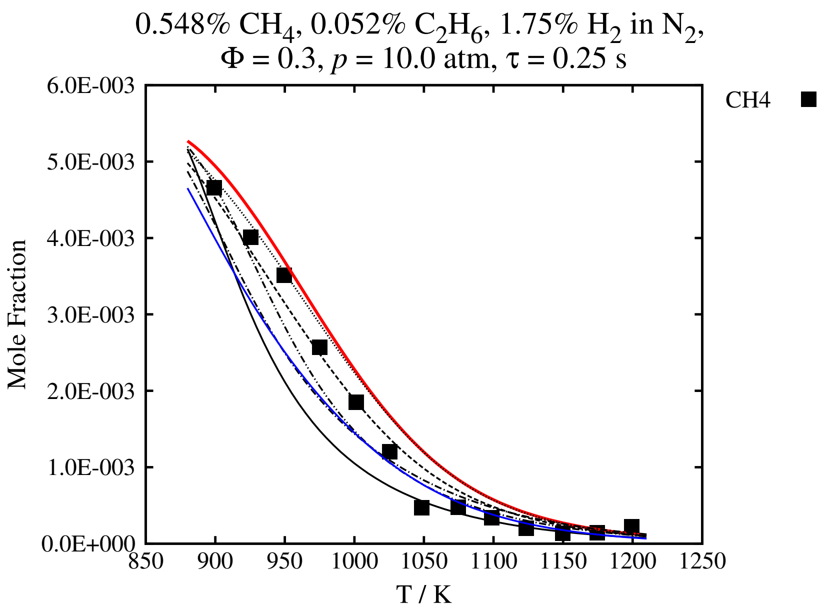


(g)

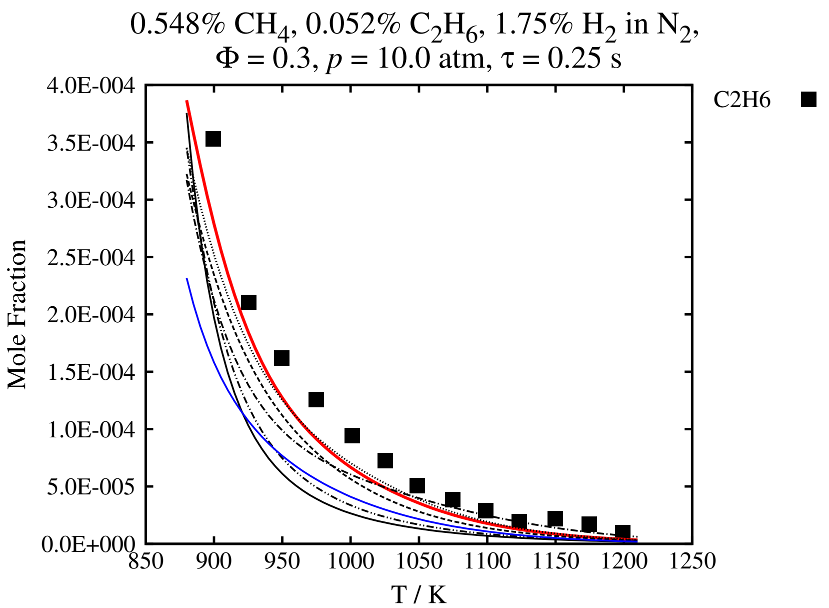


(h)

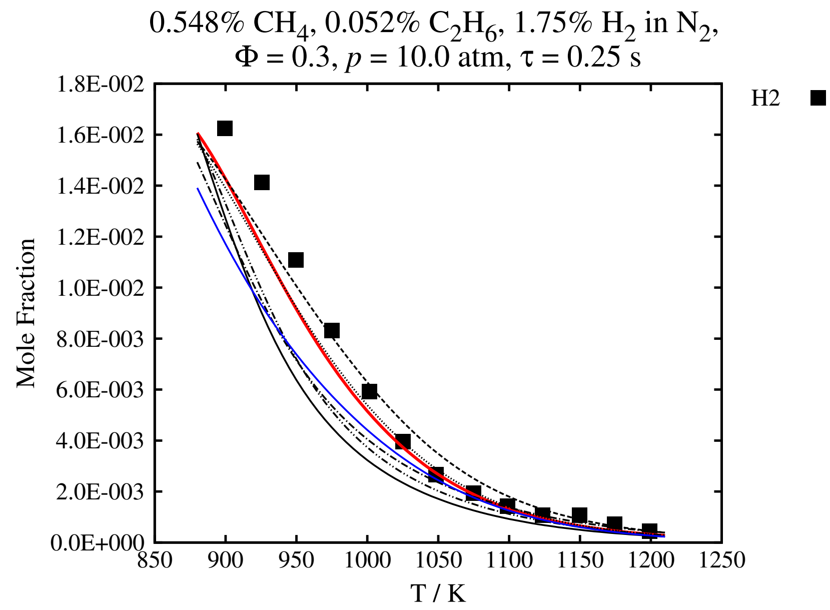
S104 Jet-stirred reactor species profiles of methane/ethane/hydrogen/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, — USC II.


0.548% CH4, 0.052% C2H6, 1.75% H2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K

(a)

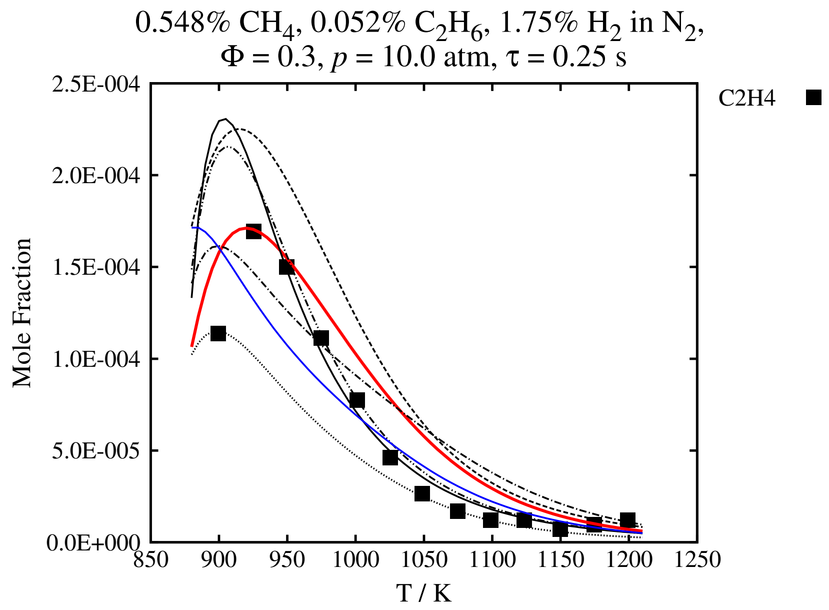

0.548% CH4, 0.052% C2H6, 1.75% H2 in N2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
C2H6
Mole Fraction
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K

