Shock-Tube Laser Absorption Measurements of CO and H_2O during Iso-Octane Combustion

O. Mathieu*, S. P. Cooper, S. A. Turaifi, C. R. Mulvihill, T. M. Atherley, and E. L. Petersen

[1]J. Mike Walker '66 Department of Mechanical Engineering, Texas A&M University, College Station, TX, USA
[2]Department of Mechanical and Industrial Engineering, Louisiana State University, Baton Rouge, LA, USA
*Corresponding Author Email: olivier.mathieu@tamu.edu

Supplemental Material Section

A/ CO measurements
A.1/ CO mole fraction time histories and model comparison
A.1.1/ Model comparison at ϕ = 0.5

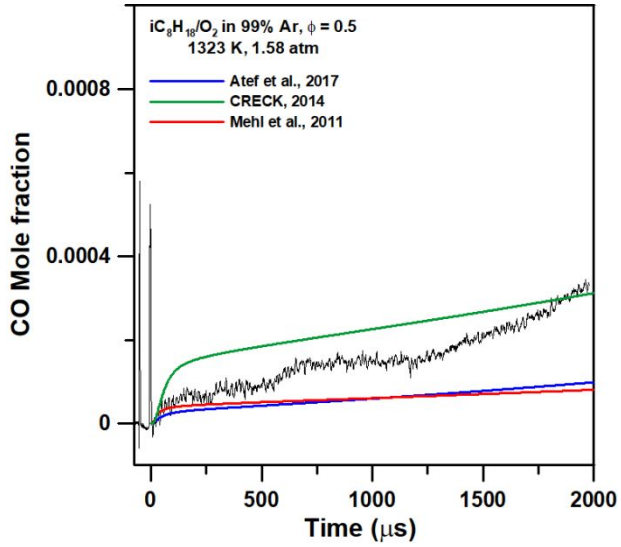

Figure SM1: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 0.5, 1323 K and 1.58 atm.

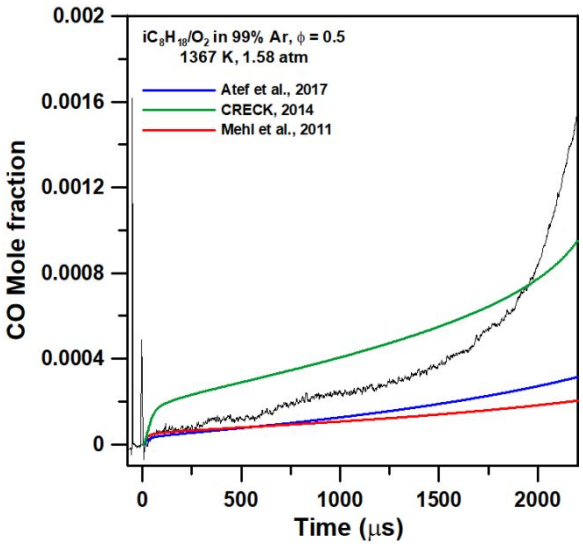

Figure SM2: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 0.5, 1367 K and 1.58 atm.

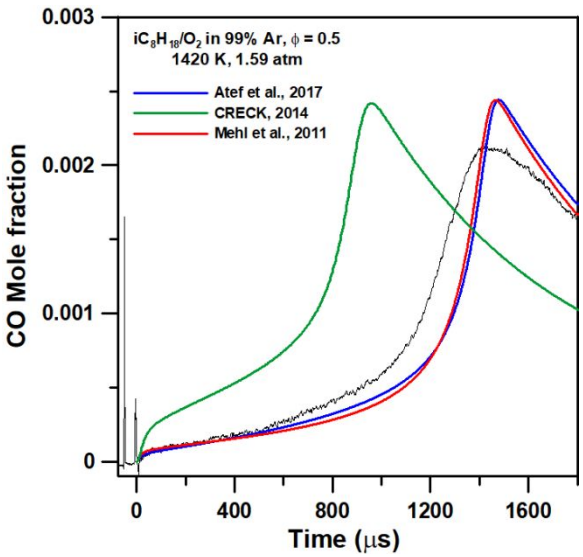

Figure SM3: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 0.5, 1420 K and 1.59 atm.

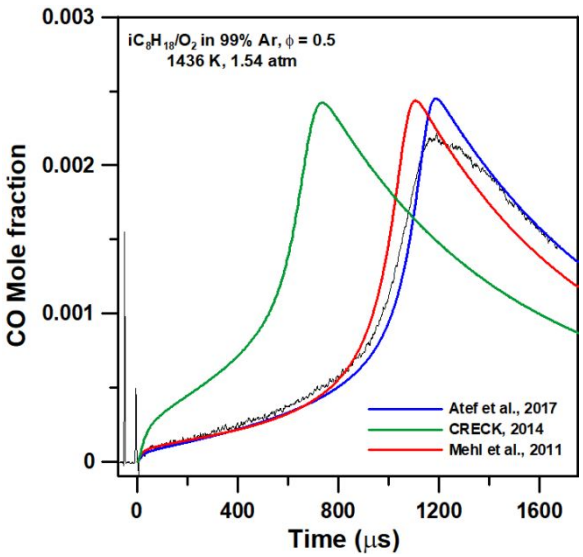

Figure SM4: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 0.5, 1436 K and 1.54 atm.

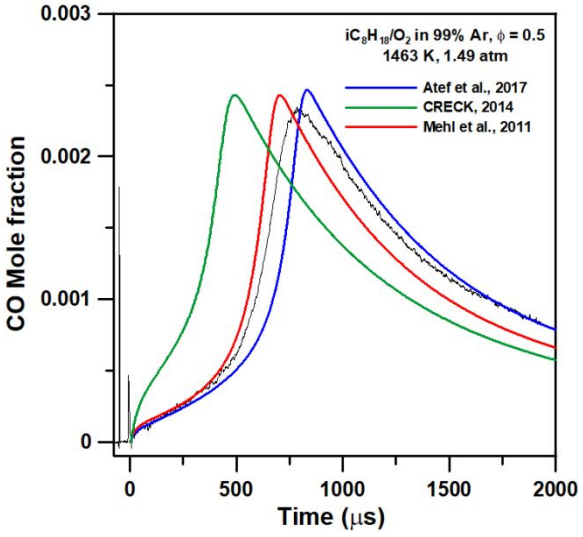

Figure SM5: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 0.5, 1463 K and 1.49 atm.

