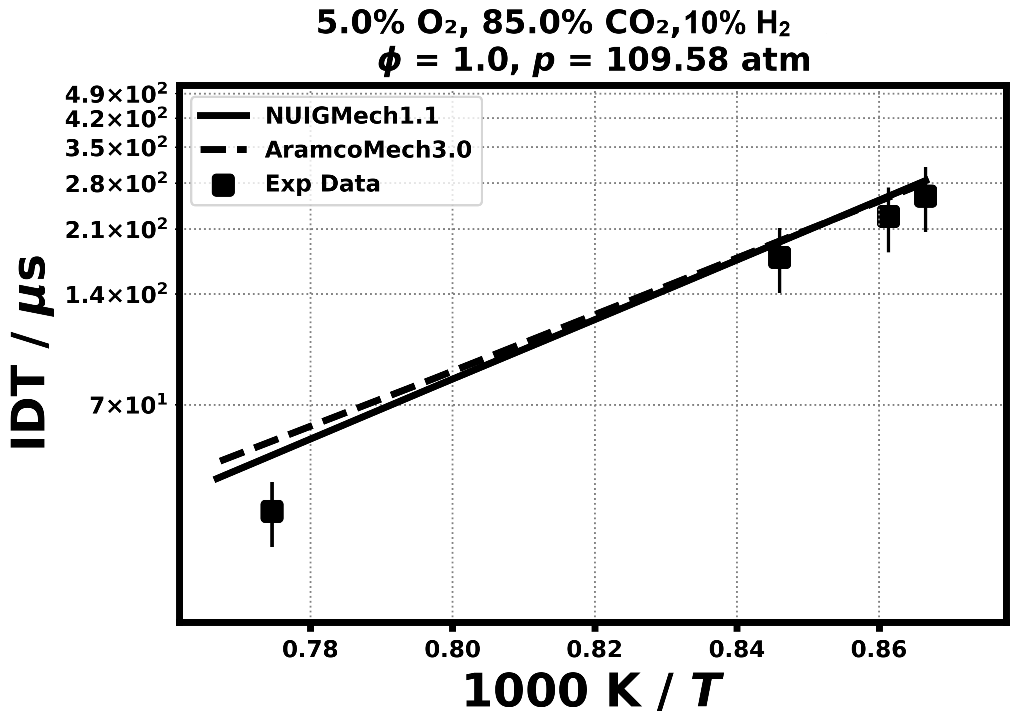
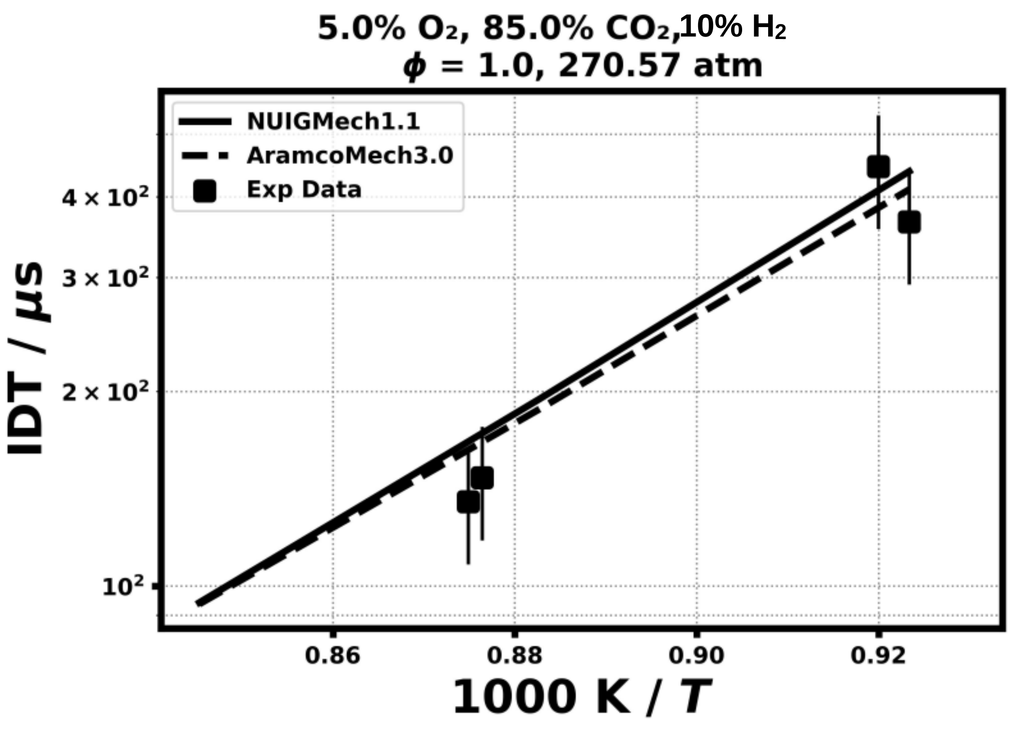
1. Validation for H_2

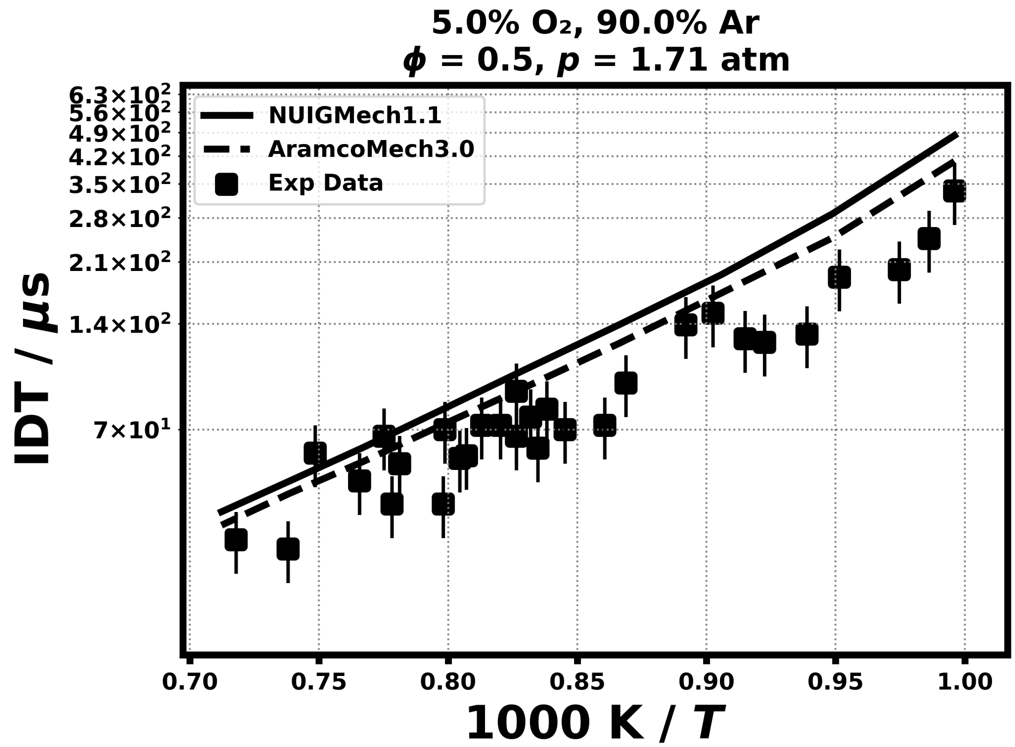
Shock tube ignition delay time

1.1) Shao, J., Choudhary, R., Davidson, D. F., Hanson, R. K., Barak, S., & Vasu, S. Proceedings of the Combustion Institute, 37(4) (2019) 4555-4562.

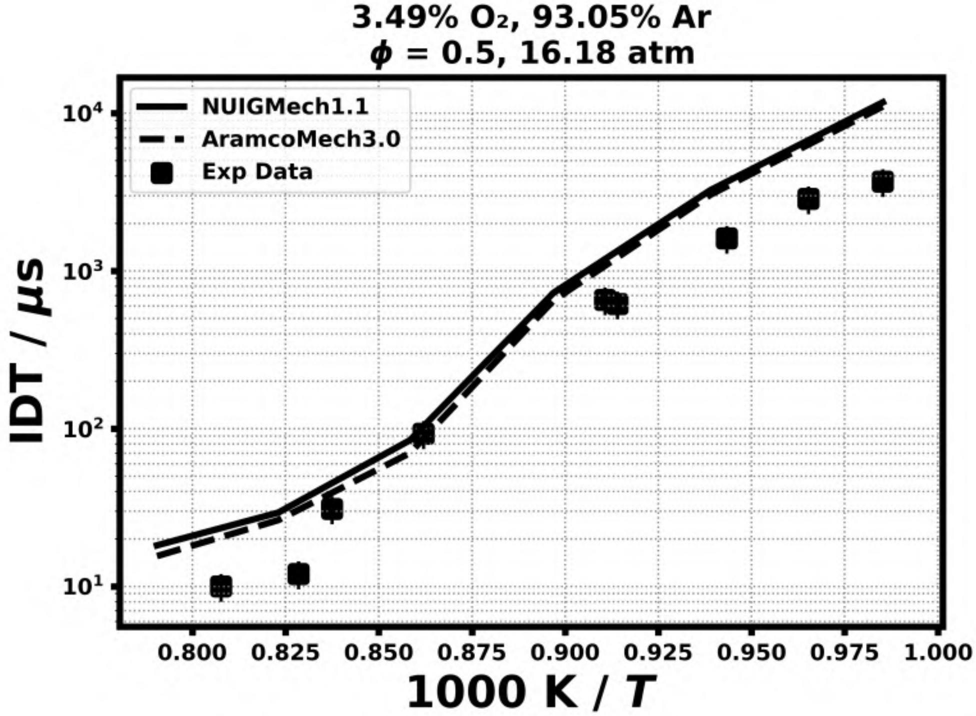




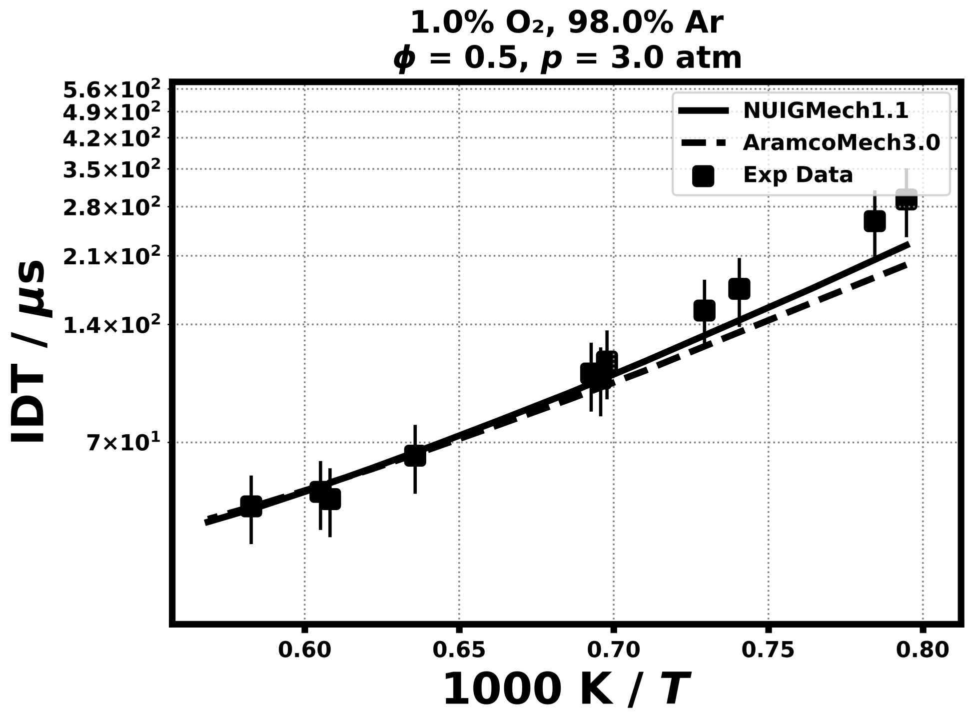
1.2) Cheng, R. K., & Oppenheim, A. K., Combustion and flame 58(2) (1984) 125-139.



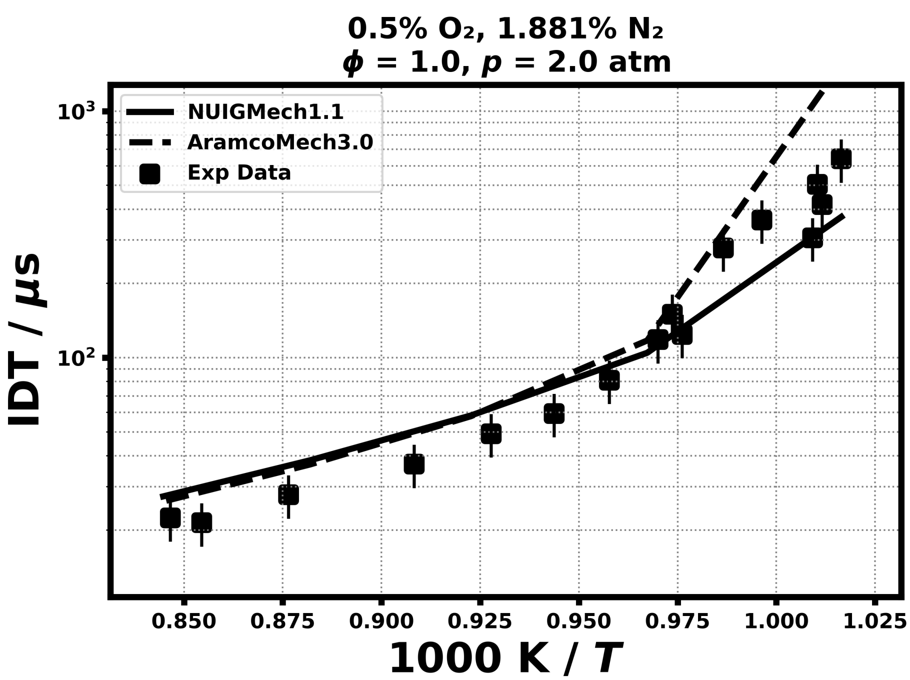
1.3) Herzler, J., & Naumann, C., Proceedings of the combustion institute, 32(1) (2009) 213-220.