(b)



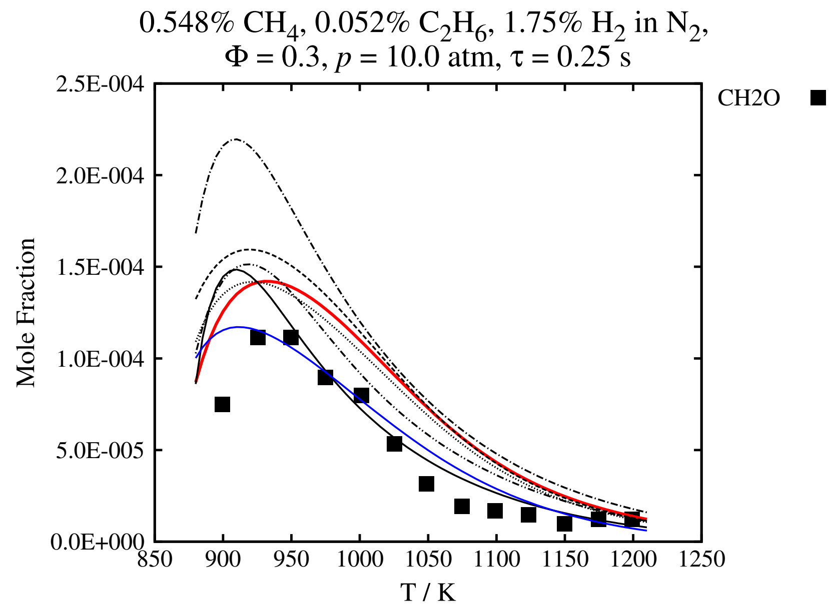
0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
$\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s
H2
Mole Fraction
T / K
1.8E-002
1.6E-002
1.4E-002
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250

(c)



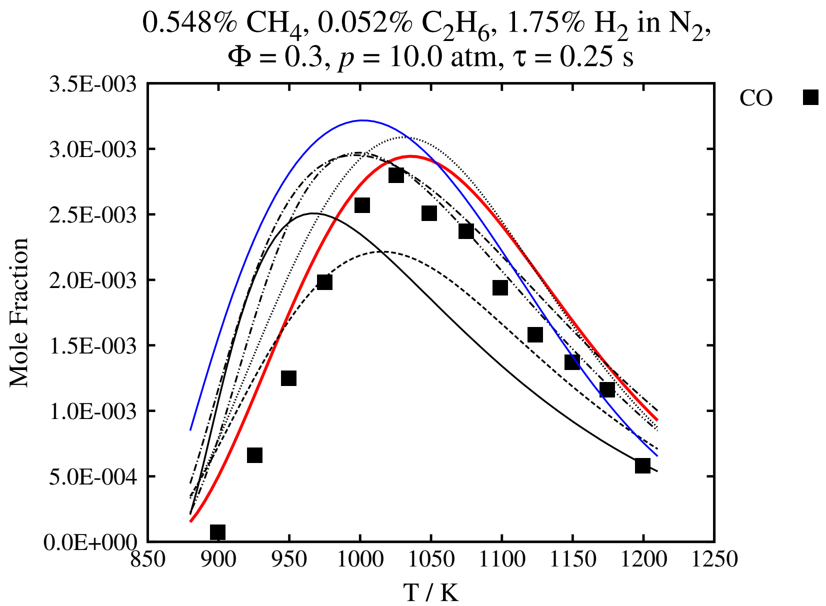
0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
$\Phi = 0.3$, $p = 10.0$ atm, $\tau = 0.25$ s
C2H4
Mole Fraction
T / K
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250

(d)



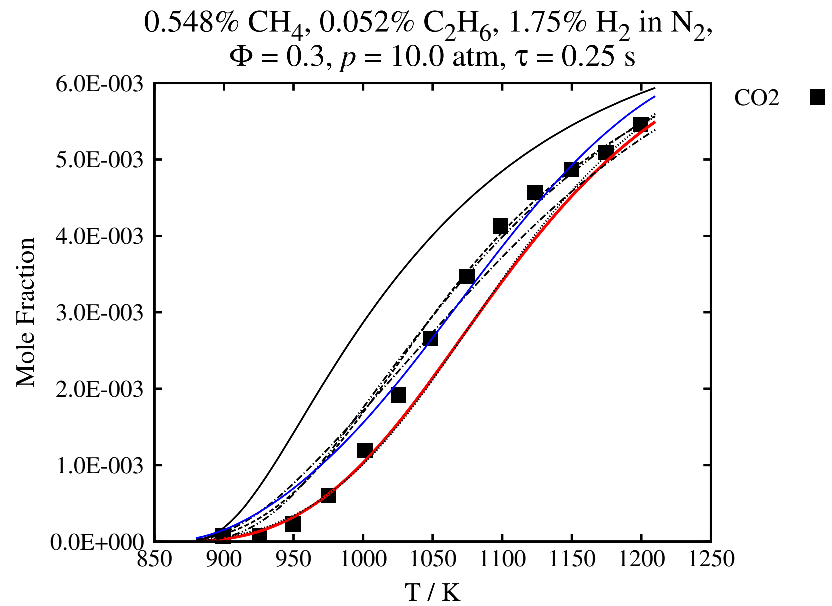
0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K

(e)

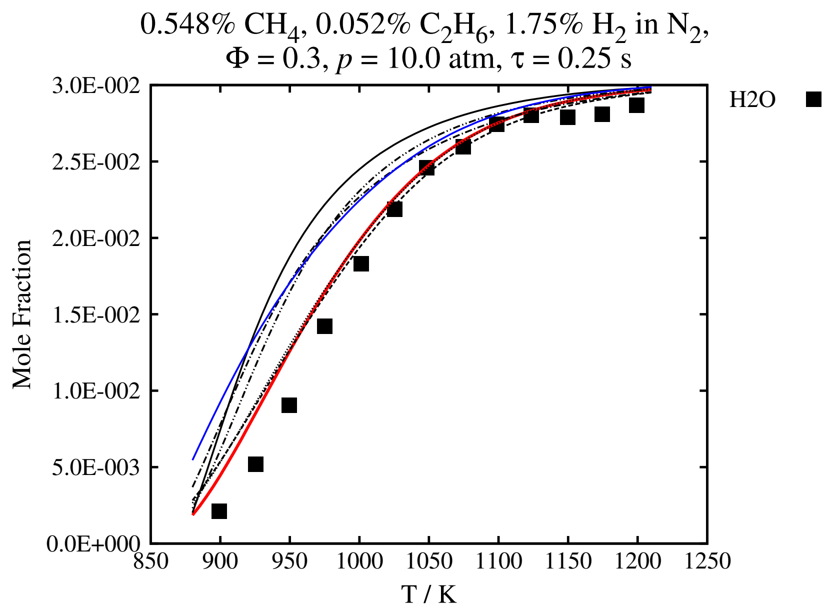


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 0.3, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850 900 950 1000 1050 1100 1150 1200 1250
T / K