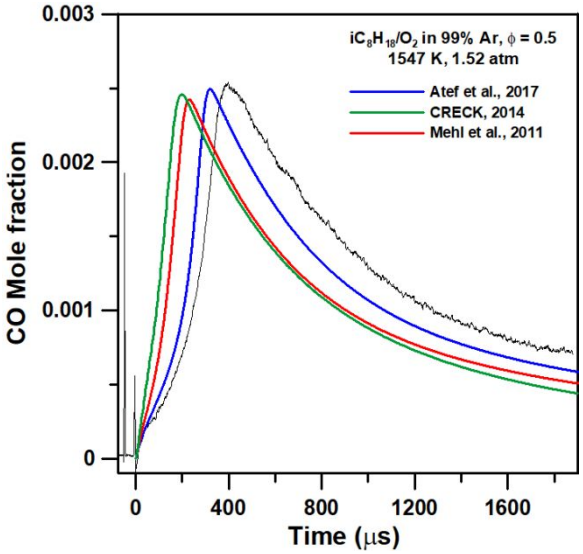

Figure SM6: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 0.5, 1547 K and 1.52 atm.

A.1.2/ Model comparison at $\phi = 1.0$

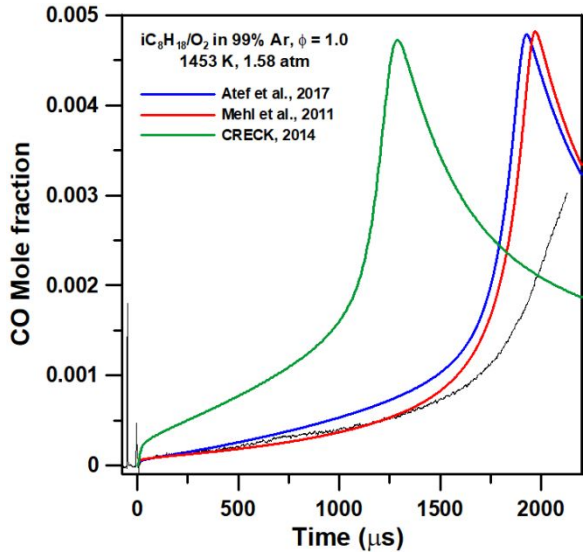

Figure SM7: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at $\phi = 1.0$, 1453 K and 1.58 atm.

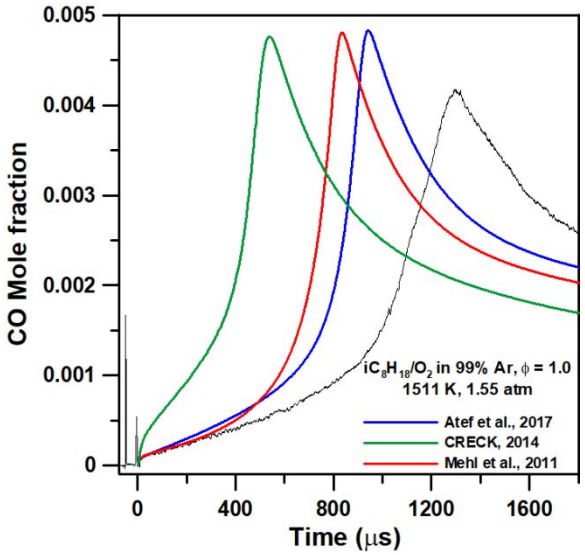

Figure SM8: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at $\phi = 1.0$, 1511 K and 1.55 atm.

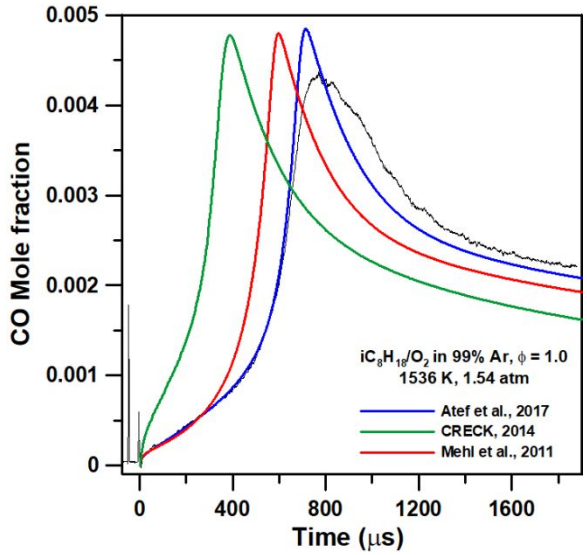

Figure SM9: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at $\phi = 1.0$, 1536 K and 1.54 atm.

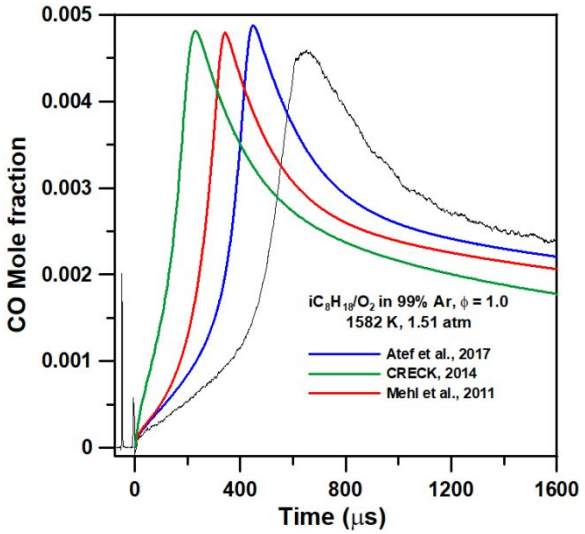

Figure SM10: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at $\phi = 1.0$, 1582 K and 1.51 atm.

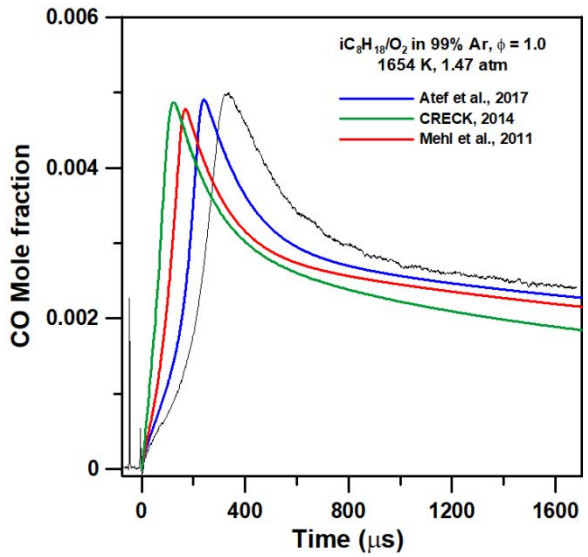

Figure SM11: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 1.0, 1654 K and 1.47 atm.