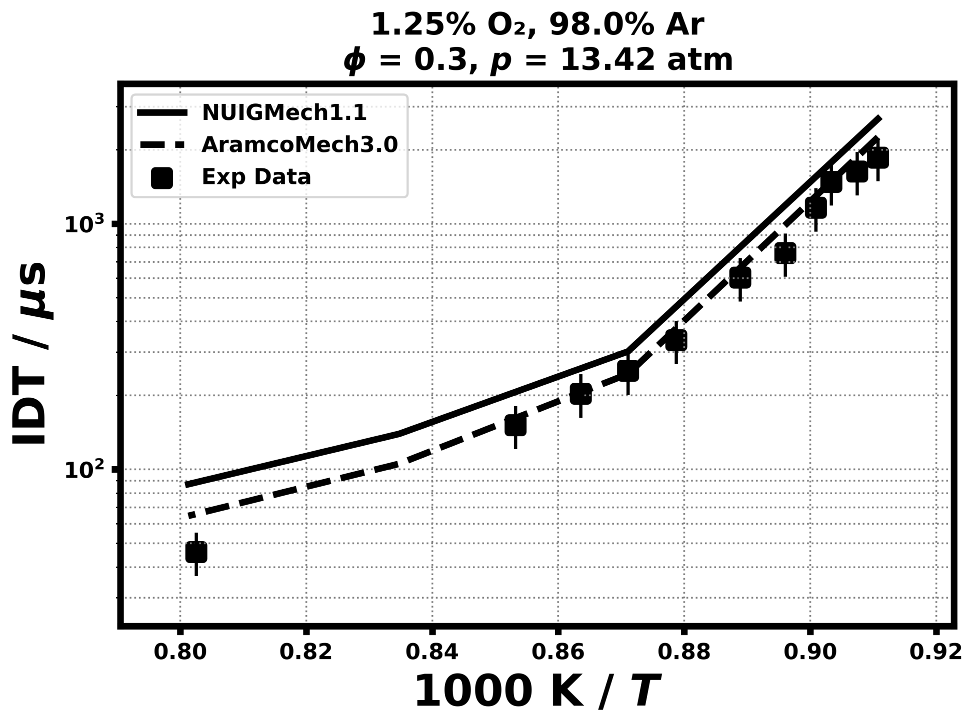
1.4) Hidaka, Y., Sato, K., Henmi, Y., Tanaka, H., & Inami, K., Combustion and flame, 118(3) (1999) 340-358.

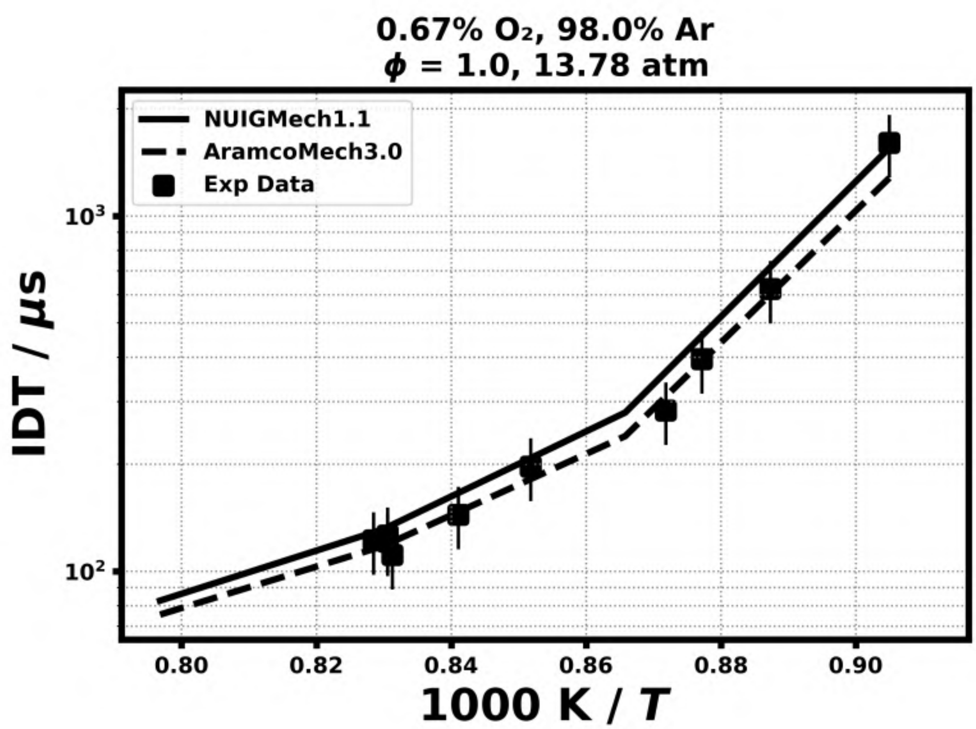


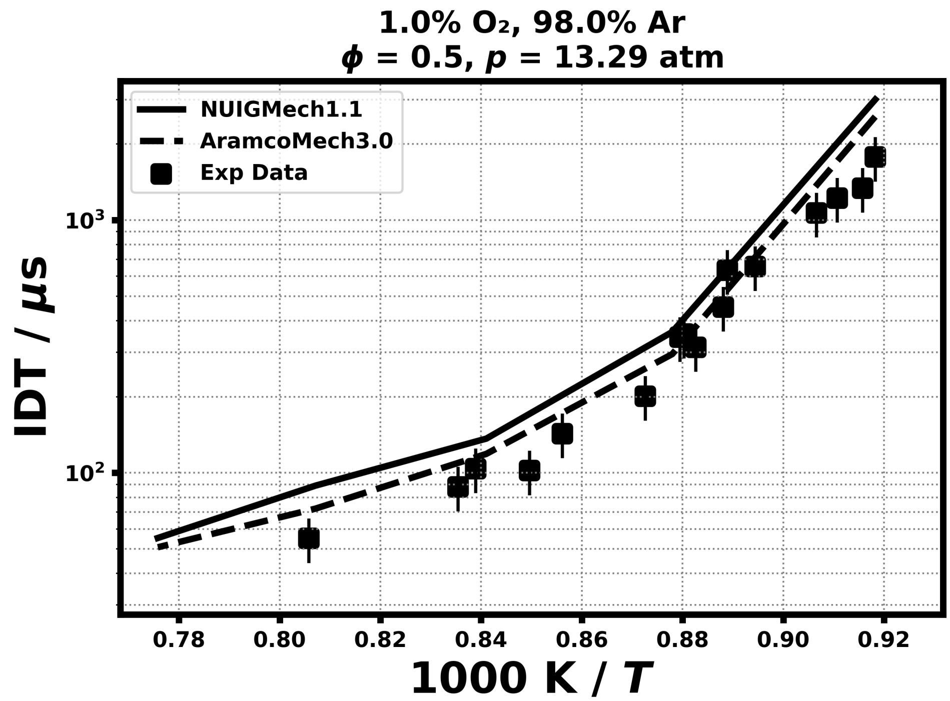
1.5) M. W. Slack, Combustion and Flame, 28 (1977) 241-249.

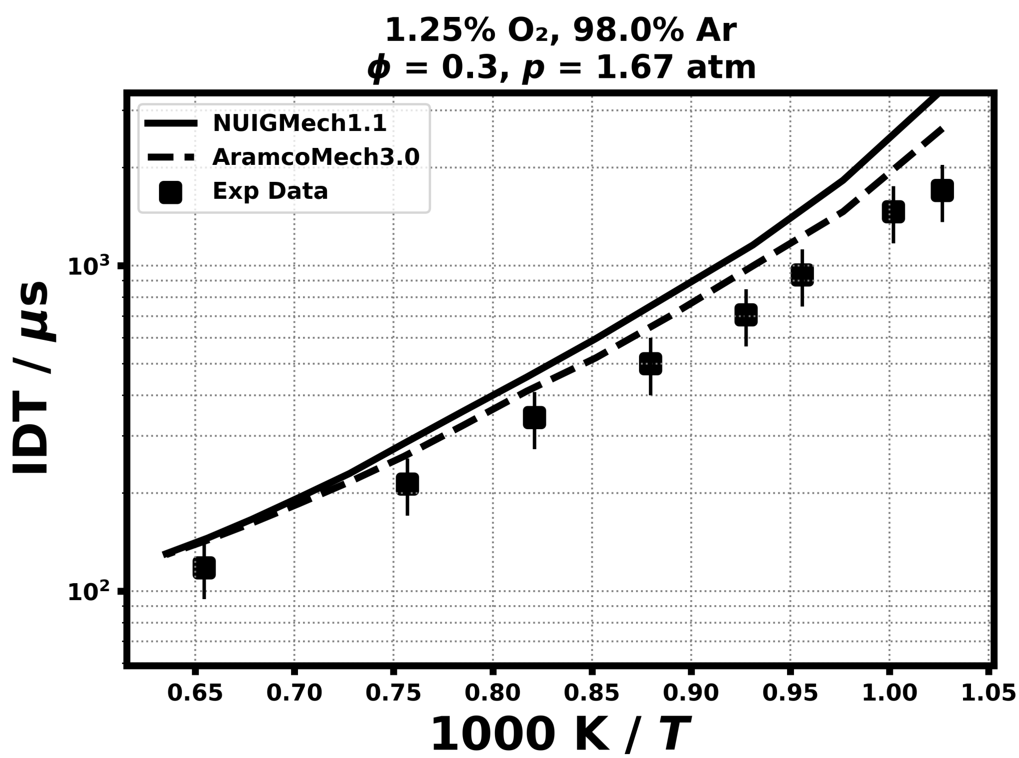


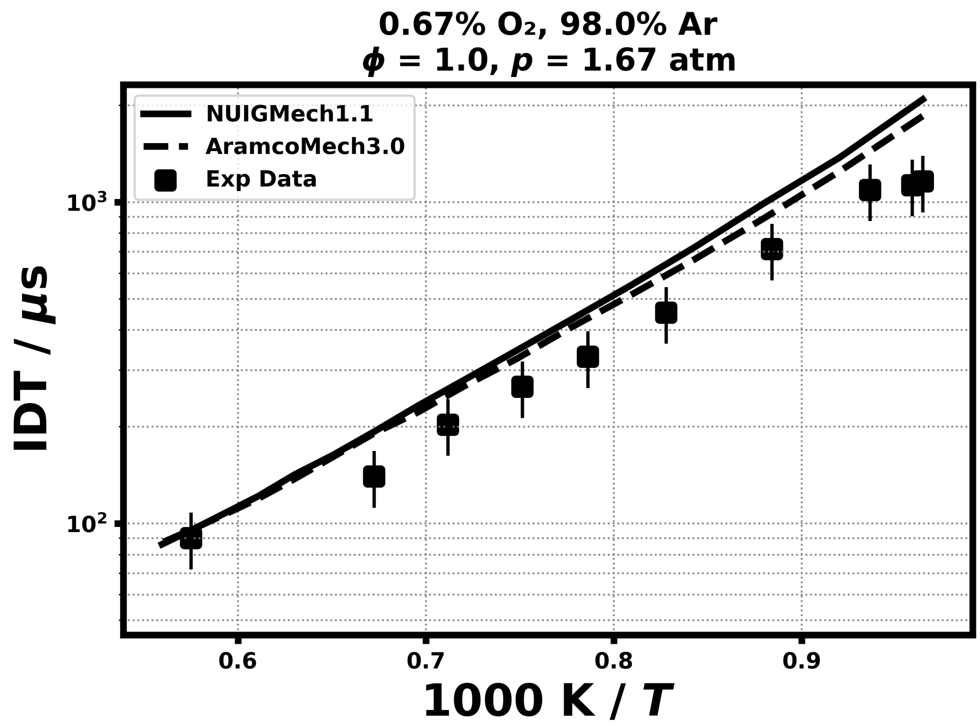
1.6) Kéromnès, A., Metcalfe, W. K., Heufer, K. A., Donohoe, N., Das, A. K., Sung, C. J., & Krejci, M. C., Combustion and Flame, 160(6), (2013) 995-1011.