(f)

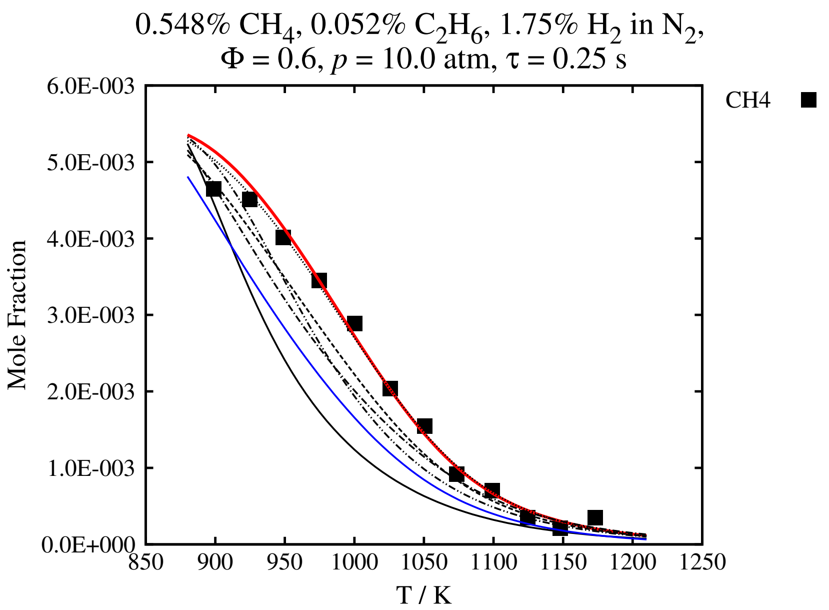


(g)

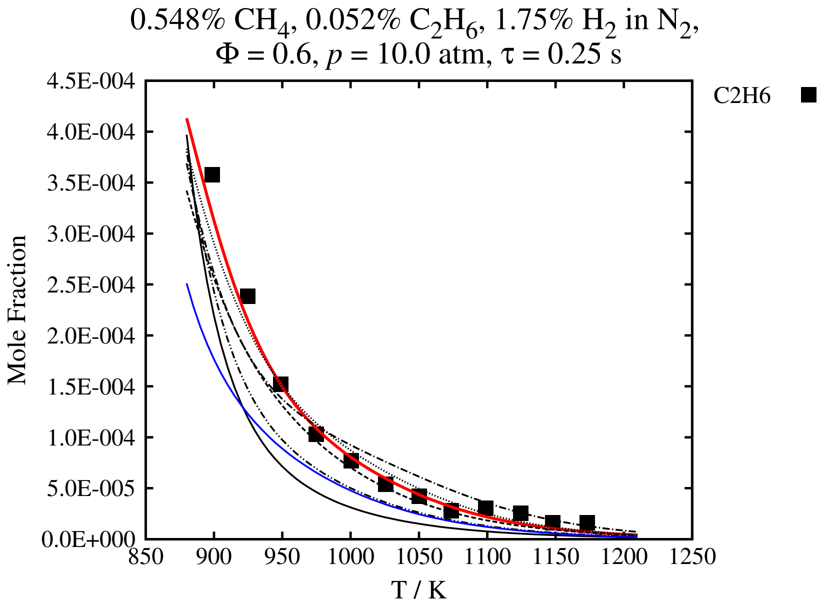


(h)

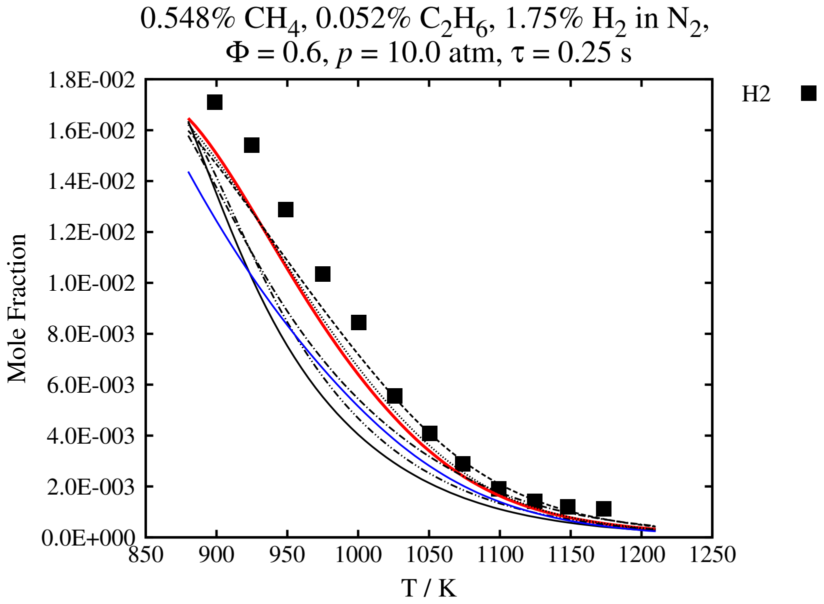
S105 Jet-stirred reactor species profiles of methane/ethane/hydrogen/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, — USC II.