A.1.3/ Model comparison at ϕ = 2.0

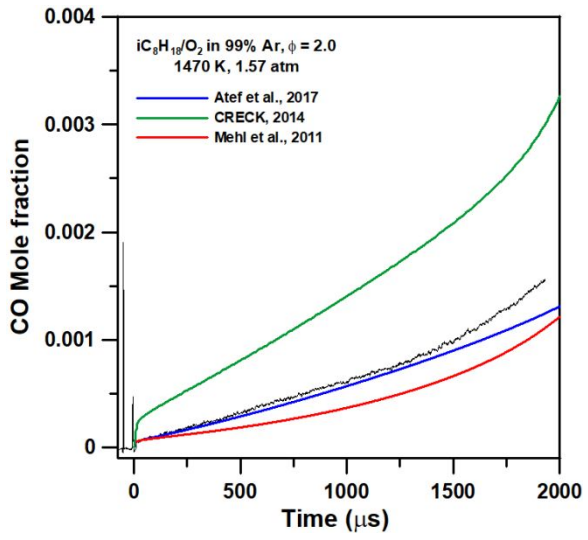

Figure SM12: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 2.0, 1470 K and 1.57 atm.

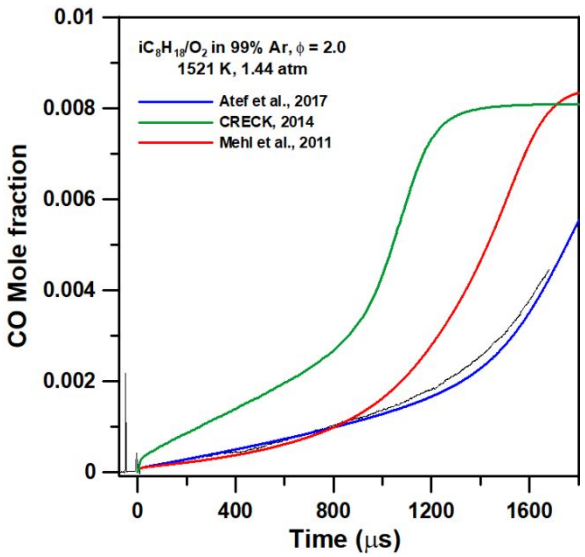

Figure SM13: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 2.0, 1521 K and 1.44 atm.

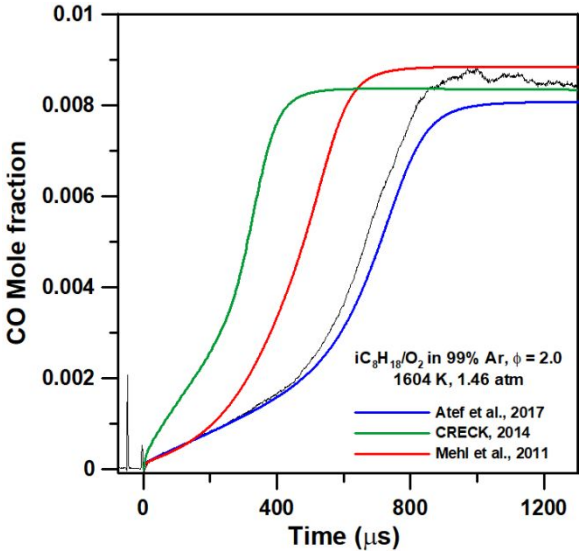

Figure SM14: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 2.0, 1604 K and 1.46 atm.

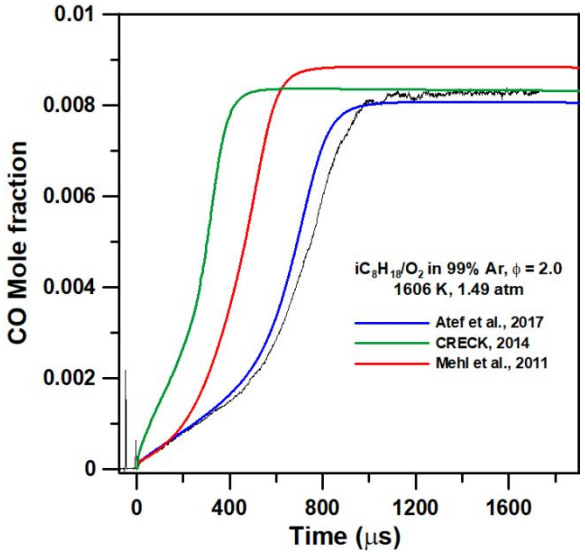

Figure SM15: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 2.0, 1606 K and 1.49 atm.

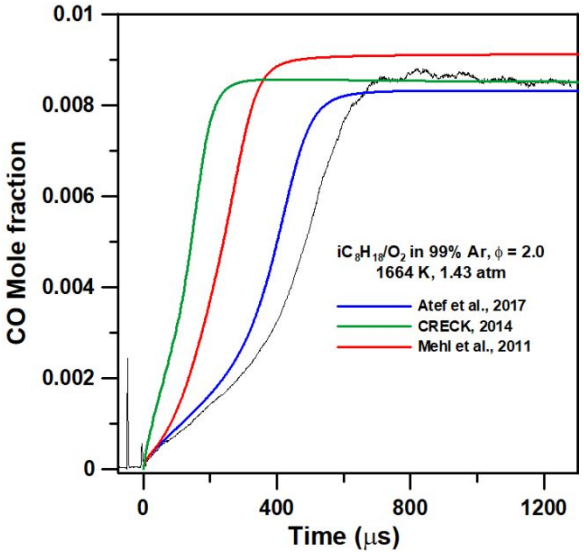

Figure SM16: CO time histories for an iso-octane/O_2 mixture in 99% inert gases at ϕ = 2.0, 1664 K and 1.43 atm.

A.2/ CO induction delay time and time-at-peak CO

Table S1: CO induction delay time (τ_{ind}), time-at-peak CO (τ_{peak}), and associated conditions behind reflected shock waves for a mixture of iso-octane/O_2 in 99% Ar diluent at ϕ = 0.5.

T_5 (K)	**P_5 (atm)**	**τ_{ind} (μs)**	**τ_{peak} (μs)**
1411	1.62	1237.8	1690
1420	1.59	995	1422
1436	1.54	853.6	1186
1463	1.49	526	788
1504	1.50	325	533
1547	1.52	196	396
1601	1.51	85.3	241

Table S2: CO induction delay time (τ_{ind}), time-at-peak CO (τ_{peak}), and associated conditions behind reflected shock waves for a mixture of iso-octane/O_2 in 99% Ar diluent at ϕ = 1.0.