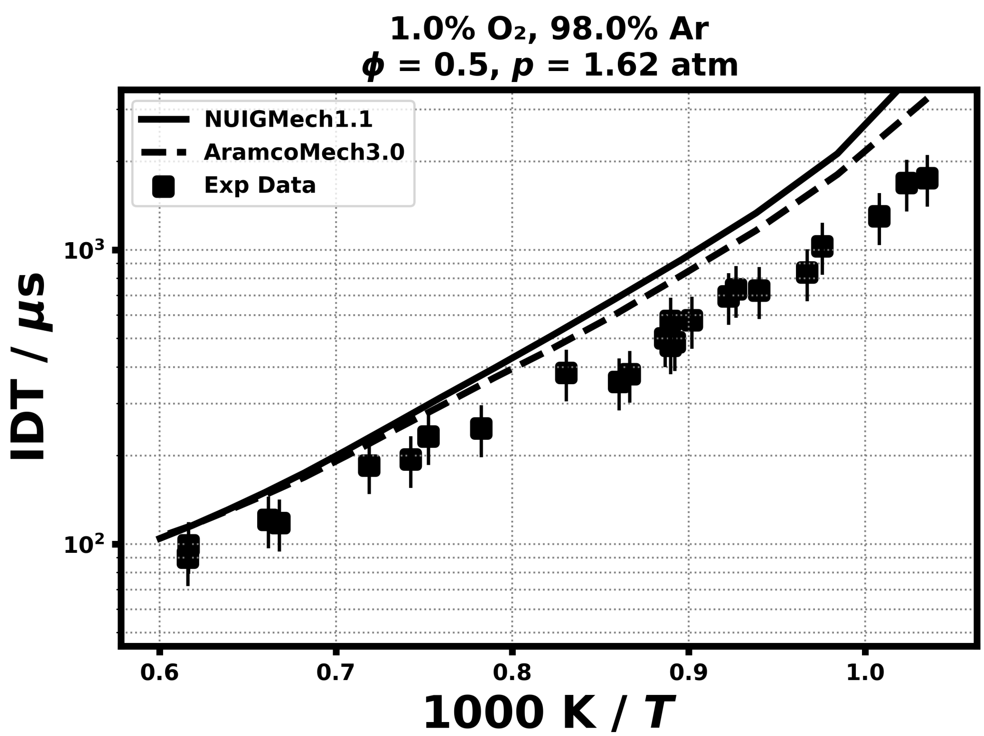


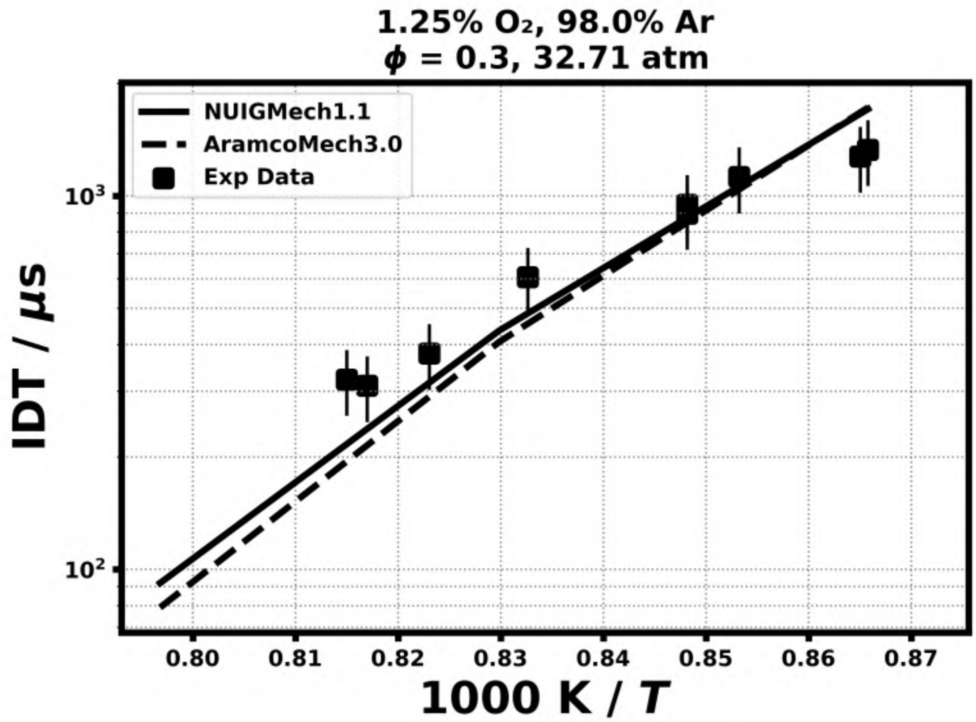


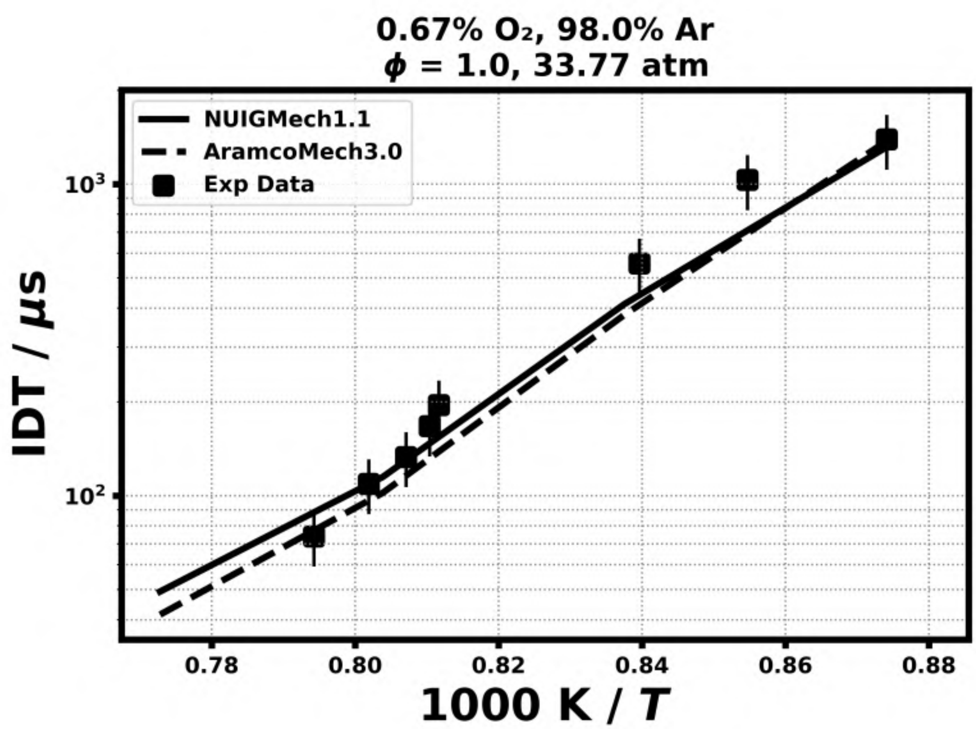

1.0% O₂, 98.0% Ar
ϕ = 0.5, p = 13.29 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.78
0.80
0.82
0.84
0.86
0.88
0.90
0.92
1000 K / T

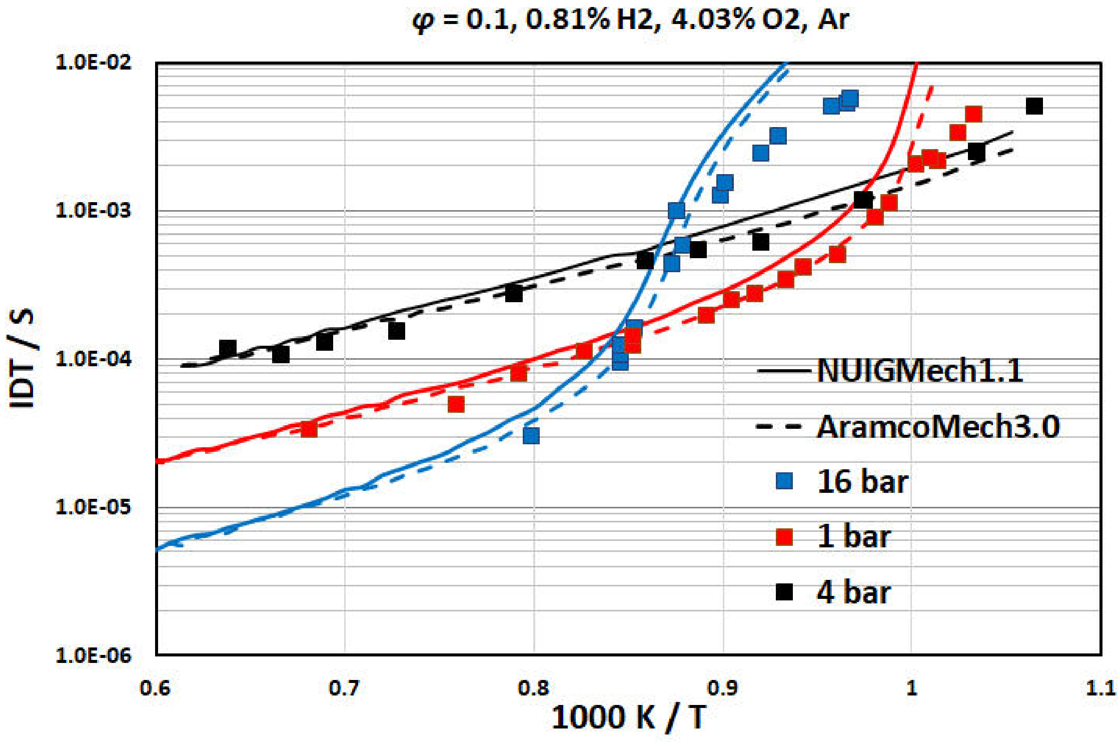

1.25% O₂, 98.0% Ar
ϕ = 0.3, p = 1.67 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.65
0.70
0.75
0.80
0.85
0.90
0.95
1.00
1.05
1000 K / T


0.67% O₂, 98.0% Ar
ϕ = 1.0, p = 1.67 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.6
0.7
0.8
0.9
1000 K / T


1.0% O₂, 98.0% Ar
ϕ = 0.5, p = 1.62 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.6
0.7
0.8
0.9
1.0
1000 K / T

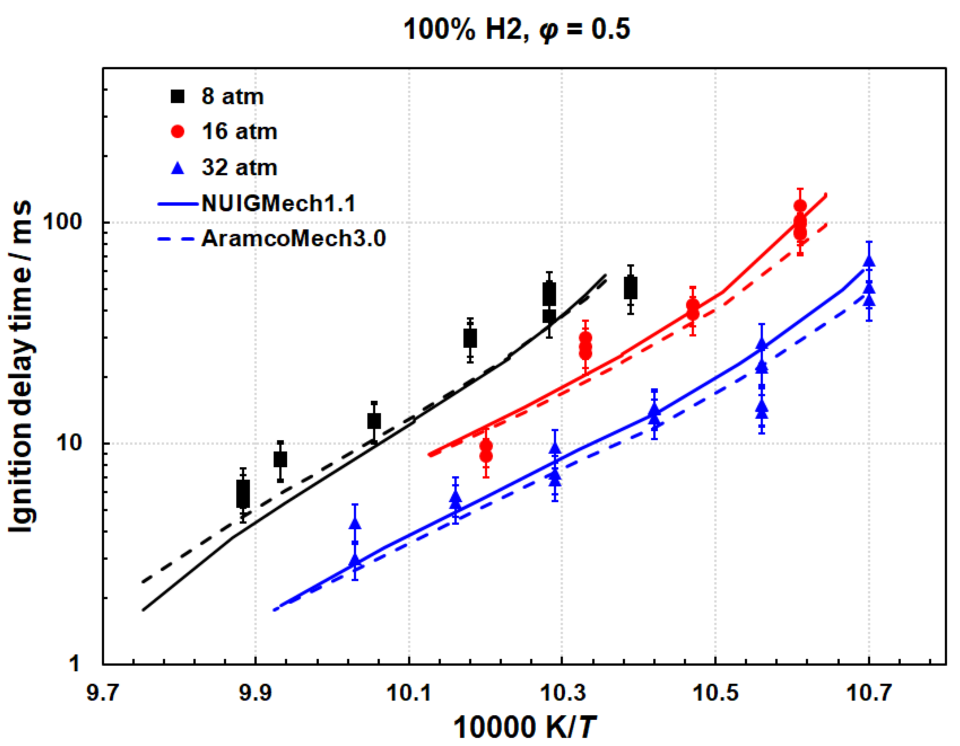

1.25% O₂, 98.0% Ar
ϕ = 0.3, 32.71 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
10³
10²
0.80
0.81
0.82
0.83
0.84
0.85
0.86
0.87


0.67% O₂, 98.0% Ar
ϕ = 1.0, 33.77 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
10³
10²
0.78
0.80
0.82
0.84
0.86
0.88



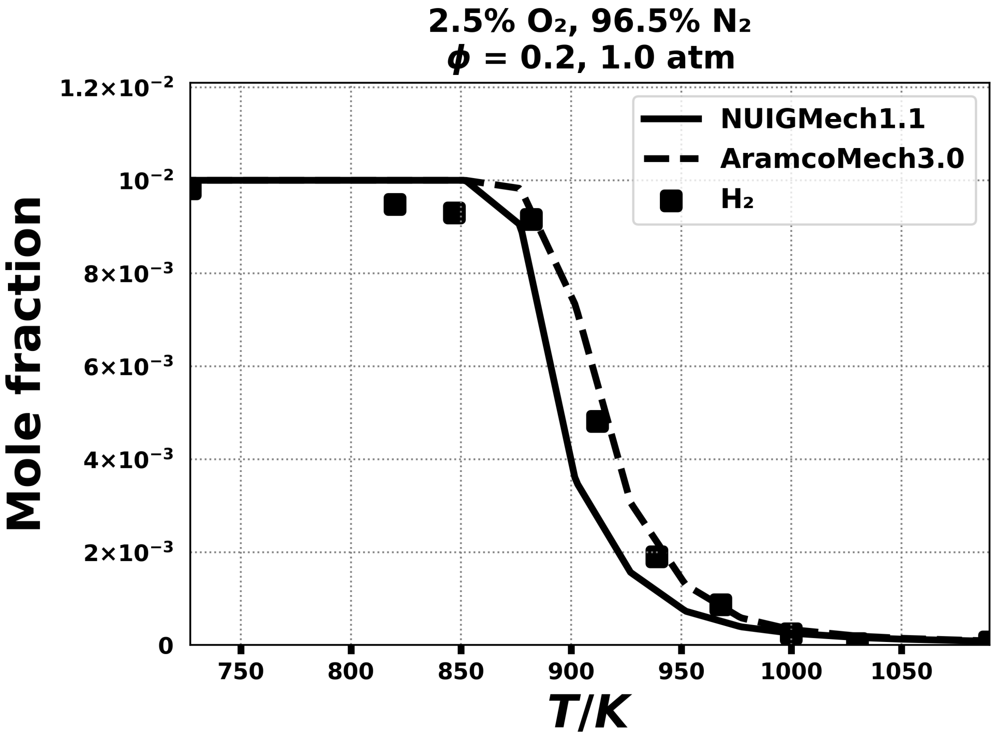
RCM Ignition delay time

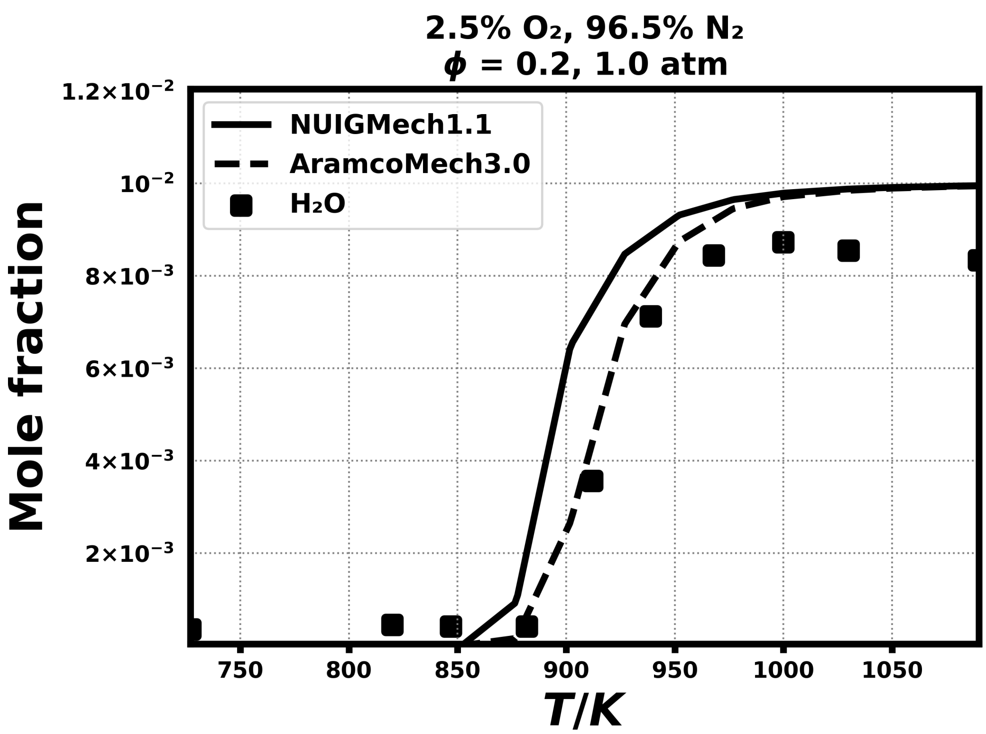
1.7) Kéromnès, A., Metcalfe, W. K., Heufer, K. A., Donohoe, N., Das, A. K., Sung, C. J., & Krejci, M. C., Combustion and Flame, 160(6), (2013) 995-1011.