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
$\Phi = 0.6$, $p = 10.0$ atm, $\tau = 0.25$ s
CH4
Mole Fraction
T / K

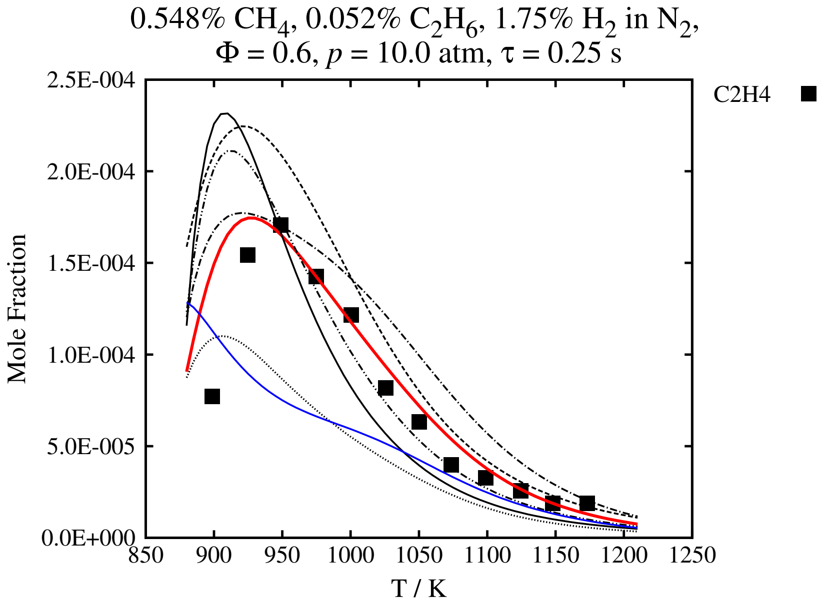
(a)


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
$\Phi = 0.6$, $p = 10.0$ atm, $\tau = 0.25$ s
C2H6
Mole Fraction
T / K

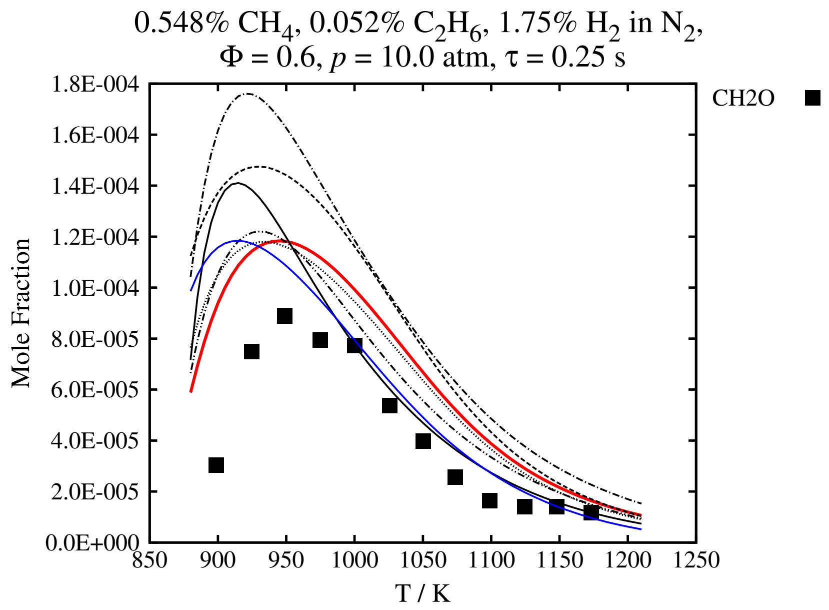
(b)


0.548% CH4, 0.052% C2H6, 1.75% H2 in N2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
Mole Fraction
T / K
H2
1.8E-002
1.6E-002
1.4E-002
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

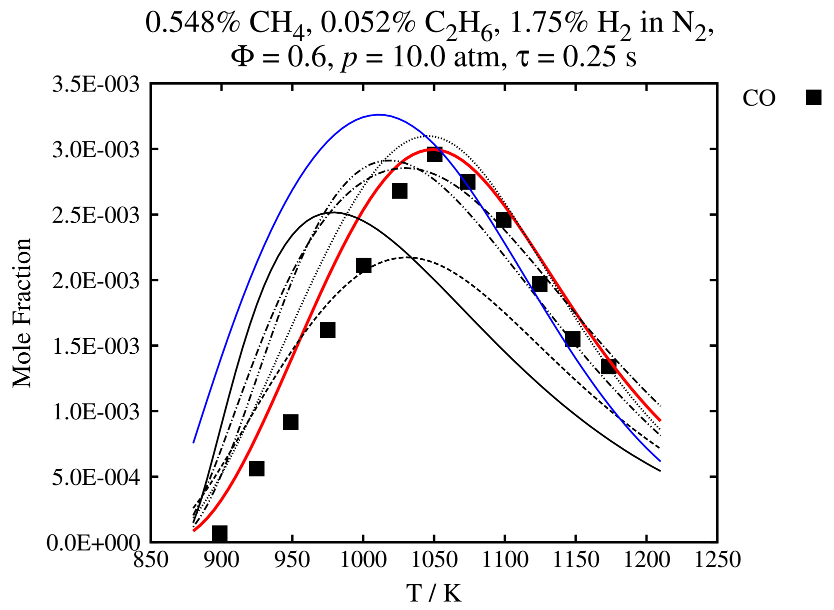
(c)


0.548% CH4, 0.052% C2H6, 1.75% H2 in N2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
Mole Fraction
T / K
C2H4
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

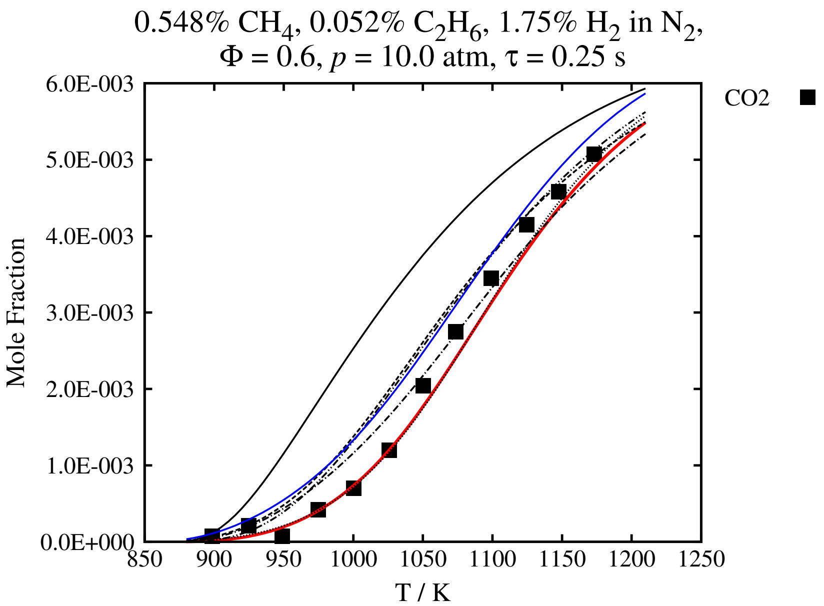
(d)


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
T / K
1.8E-004
1.6E-004
1.4E-004
1.2E-004
1.0E-004
8.0E-005
6.0E-005
4.0E-005
2.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