T_5 (K)	**P_5 (atm)**	**τ_{ind} (μs)**	**τ_{peak} (μs)**
1496	1.57	1144	1464
1511	1.55	871	1295
1536	1.54	517	776
1582	1.51	416	656
1625	1.49	194	437
1654	1.47	159	332
1706	1.44	89	222

Table S3: CO induction delay time (τ_{ind}) and associated conditions behind reflected shock waves for a mixture of iso-octane/O_2 in 99% Ar diluent at ϕ = 2.0.

T_5 (K)	P_5 (atm)	τ_{ind} (μs)
1557	1.44	700
1604	1.46	446
1606	1.49	501
1664	1.43	301
1718	1.37	118
1815	1.37	29

B/ H_2O measurements

B.1/ H_2O mole fraction time histories and model comparison

B.1.1/ Model comparison at $\phi = 0.5$

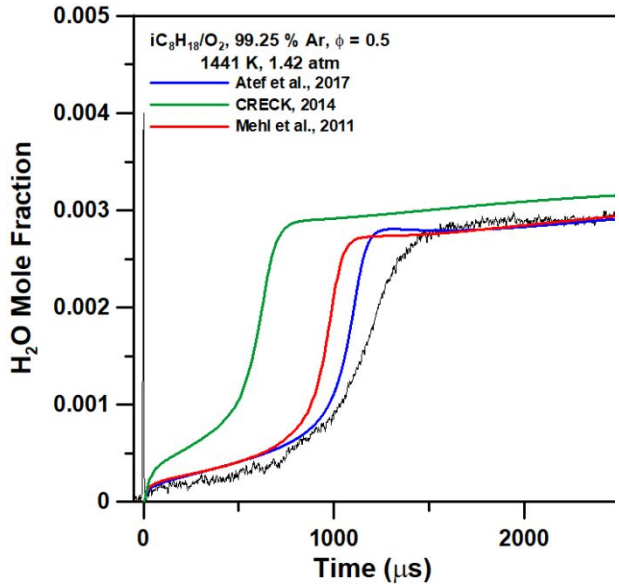

Figure SM17: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 0.5$, 1441 K and 1.42 atm.

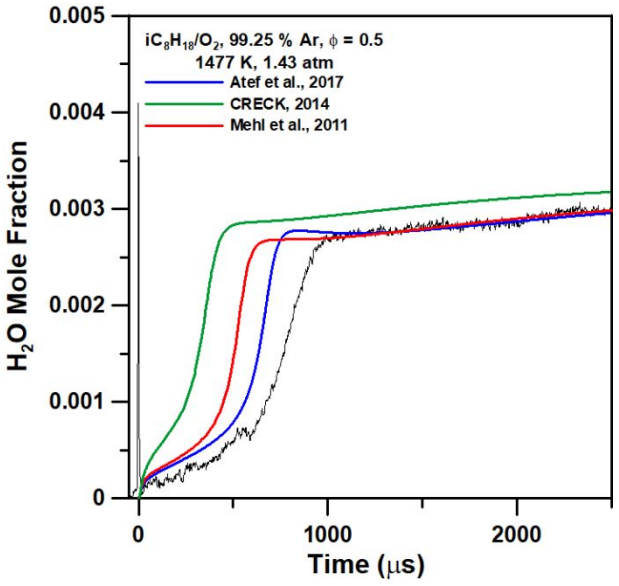

Figure SM18: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 0.5$, 1477 K and 1.43 atm.

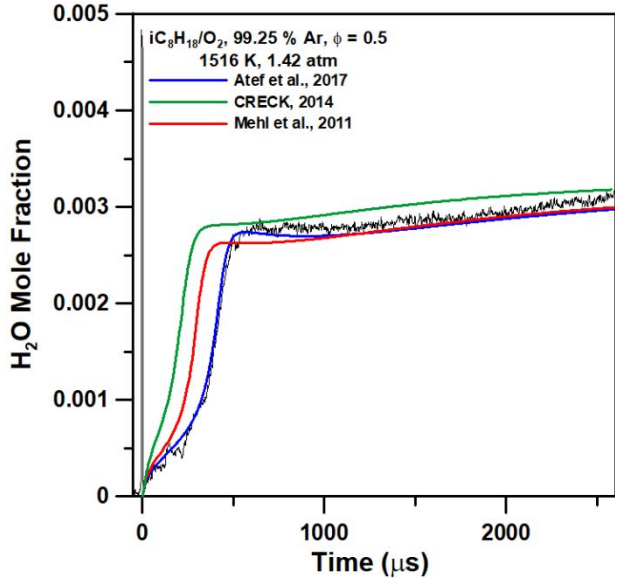

Figure SM19: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 0.5$, 1516 K and 1.42 atm.

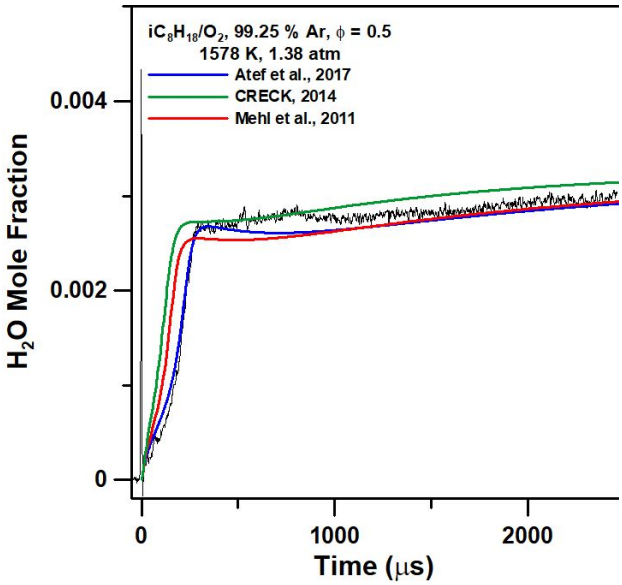

Figure SM20: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 0.5$, 1578 K and 1.38 atm.