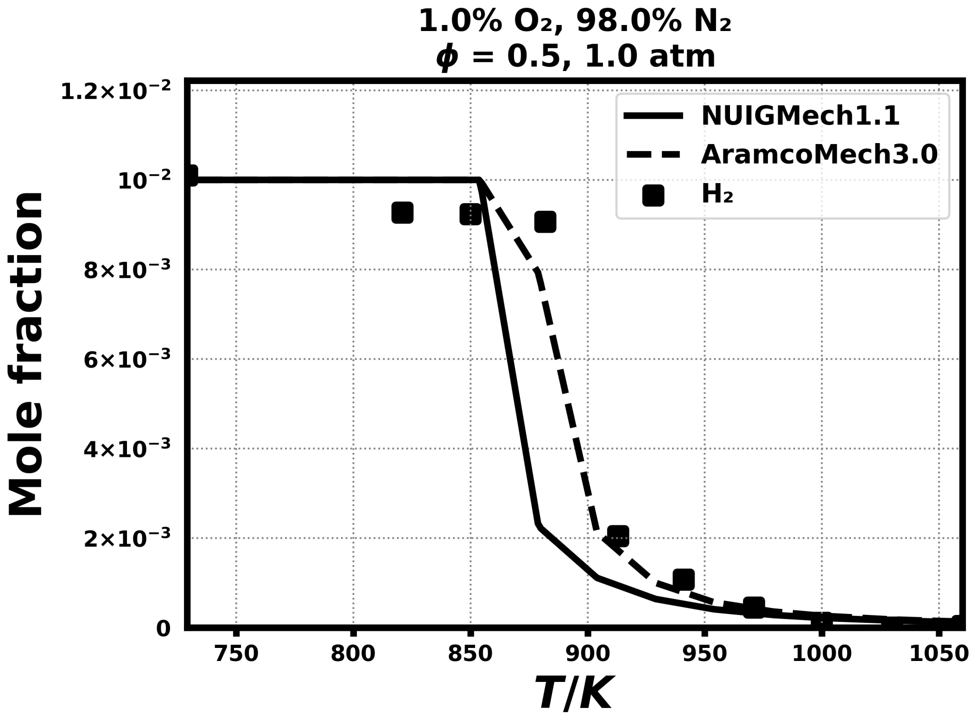


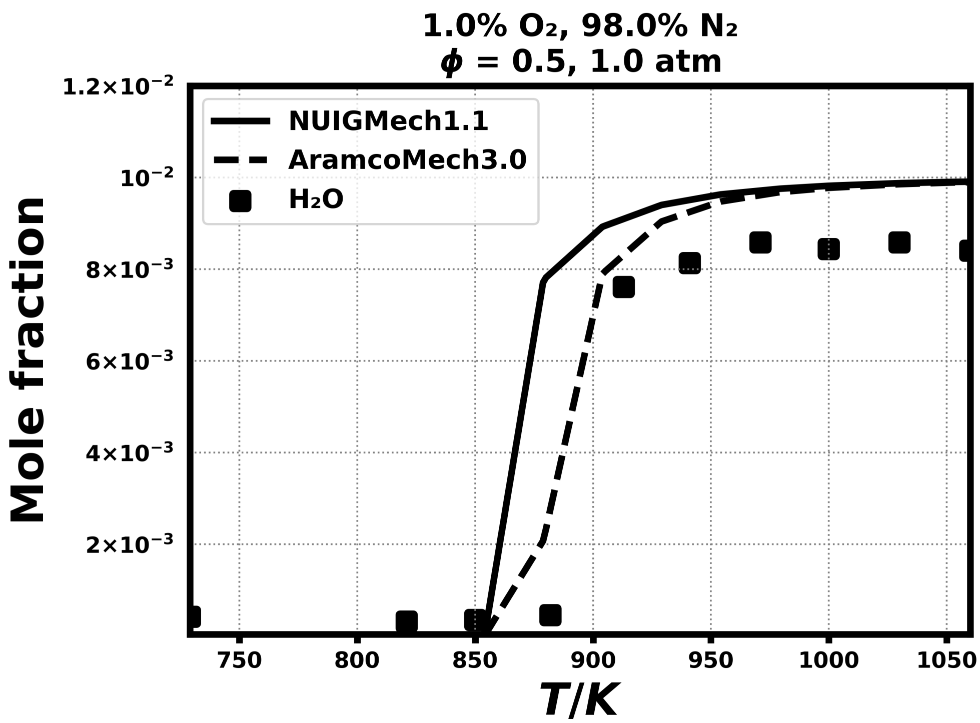
Speciation in Jet-stirred reactor

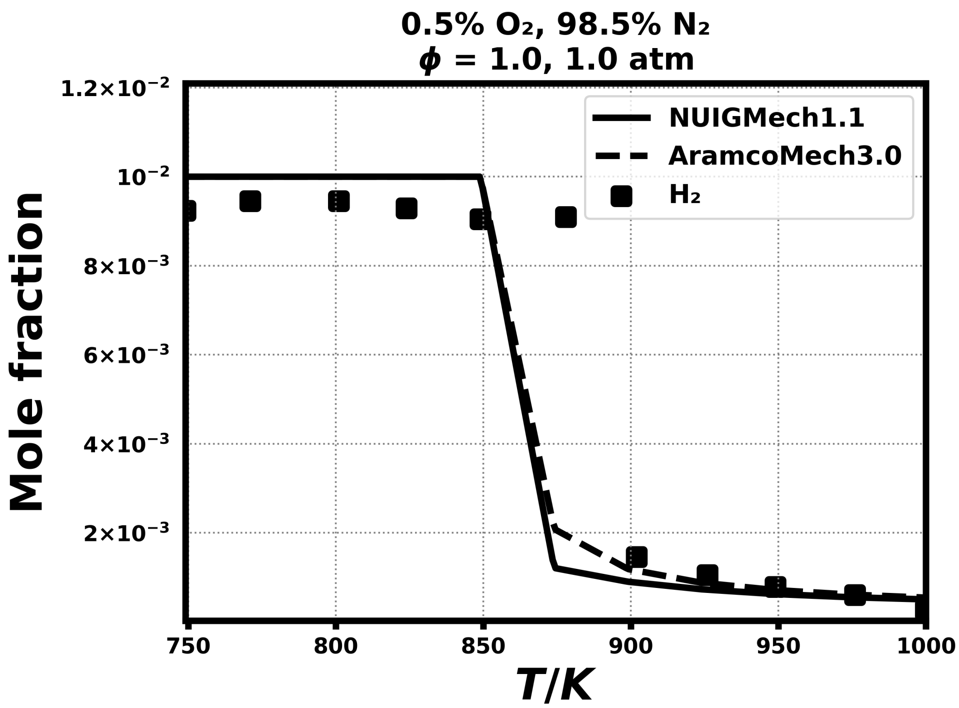
1.8) G. Dayma et al., Combustion science and technology, 178(10-11), 1999-2024.



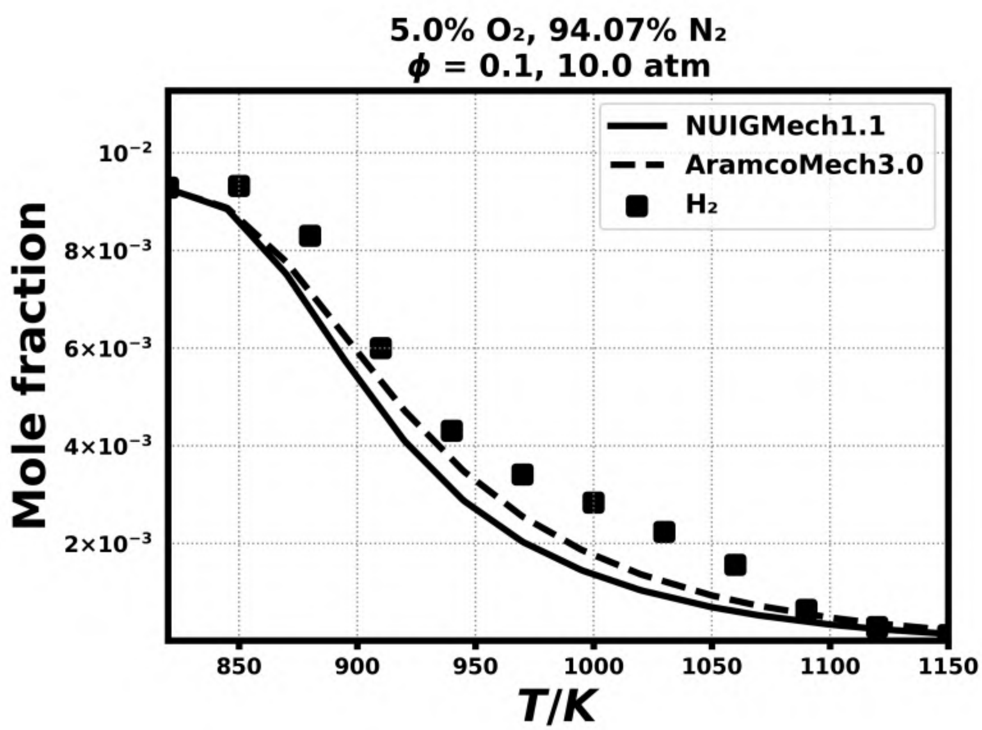


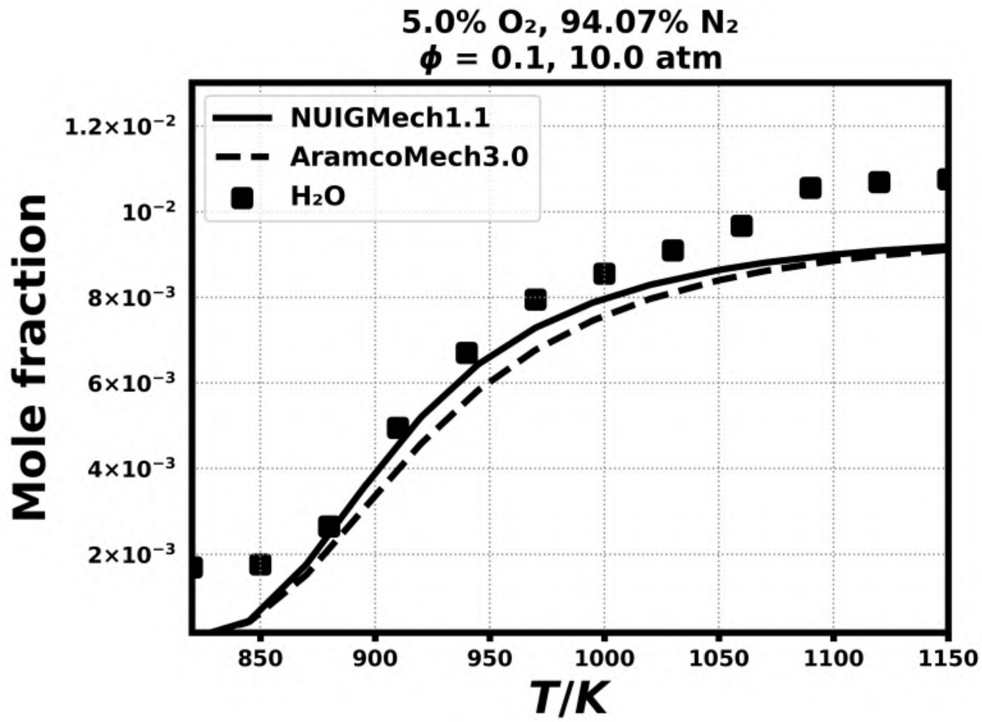

1.0% O₂, 98.0% N₂
ϕ = 0.5, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
H₂
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
0
750
800
850
900
950
1000
1050

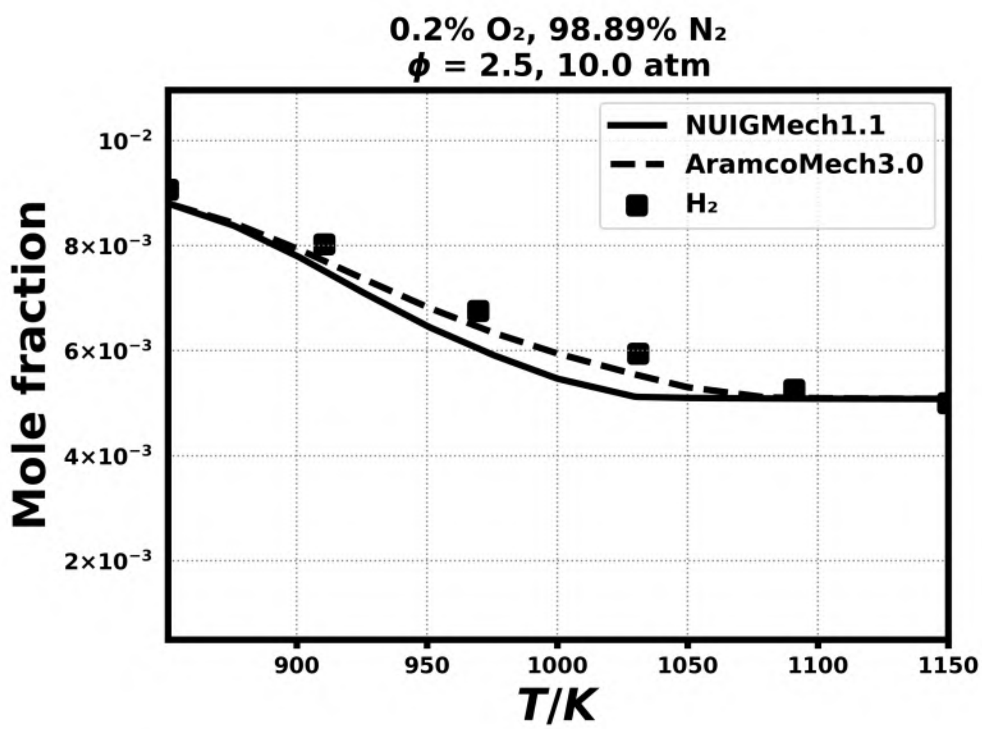

1.0% O₂, 98.0% N₂
ϕ = 0.5, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
H₂O
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
750
800
850
900
950
1000
1050

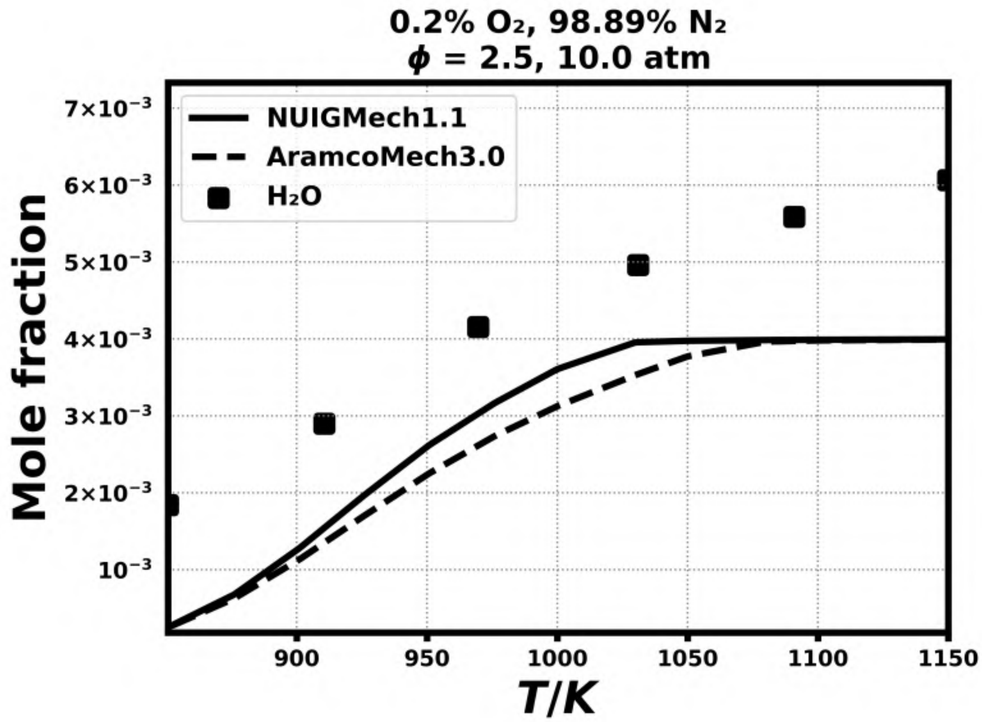


1.9) Le Cong, T., & Dagaut, P., Energy & Fuels, 23(2) (2009) 725-734.