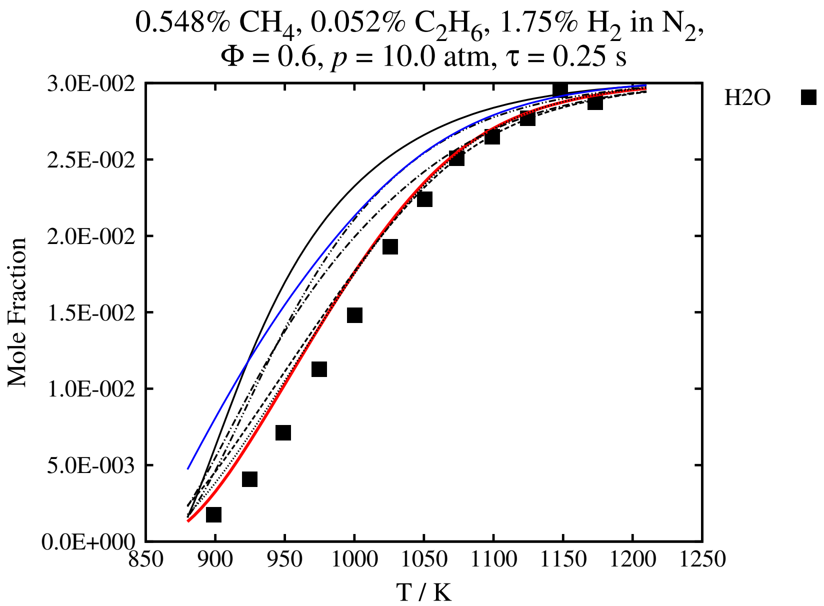
(e)


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 0.6, p = 10.0 atm, τ = 0.25 s
CO
Mole Fraction
T / K
3.5E-003
3.0E-003
2.5E-003
2.0E-003
1.5E-003
1.0E-003
5.0E-004
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

(f)

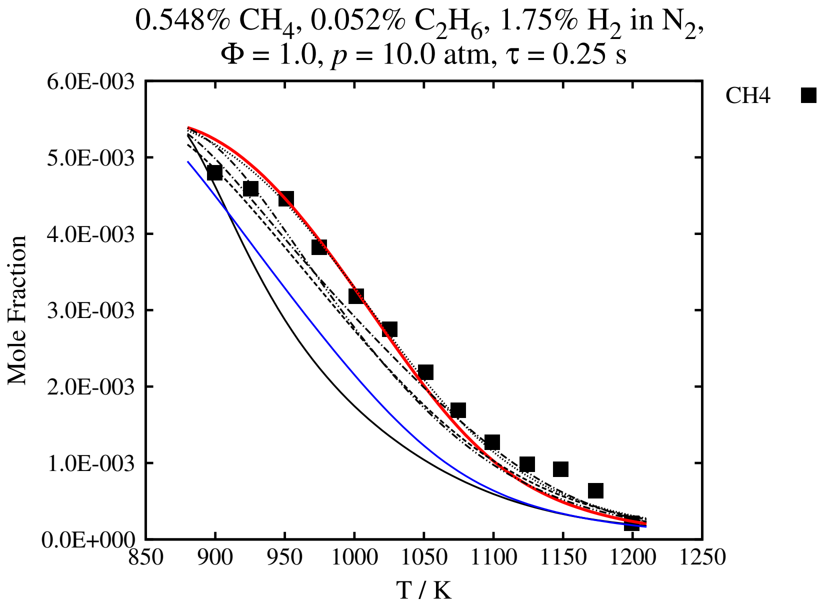


(g)

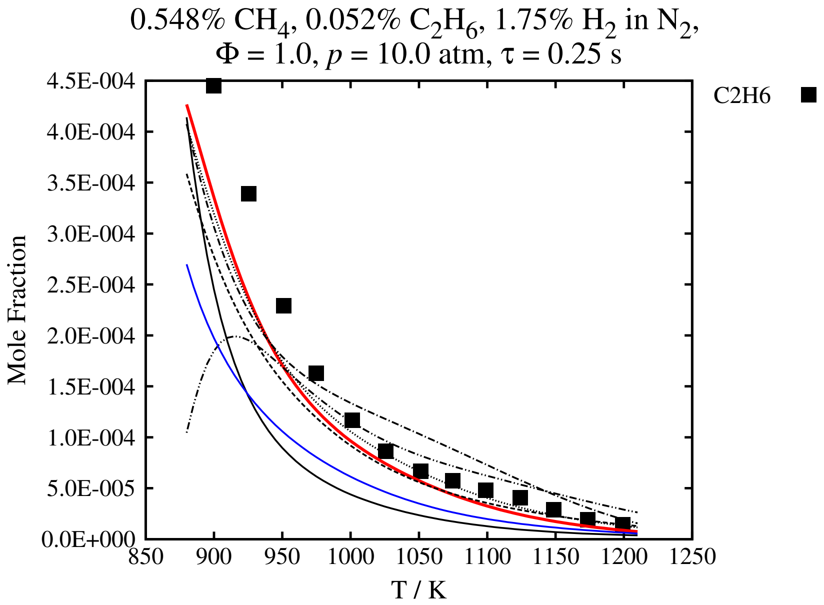


(h)

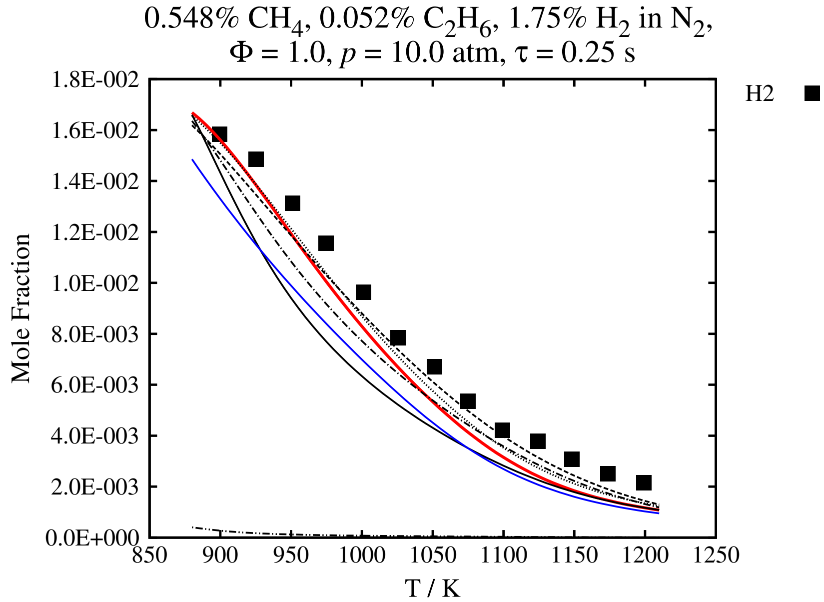
S106 Jet-stirred reactor species profiles of methane/ethane/hydrogen/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, — · — Ranzi, — · · San Diego Mech, — USC II.