B.1.2/ Model comparison at $\phi = 1.0$

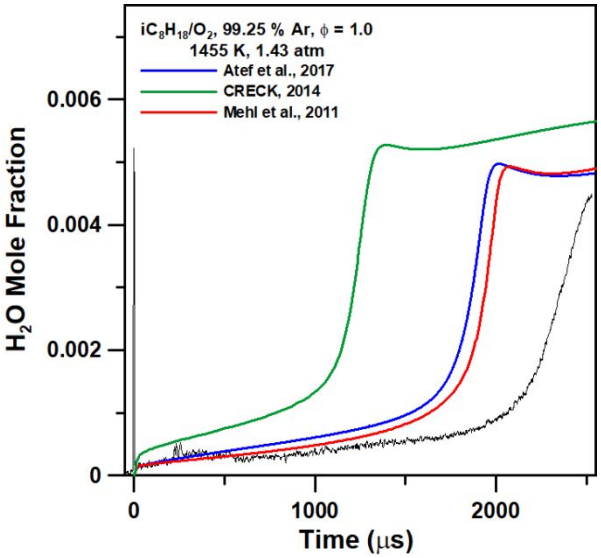

Figure SM21: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 1.0$, 1455 K and 1.43 atm.

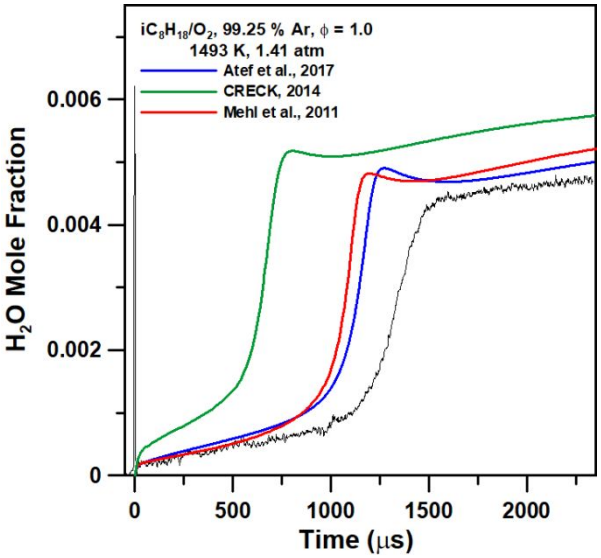

Figure SM22: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 1.0$, 1493 K and 1.41 atm.

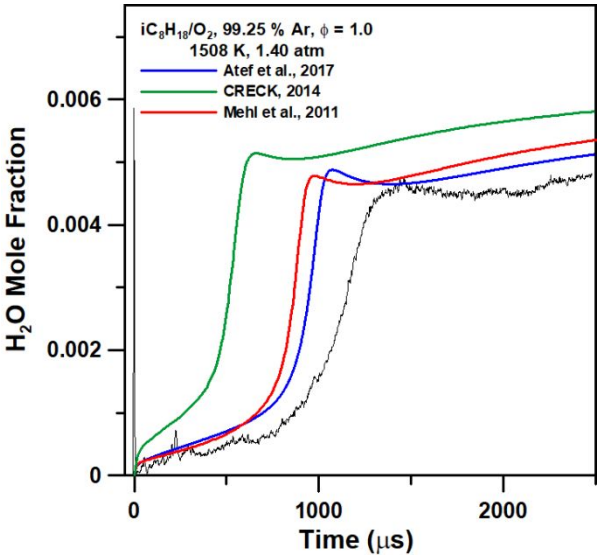

Figure SM23: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 1.0$, 1508 K and 1.40 atm.

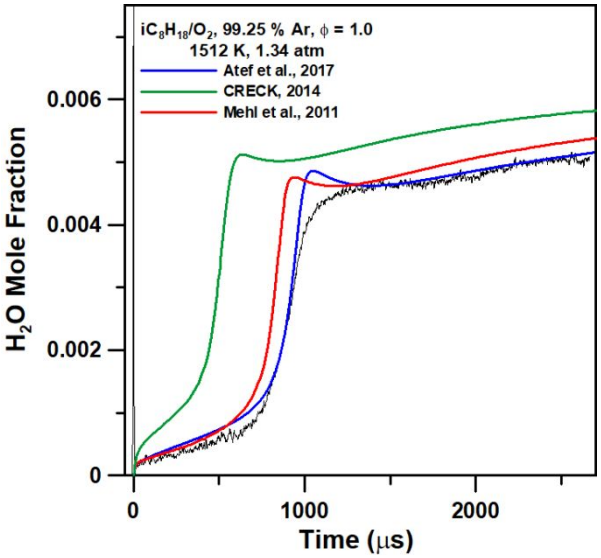

Figure SM24: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 1.0$, 1512 K and 1.34 atm.

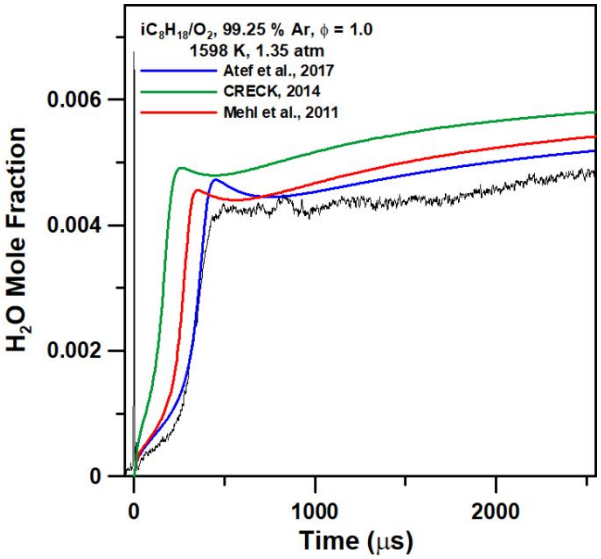

Figure SM25: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at ϕ = 1.0, 1598 K and 1.35 atm.

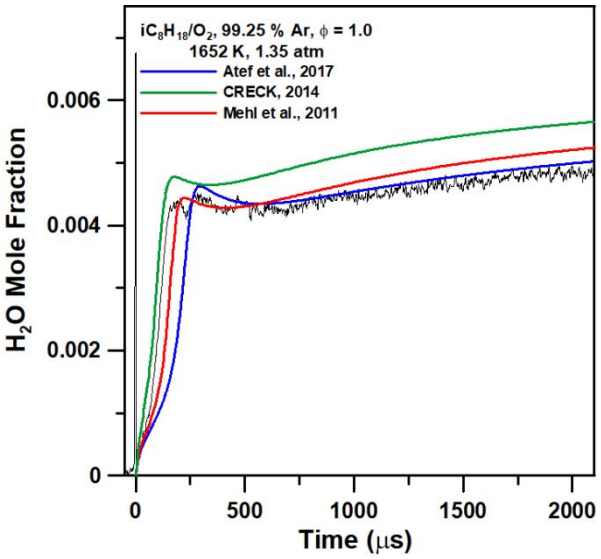

Figure SM26: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at ϕ = 1.0, 1652 K and 1.35 atm.