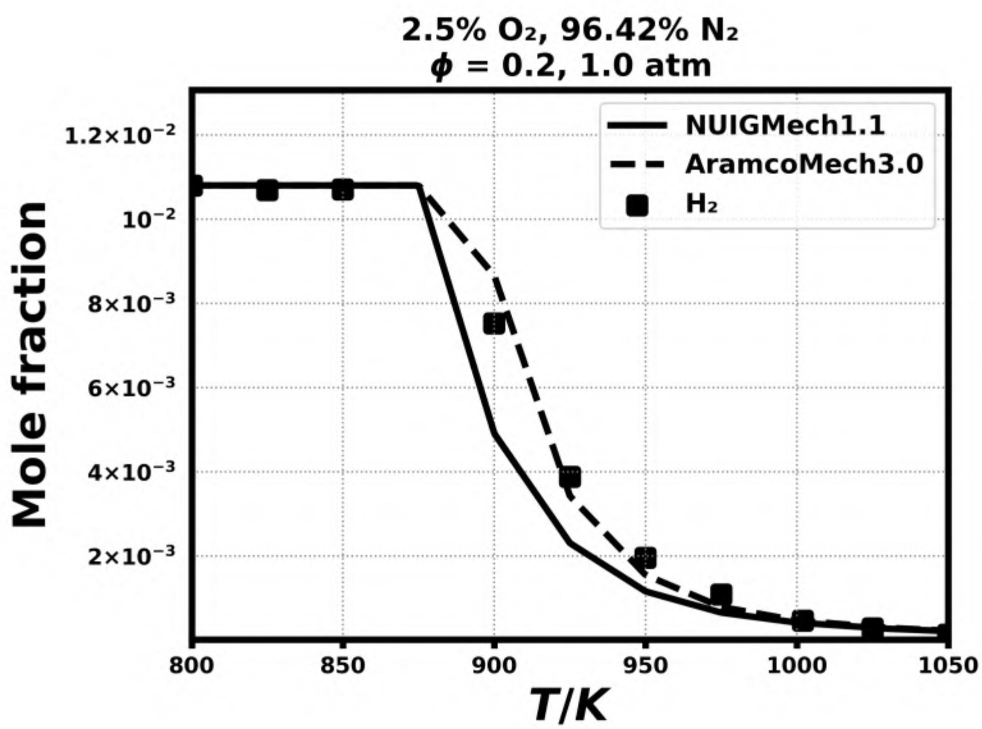



5.0% O₂, 94.07% N₂
ϕ = 0.1, 10.0 atm
NUIGMech1.1
AramcoMech3.0
H₂O
Mole fraction
T/K
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
850
900
950
1000
1050
1100
1150

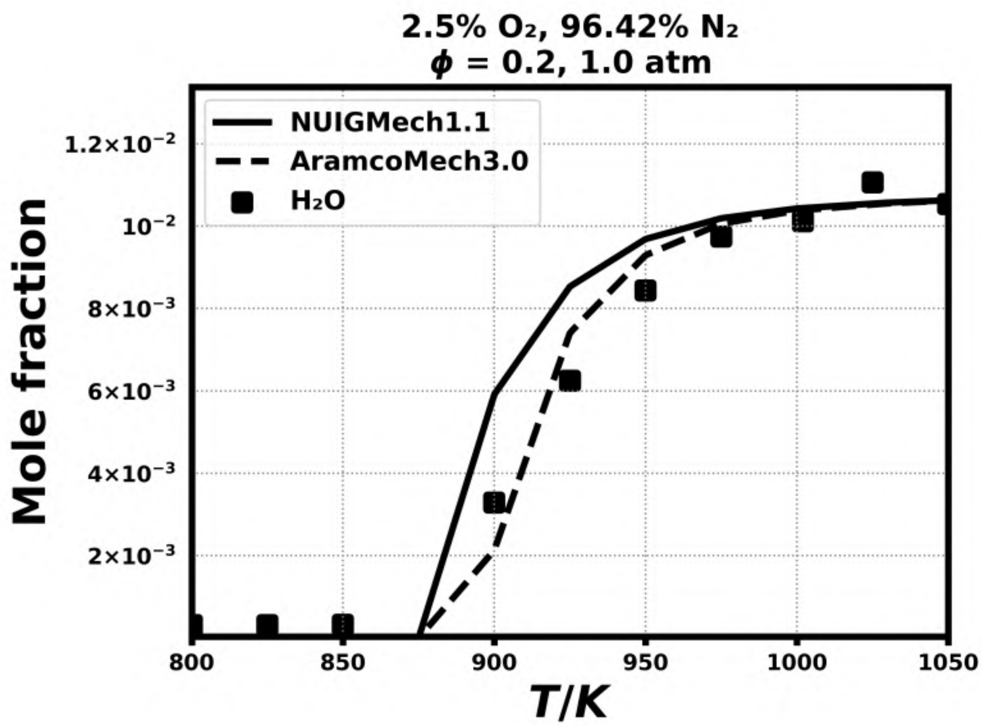

0.2% O₂, 98.89% N₂
ϕ = 2.5, 10.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
900
950
1000
1050
1100
1150

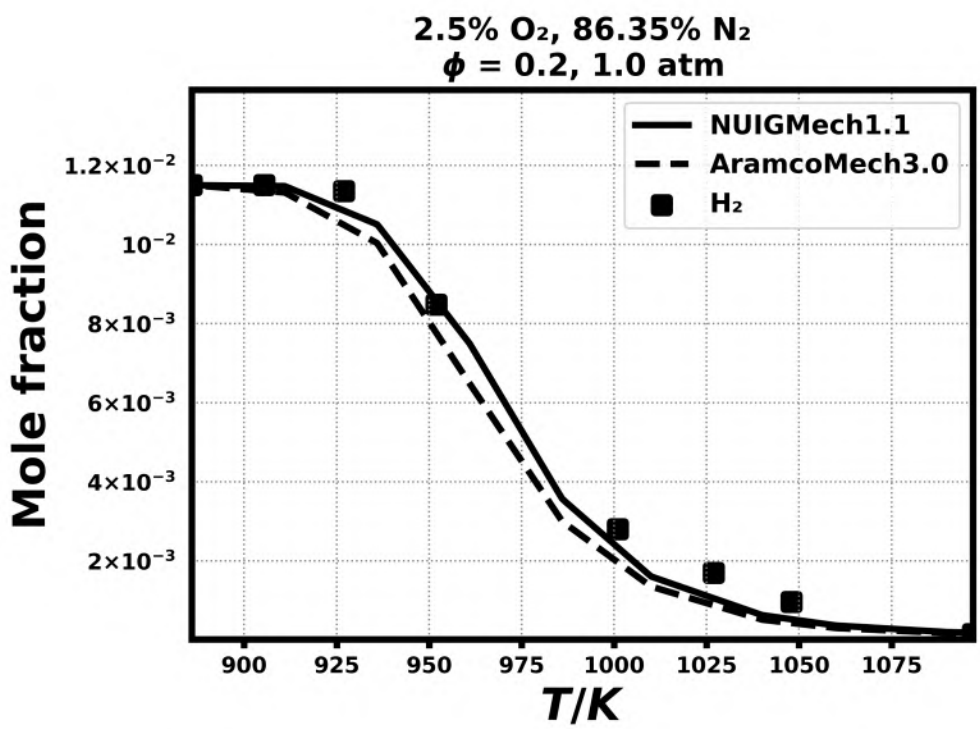


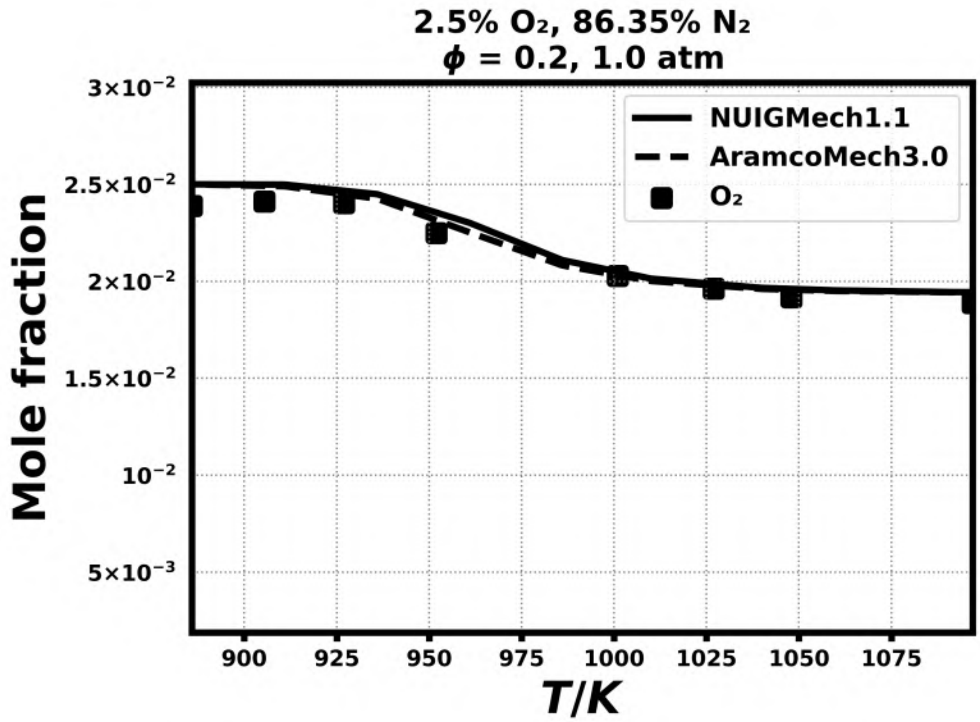
0.2% O₂, 98.89% N₂
ϕ = 2.5, 10.0 atm
NUIGMech1.1
AramcoMech3.0
H₂O
Mole fraction
T/K

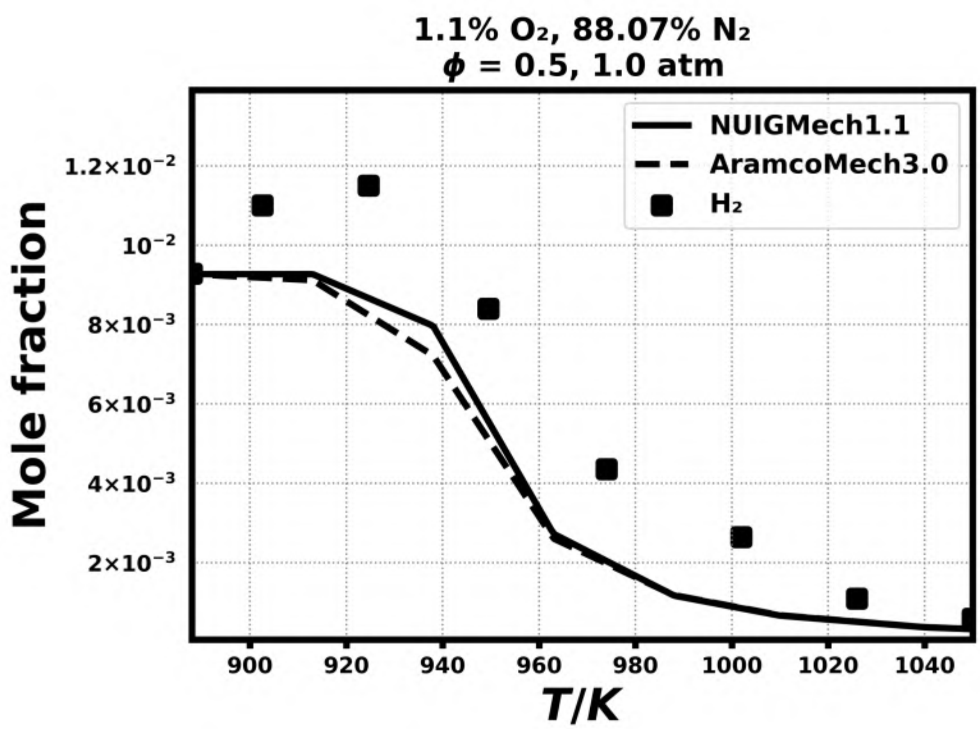


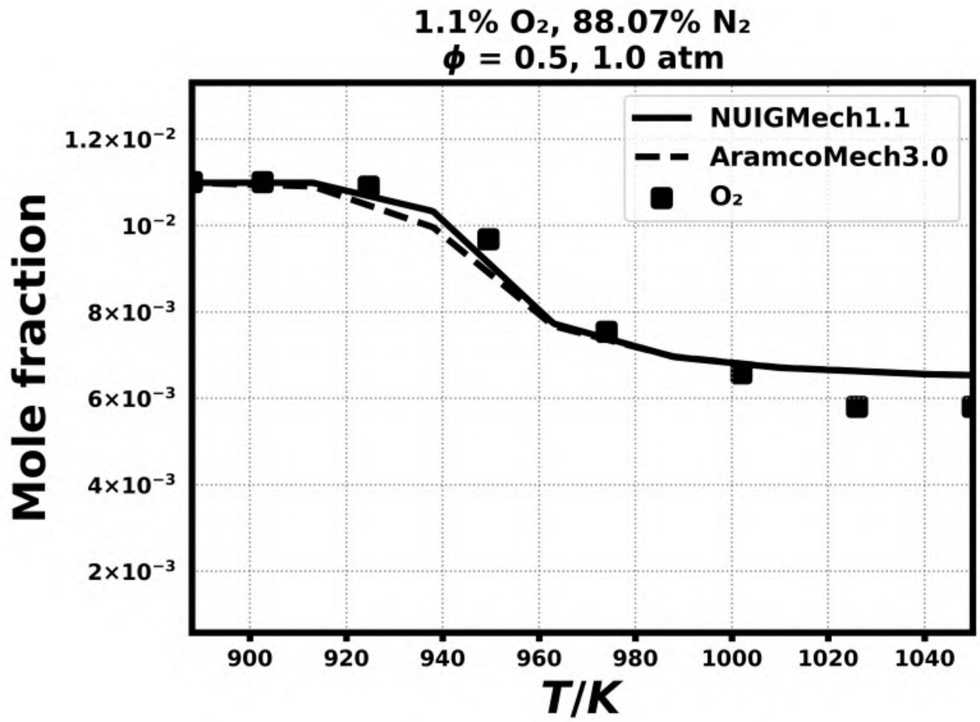
2.5% O₂, 96.42% N₂
ϕ = 0.2, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K