0.548% CH4, 0.052% C2H6, 1.75% H2 in N2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CH4
Mole Fraction
T / K
6.0E-003
5.0E-003
4.0E-003
3.0E-003
2.0E-003
1.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

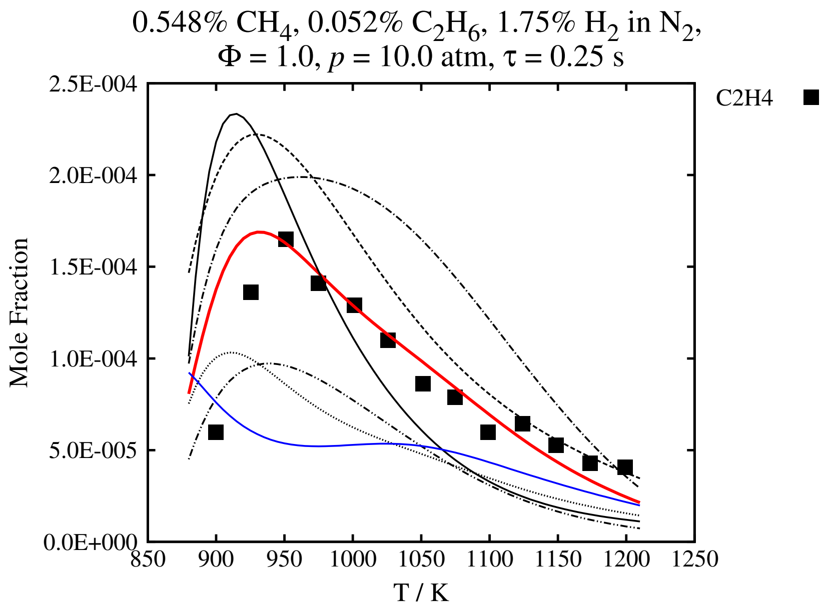
(a)


0.548% CH4, 0.052% C2H6, 1.75% H2 in N2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
C2H6
Mole Fraction
T / K
4.5E-004
4.0E-004
3.5E-004
3.0E-004
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

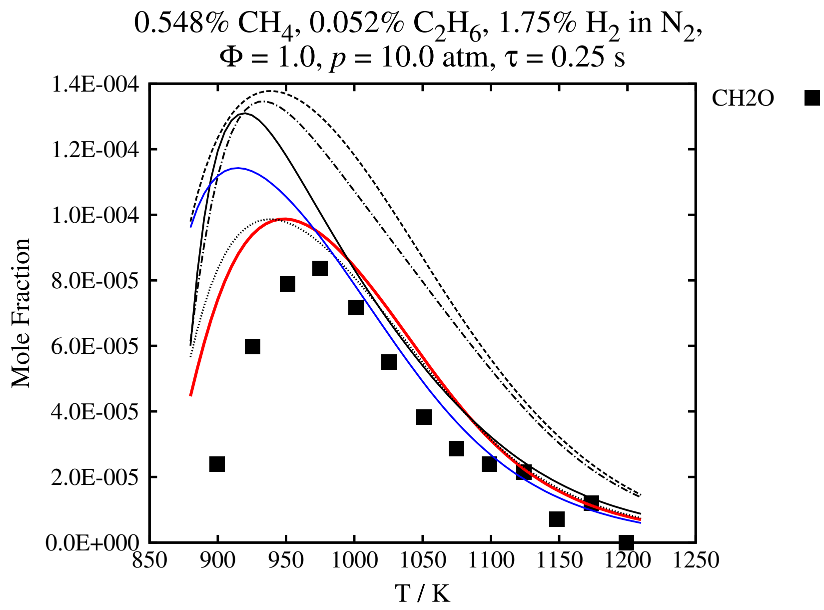
(b)


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
H2
Mole Fraction
T / K
1.8E-002
1.6E-002
1.4E-002
1.2E-002
1.0E-002
8.0E-003
6.0E-003
4.0E-003
2.0E-003
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

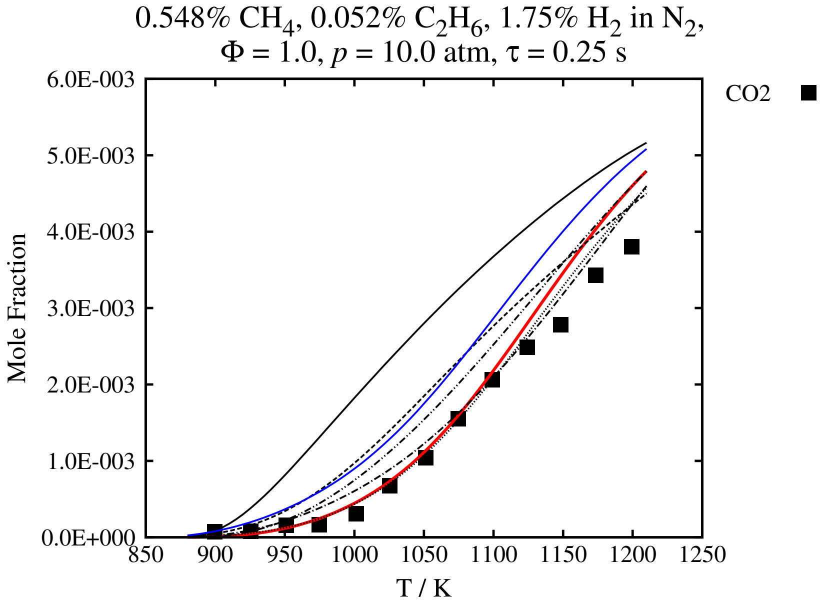
(c)


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
C2H4
Mole Fraction
T / K
2.5E-004
2.0E-004
1.5E-004
1.0E-004
5.0E-005
0.0E+000
850
900
950
1000
1050
1100
1150
1200
1250