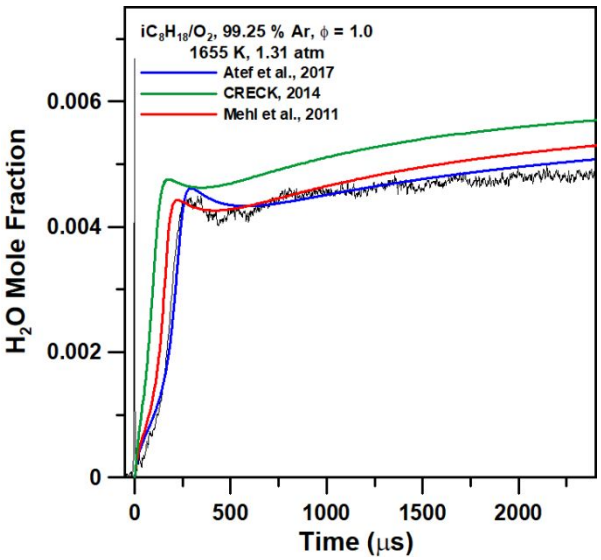

Figure SM27: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at ϕ = 1.0, 1655 K and 1.31 atm.

B.1.3/ Model comparison at $\phi = 2.0$

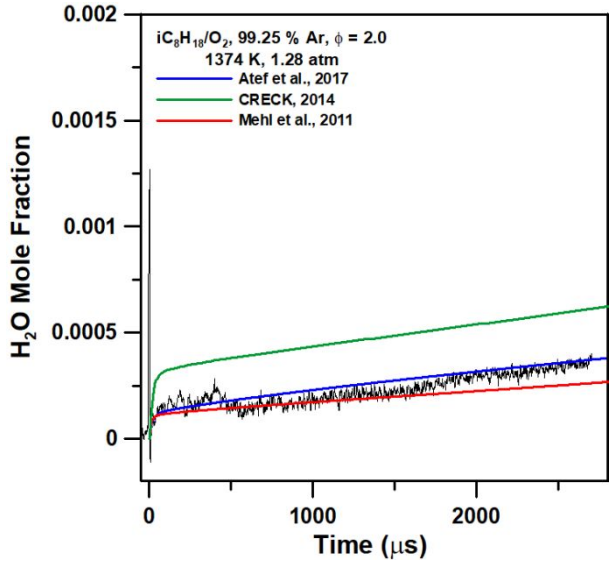

Figure SM28: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 2.0$, 1374 K and 1.28 atm.

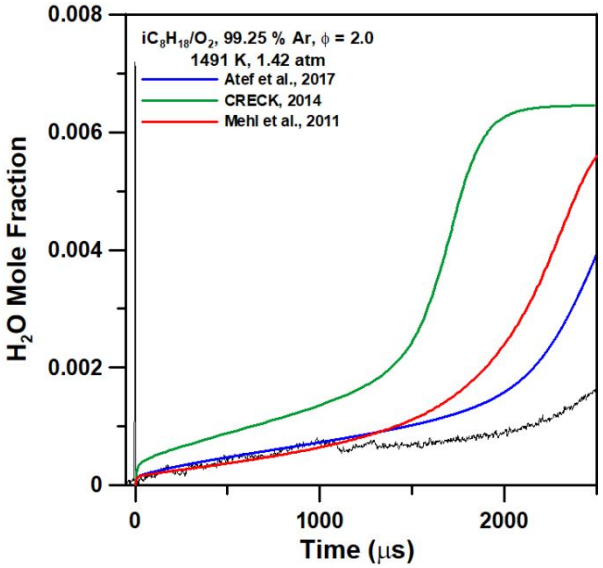

Figure SM29: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 2.0$, 1491 K and 1.42 atm.

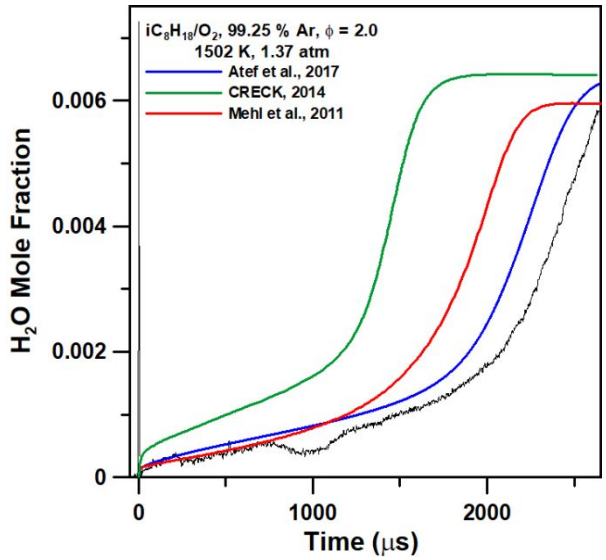

Figure SM29: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 2.0$, 1502 K and 1.37 atm.

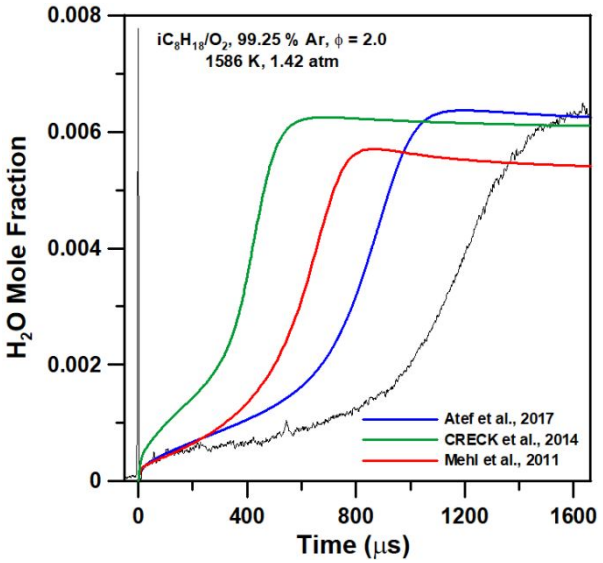

Figure SM30: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at $\phi = 2.0$, 1586 K and 1.42 atm.