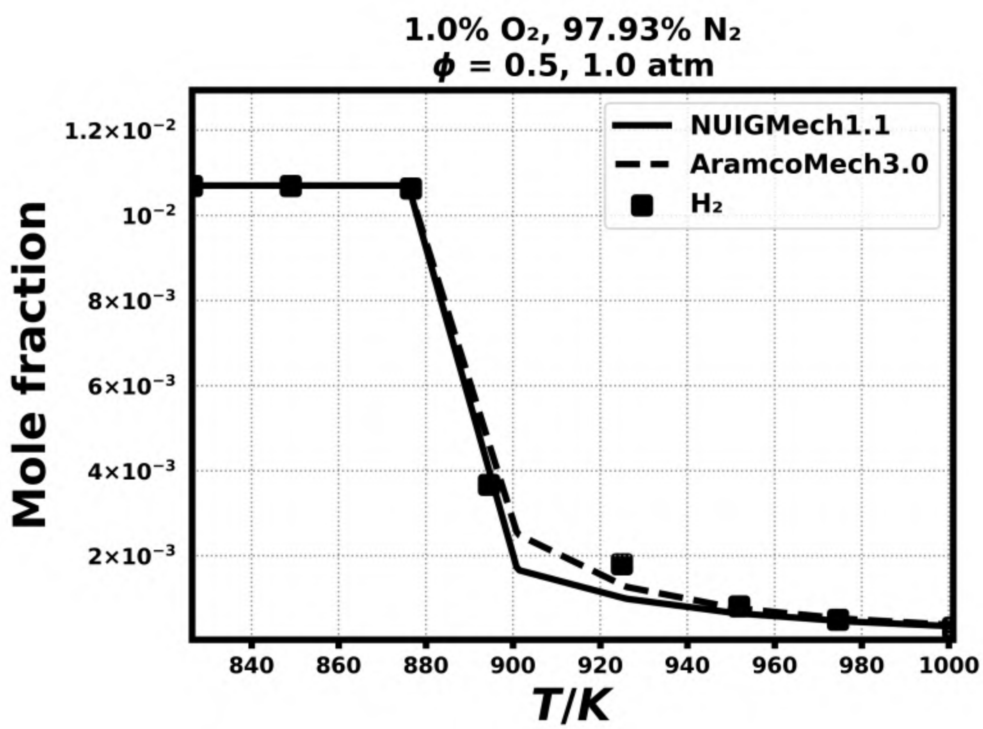

2.5% O₂, 96.42% N₂
ϕ = 0.2, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂O
Mole fraction
T/K

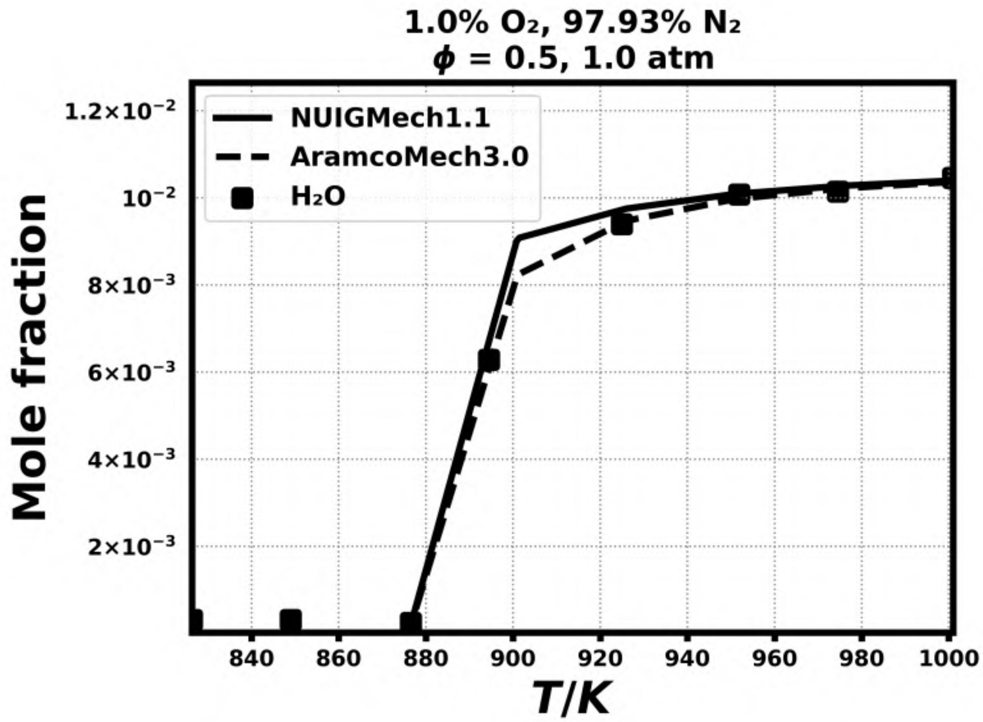

2.5% O₂, 86.35% N₂
ϕ = 0.2, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K

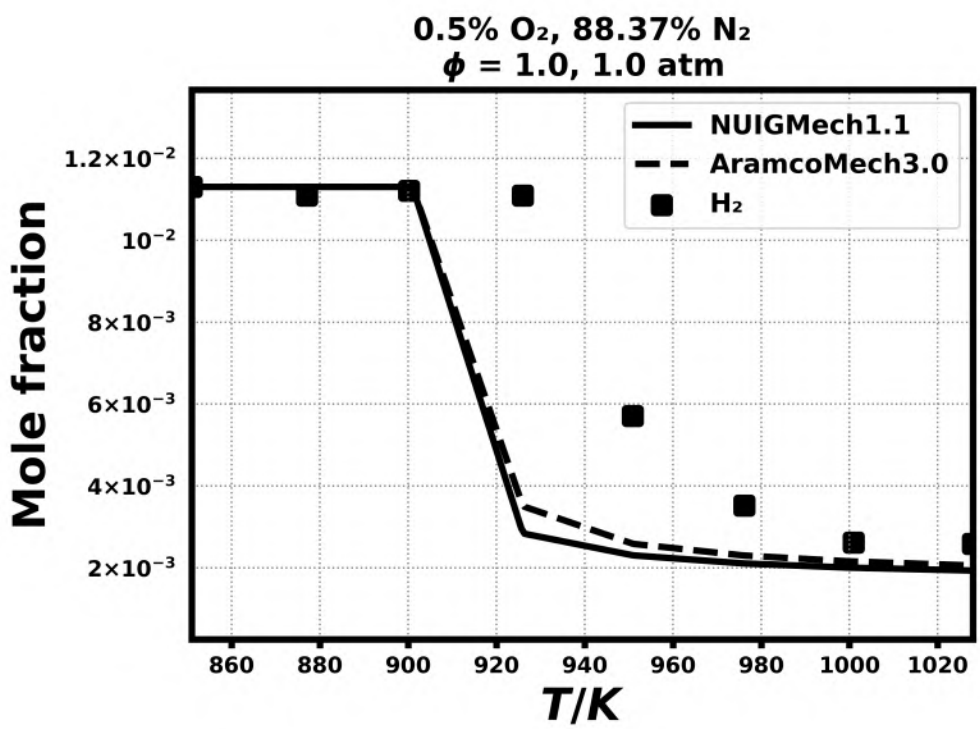

2.5% O₂, 86.35% N₂
ϕ = 0.2, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
O₂
3×10⁻²
2.5×10⁻²
2×10⁻²
1.5×10⁻²
10⁻²
5×10⁻³
900
925
950
975
1000
1025
1050
1075

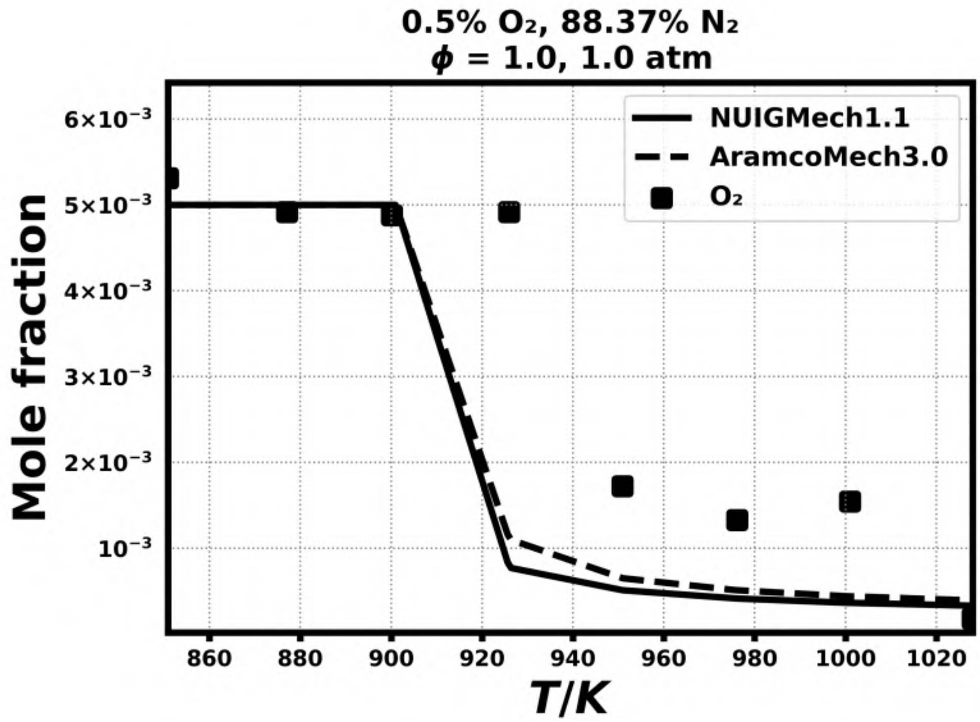

1.1% O₂, 88.07% N₂
ϕ = 0.5, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
H₂
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
900
920
940
960
980
1000
1020
1040


1.1% O₂, 88.07% N₂
ϕ = 0.5, 1.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
T/K
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
900
920
940
960
980
1000
1020
1040

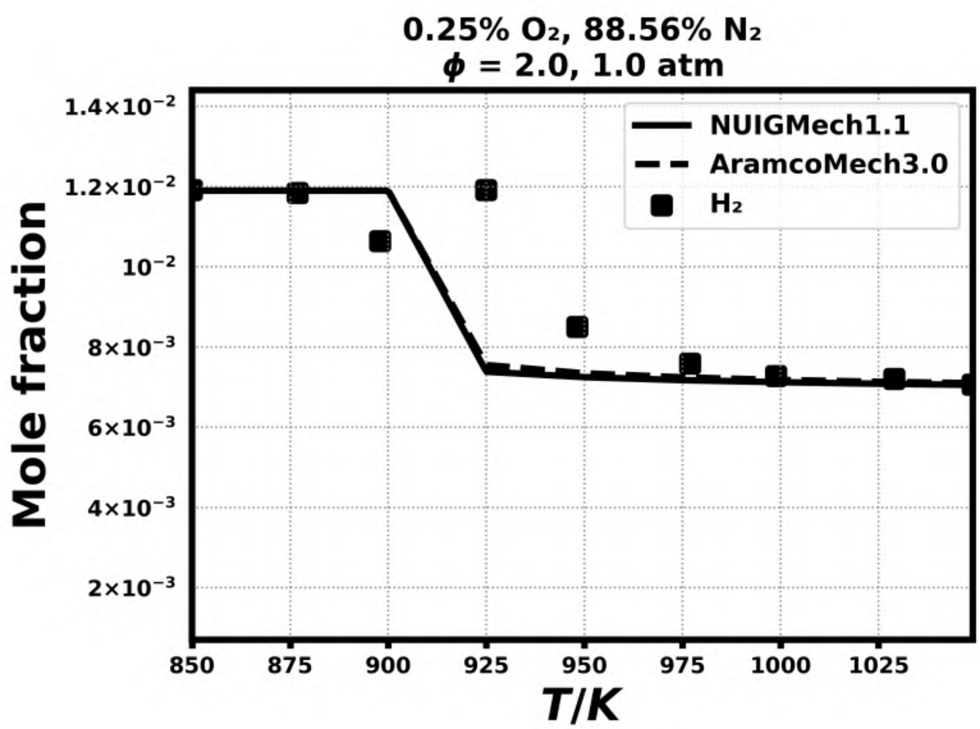

1.0% O₂, 97.93% N₂
ϕ = 0.5, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
840
860
880
900
920
940
960
980
1000


1.0% O₂, 97.93% N₂
ϕ = 0.5, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂O
Mole fraction
T/K