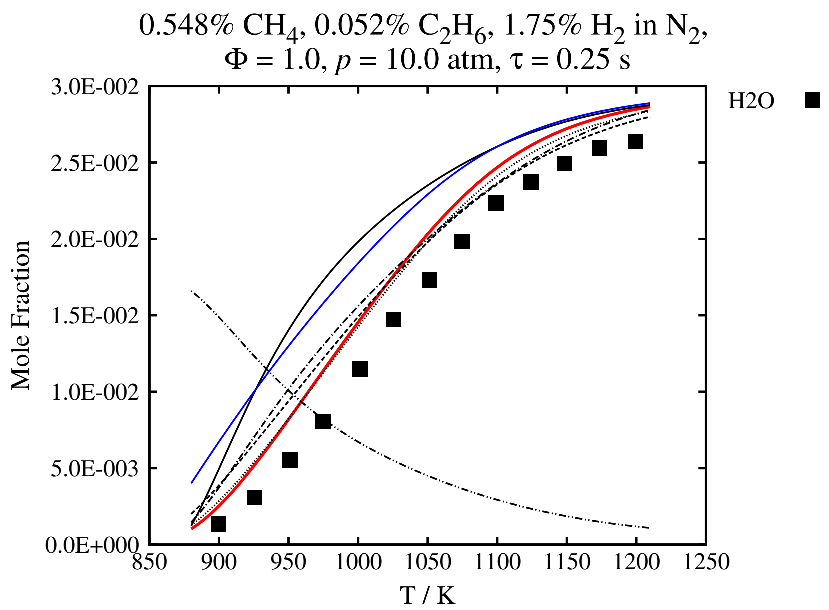
(d)


0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CH2O
Mole Fraction
T / K

(e)

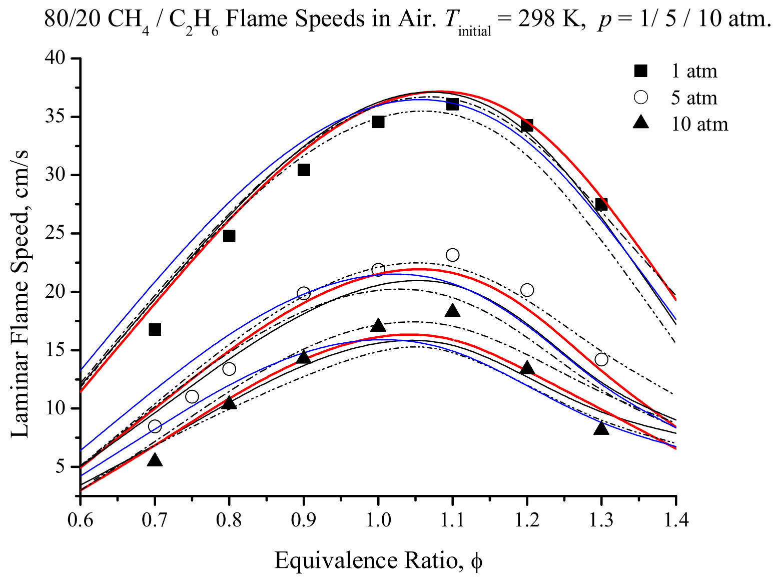

0.548% CH_4, 0.052% C_2H_6, 1.75% H_2 in N_2,
Φ = 1.0, p = 10.0 atm, τ = 0.25 s
CO2
Mole Fraction
T / K

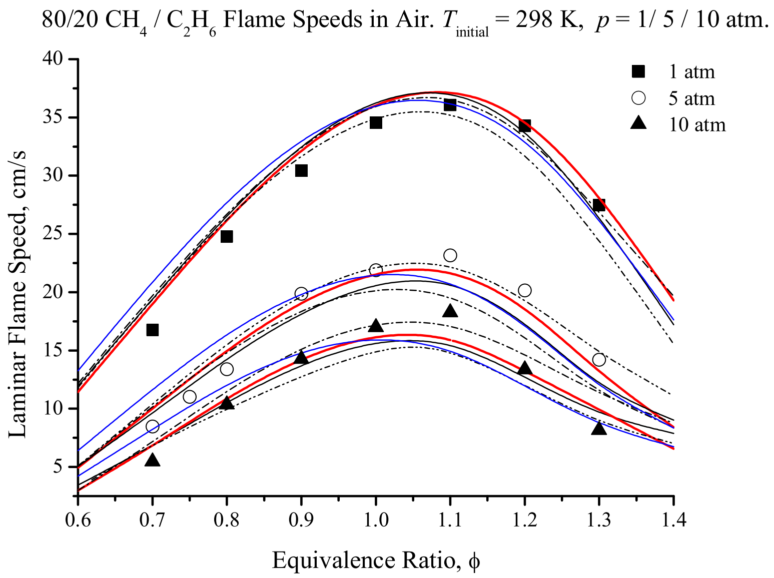
(f)

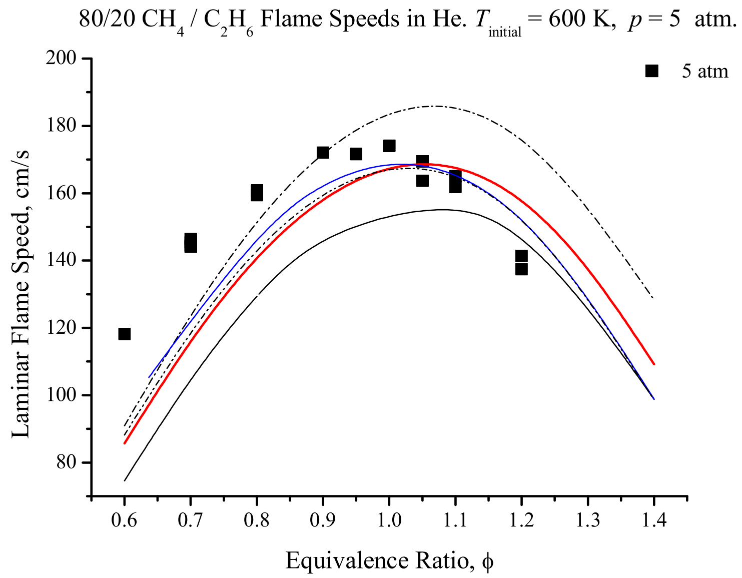


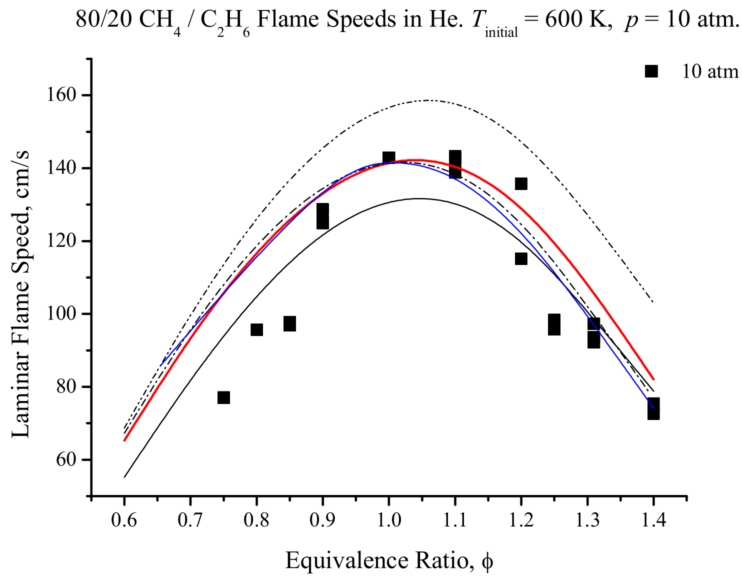
(g)