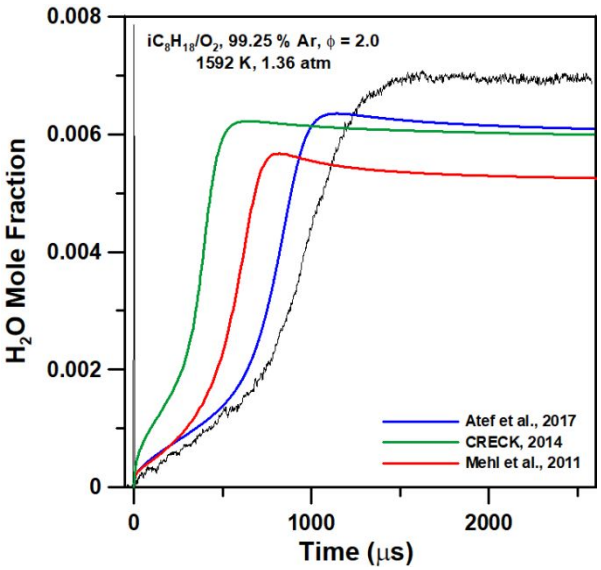

Figure SM31: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at ϕ = 2.0, 1592 K and 1.36 atm.

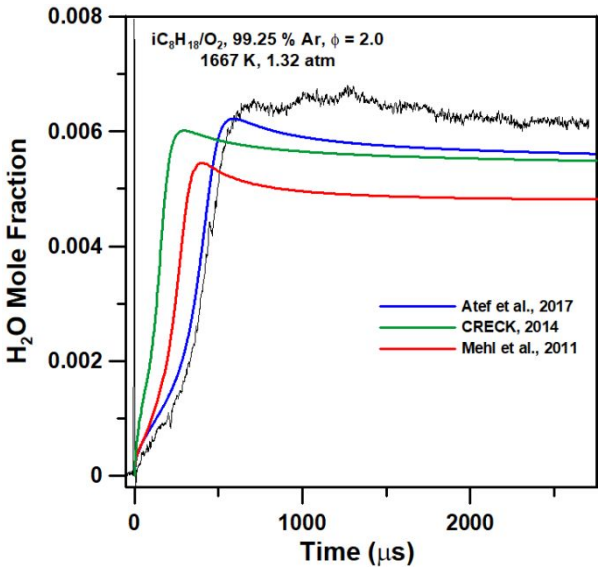

Figure SM32: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at ϕ = 2.0, 1667 K and 1.32 atm.

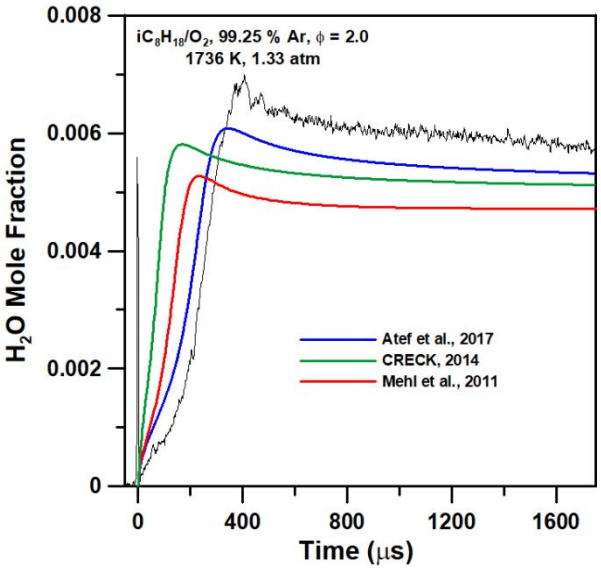

Figure SM33: H_2O time histories for an iso-octane/O_2 mixture in 99% Ar at ϕ = 2.0, 1736 K and 1.33 atm.

B.2/ H_2O induction delay time

Table S4: H_2O induction delay time (τ_{ind}) and associated conditions behind reflected shock waves for a mixture of iso-octane/O_2 in 99% Ar at ϕ = 0.5.

T_5 (K)	P_5 (atm)	τ_{ind} (μs)
1403	1.41	1612.0
1405	1.43	1486.5
1408	1.48	1895.7
1441	1.42	883.5
1477	1.43	547.8
1516	1.42	278.0
1532	1.39	167.5
1578	1.38	123.6
1600	1.35	77.4
1687	1.37	40.8

Table S5: H_2O induction delay time (τ_{ind}) and associated conditions behind reflected shock waves for a mixture of iso-octane/O_2 in 99% Ar at ϕ = 1.0.

T_5 (K)	P_5 (atm)	τ_{ind} (μs)
1455	1.43	2073.6
1460	1.40	1612
1493	1.41	1126.6
1508	1.4	805
1512	1.34	725.1
1543	1.33	400
1598	1.35	229.6
1652	1.35	107.9
1655	1.31	109.8
1728	1.36	53.4

Table S6: H_2O induction delay time (τ_{ind}) and associated conditions behind reflected shock waves for a mixture of iso-octane/O_2 in 99% Ar at ϕ = 2.0.

T_5 (K)	P_5 (atm)	τ_{ind} (μs)
1502	1.37	1921
1548	1.41	1217
1586	1.42	863
1592	1.36	598
1634	1.35	425
1667	1.32	230
1736	1.33	141
1793	1.32	59