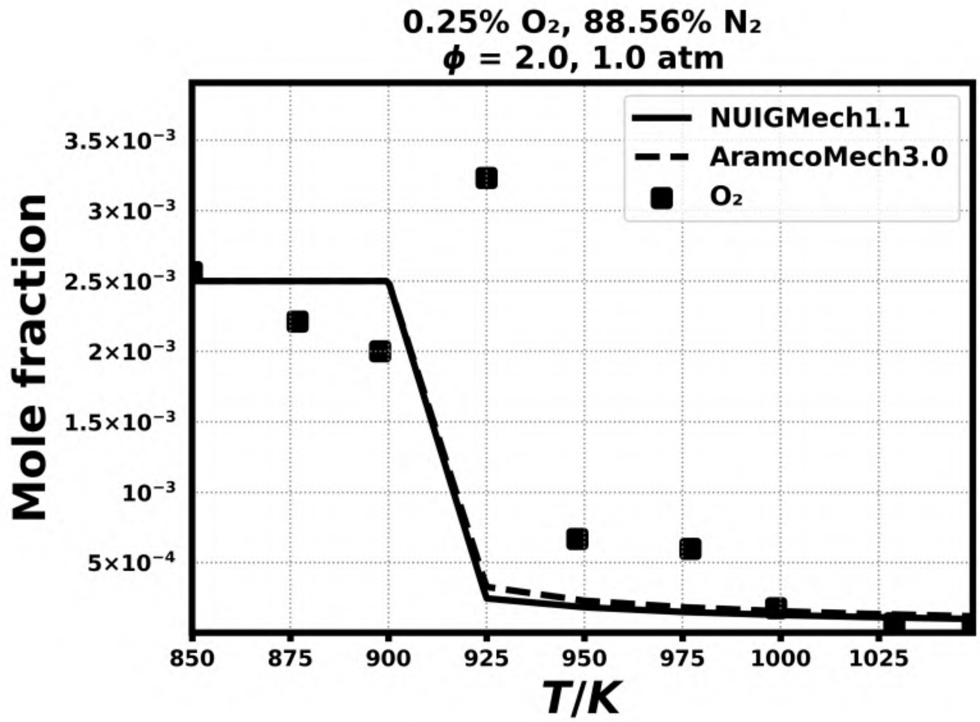

0.5% O₂, 88.37% N₂
ϕ = 1.0, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K

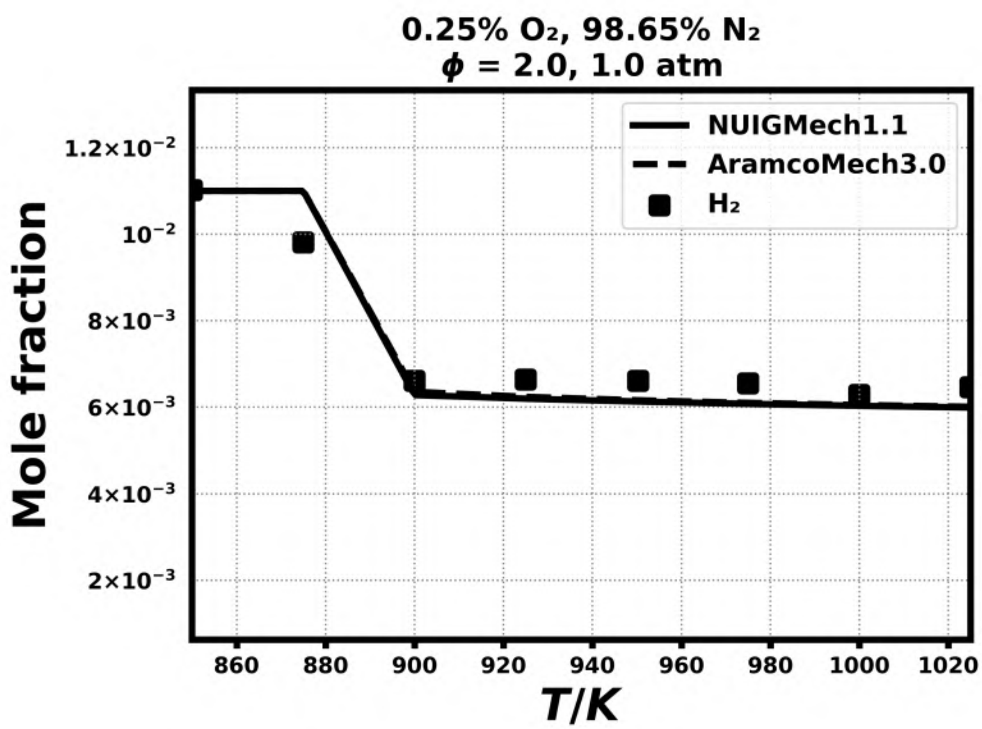


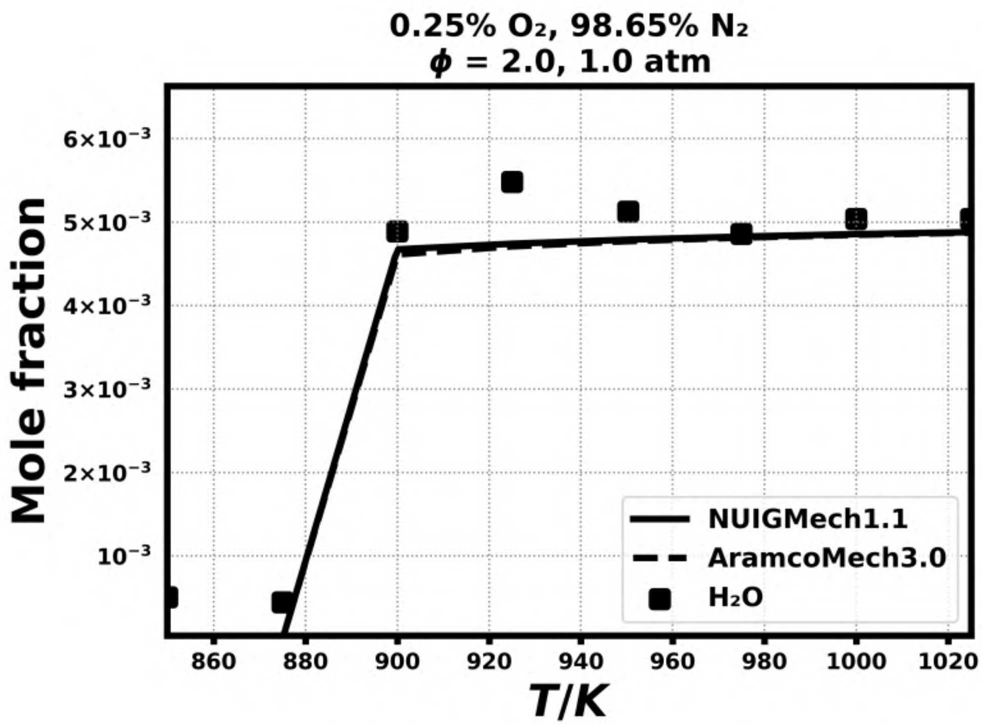
0.5% O₂, 88.37% N₂
ϕ = 1.0, 1.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
6×10⁻³
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
860
880
900
920
940
960
980
1000
1020
T/K



0.25% O₂, 88.56% N₂
ϕ = 2.0, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
1.4×10⁻²
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
850
875
900
925
950
975
1000
1025
T/K

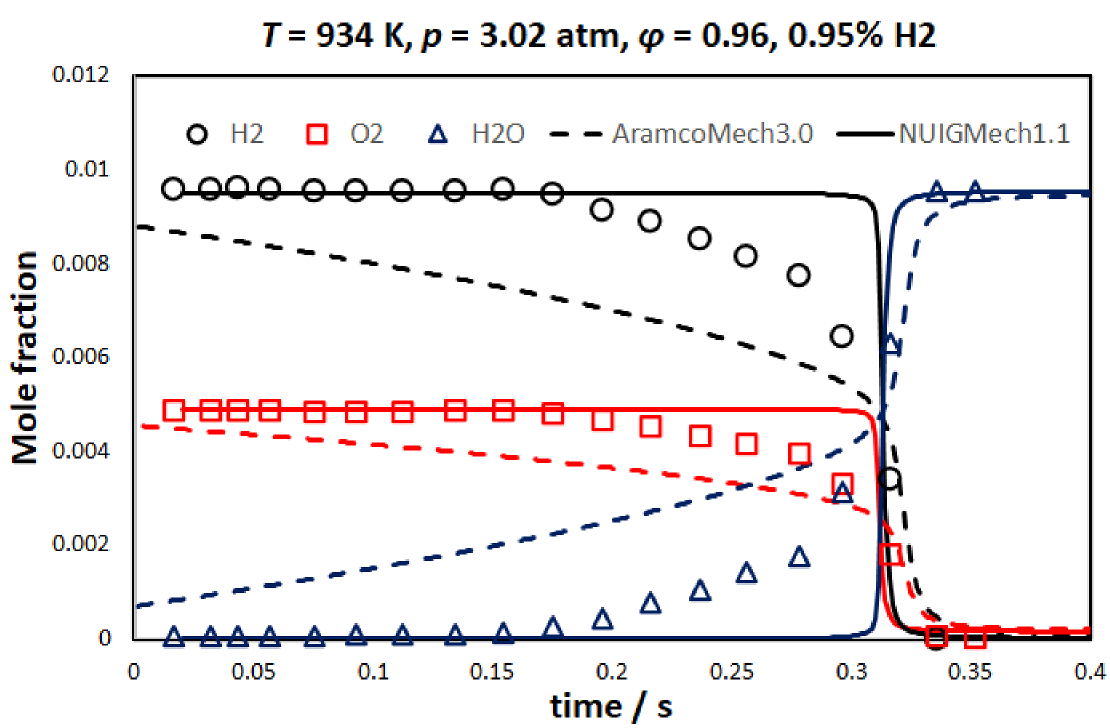

0.25% O_2, 88.56% N_2
ϕ = 2.0, 1.0 atm
NUIGMech1.1
AramcoMech3.0
O_2
Mole fraction
T/K
3.5×10⁻³
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
850
875
900
925
950
975
1000
1025

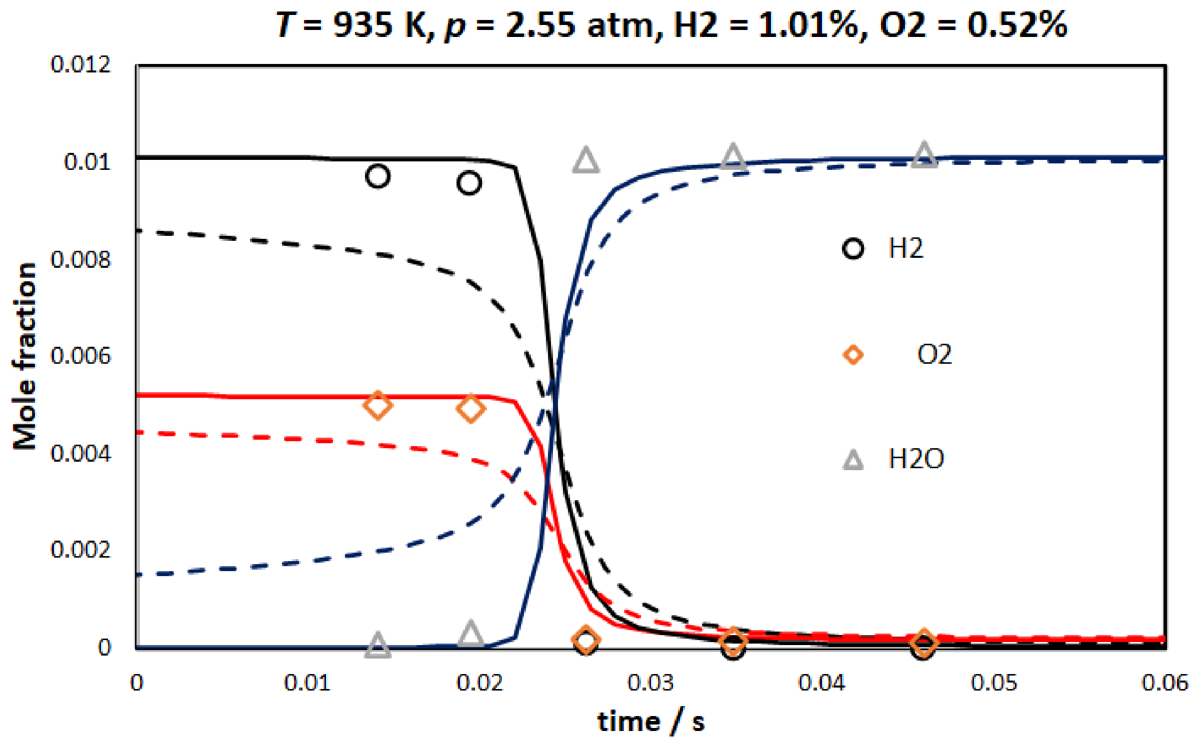

0.25% O_2, 98.65% N_2
ϕ = 2.0, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H_2
Mole fraction
T/K
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
860
880
900
920
940
960
980
1000
1020