S107 Jet-stirred reactor species profiles of methane/ethane/hydrogen/oxygen/nitrogen mixtures. Symbols are experimental data [65] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

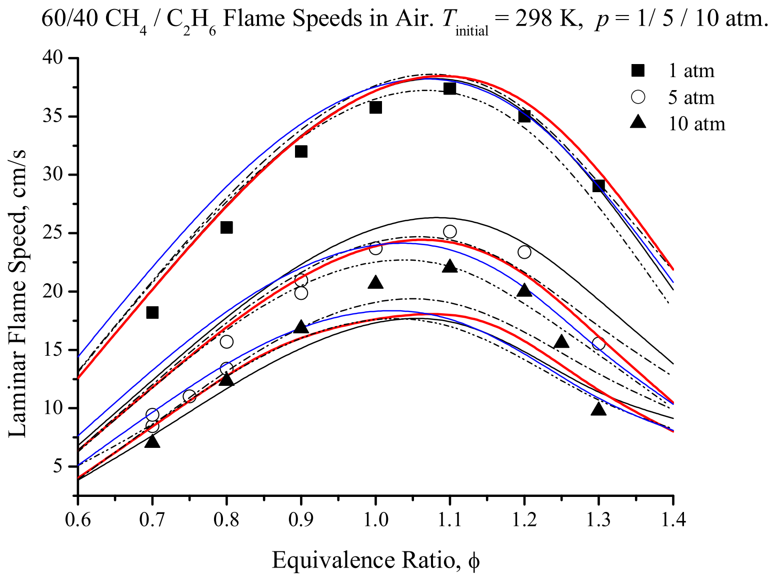

80/20 CH_4 / C_2H_6 Flame Speeds in Air. $T_{initial}$ = 298 K, p = 1/ 5 / 10 atm.
1 atm
5 atm
10 atm
Laminar Flame Speed, cm/s
Equivalence Ratio, ϕ
40
35
30
25
20
15
10
5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4


80/20 CH_4 / C_2H_6 Flame Speeds in Air. $T_{initial}$ = 298 K, p = 1/ 5 / 10 atm.
1 atm
5 atm
10 atm
Laminar Flame Speed, cm/s
Equivalence Ratio, ϕ
40
35
30
25
20
15
10
5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4

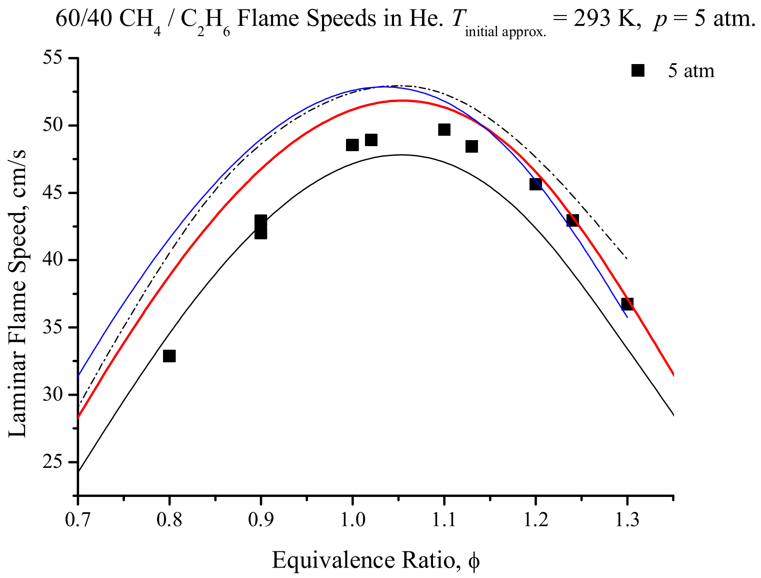


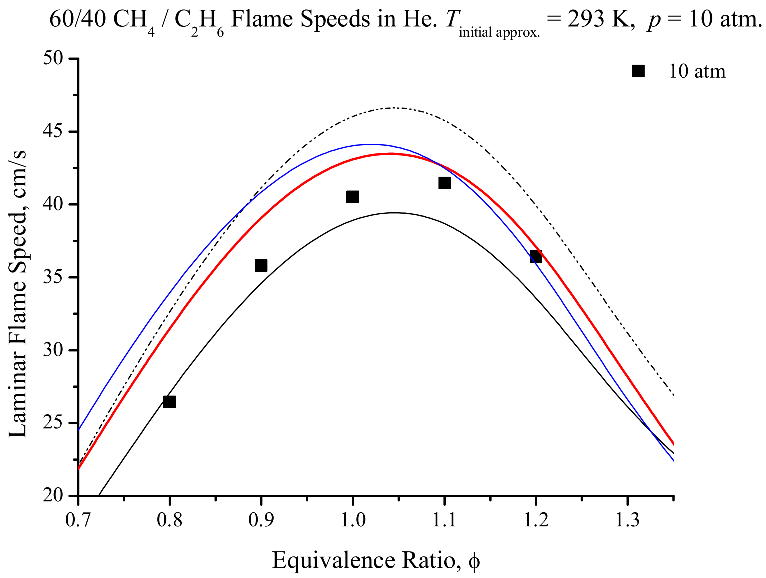


S108 Laminar flame speed measurements 80/20 methane/ethane/helium mixtures. Symbols are experimental data [16] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.



S109 Laminar flame speed measurements 60/40 methane/ethane/air mixtures. Symbols are experimental data [16] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, - - - Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.





S110 Laminar flame speed measurements 60/40 methane/ethane/helium mixtures. Symbols are experimental data [16] lines are model predictions. — AramcoMech 1.3, — GRI-Mech 3.0, – – – Leeds Mech, · · · MFC, – · – Ranzi, – · · San Diego Mech, — USC II.

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