C. Chemical Analysis

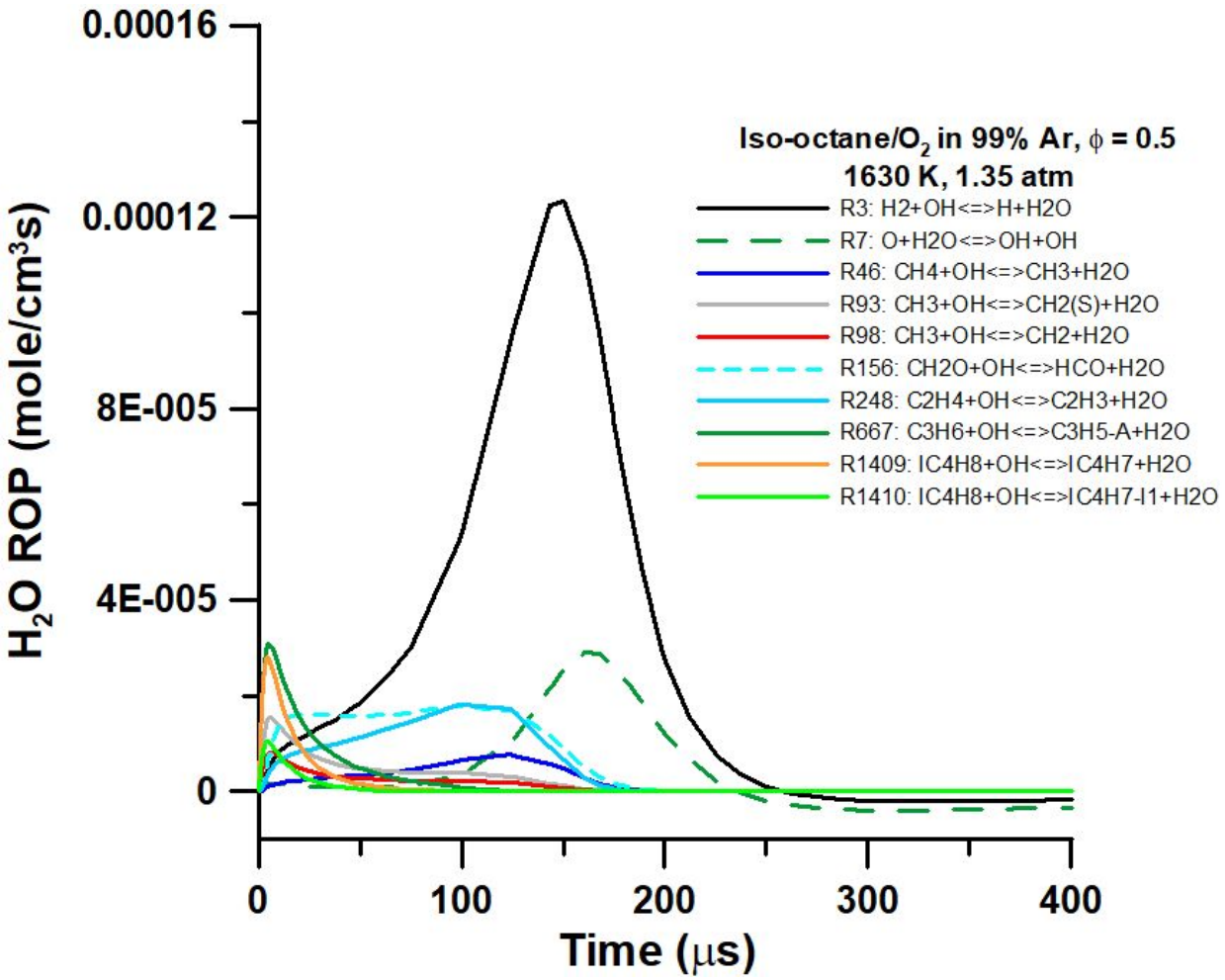

Figure SM 34: Rate of production analysis for water using the Atef et al. model from a mixture of iso-octane/O_2, ϕ = 0.5, in 99% Ar at 1630 K and 1.35 atm.

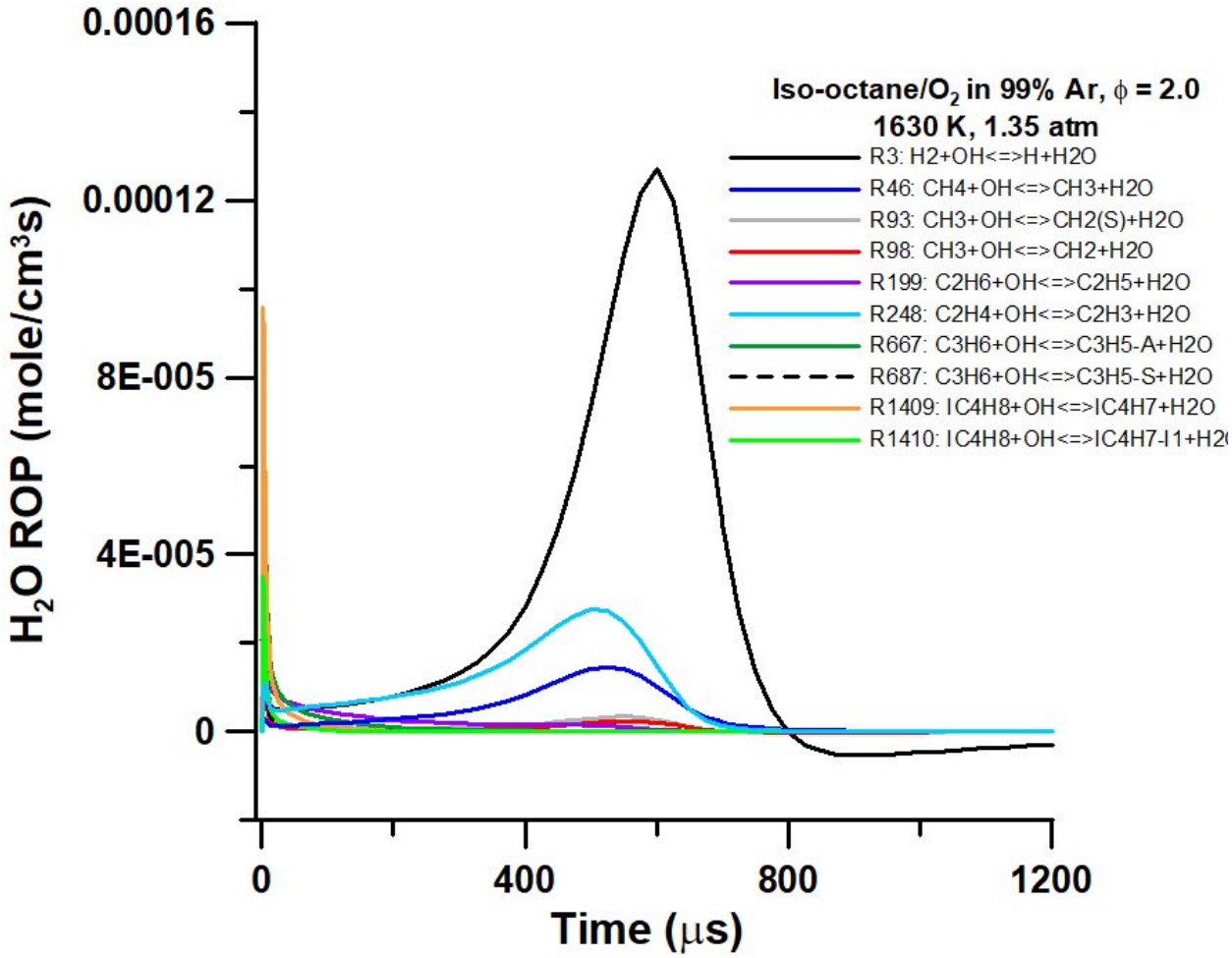

Figure SM 35: Rate of production analysis for water using the Atef et al. model from a mixture of iso-octane/O_2, ϕ = 2.0, in 99% Ar at 1630 K and 1.35 atm.