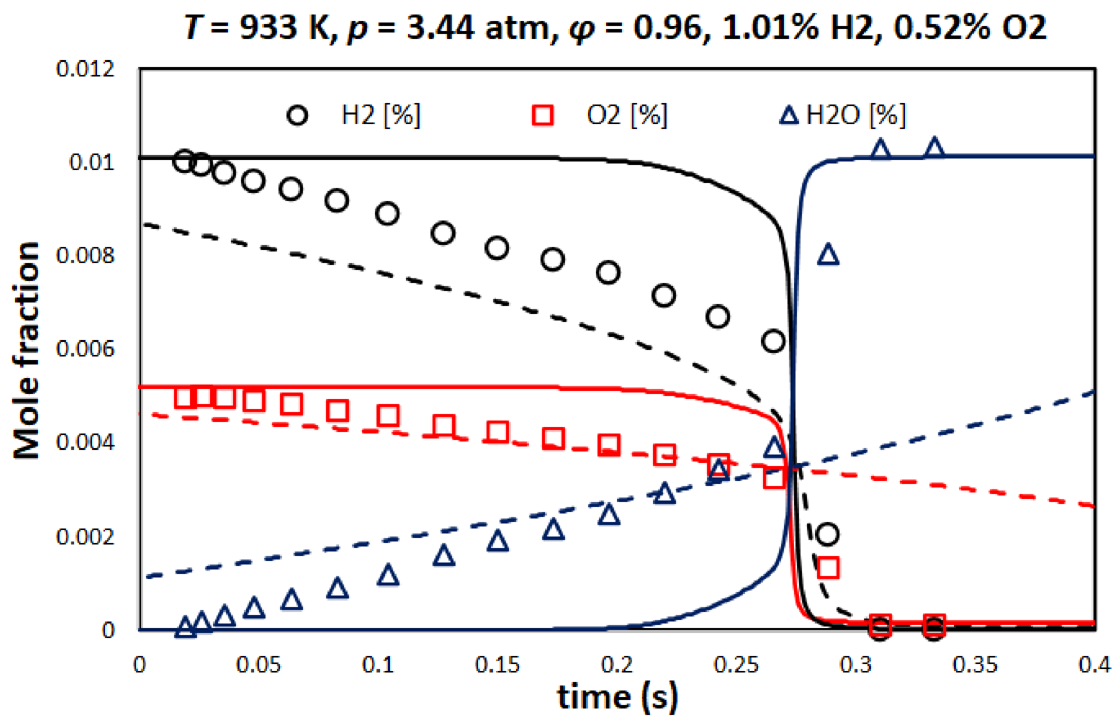


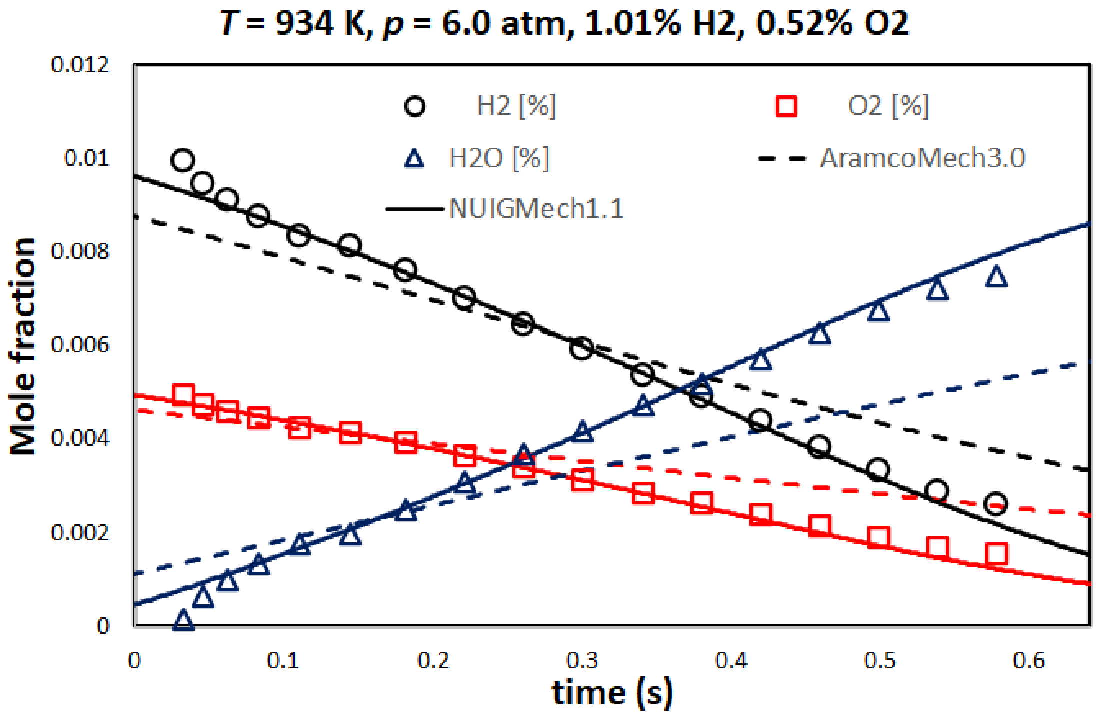
Speciation in Flow reactor

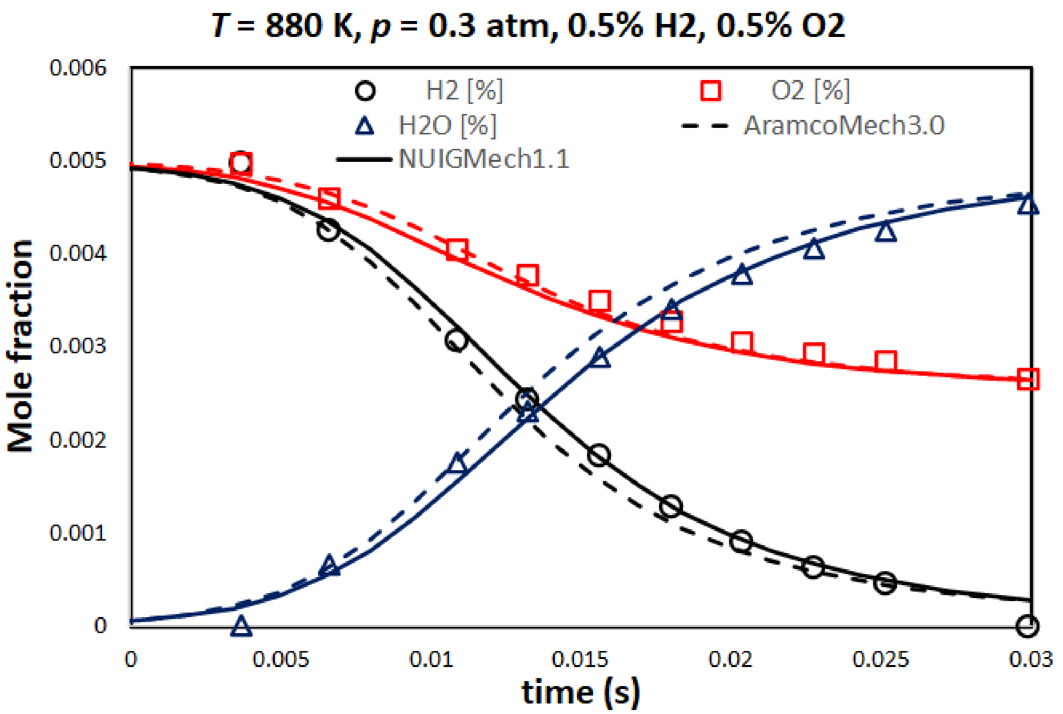
1.10) Mueller, M. A., T. J. Kim, R. A. Yetter, and F. L. Dryer, " International Journal of Chemical Kinetics 31, 2 (1999) 113-125.

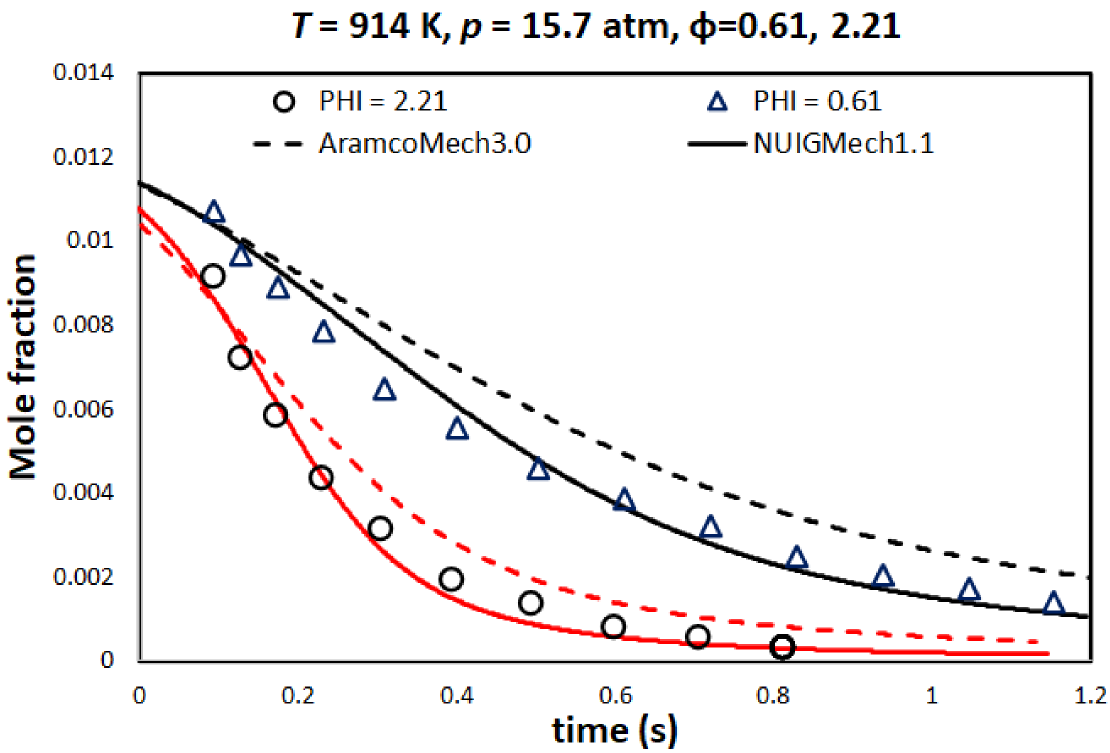



T = 935 K, p = 2.55 atm, H2 = 1.01%, O2 = 0.52%
0.012
0.01
0.008
0.006
0.004
0.002
0
Mole fraction
H2
O2
H2O
0
0.01
0.02
0.03
0.04
0.05
0.06
time / s

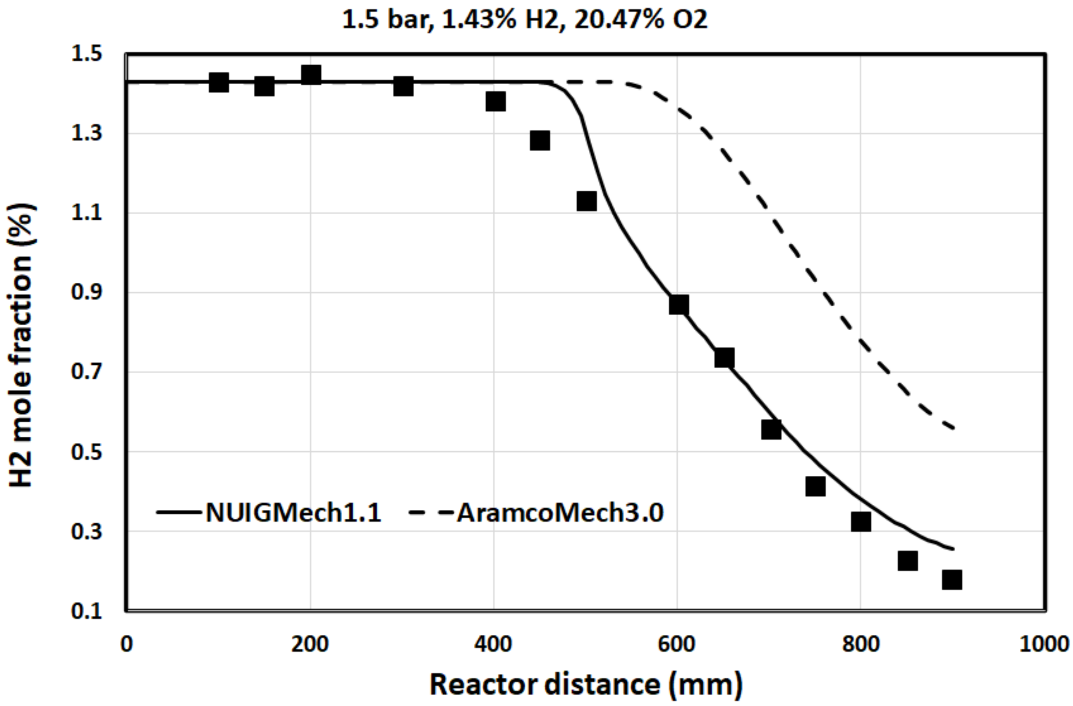

T = 933 K, p = 3.44 atm, φ = 0.96, 1.01% H2, 0.52% O2
0.012
0.01
0.008
0.006
0.004
0.002
0
Mole fraction
H2 [%]
O2 [%]
H2O [%]
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
time (s)

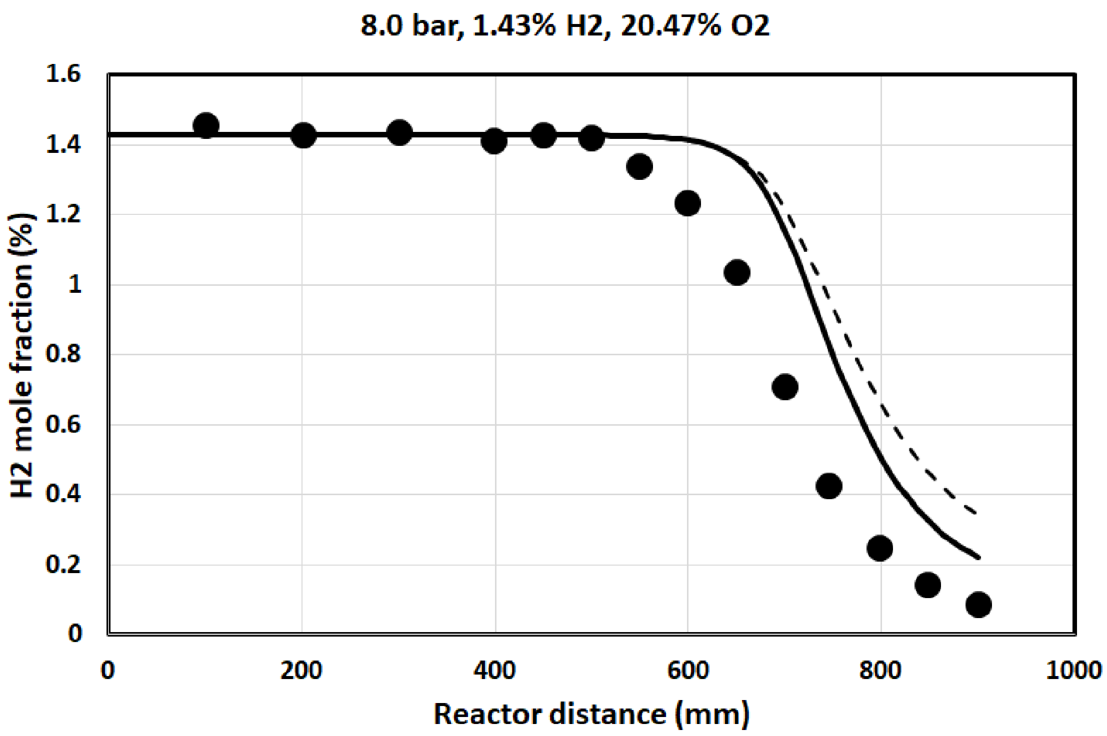

T = 934 K, p = 6.0 atm, 1.01% H2, 0.52% O2
H2 [%]
O2 [%]
H2O [%]
AramcoMech3.0
NUIGMech1.1
Mole fraction
time (s)
0.012
0.01
0.008
0.006
0.004
0.002
0
0
0.1
0.2
0.3
0.4
0.5
0.6

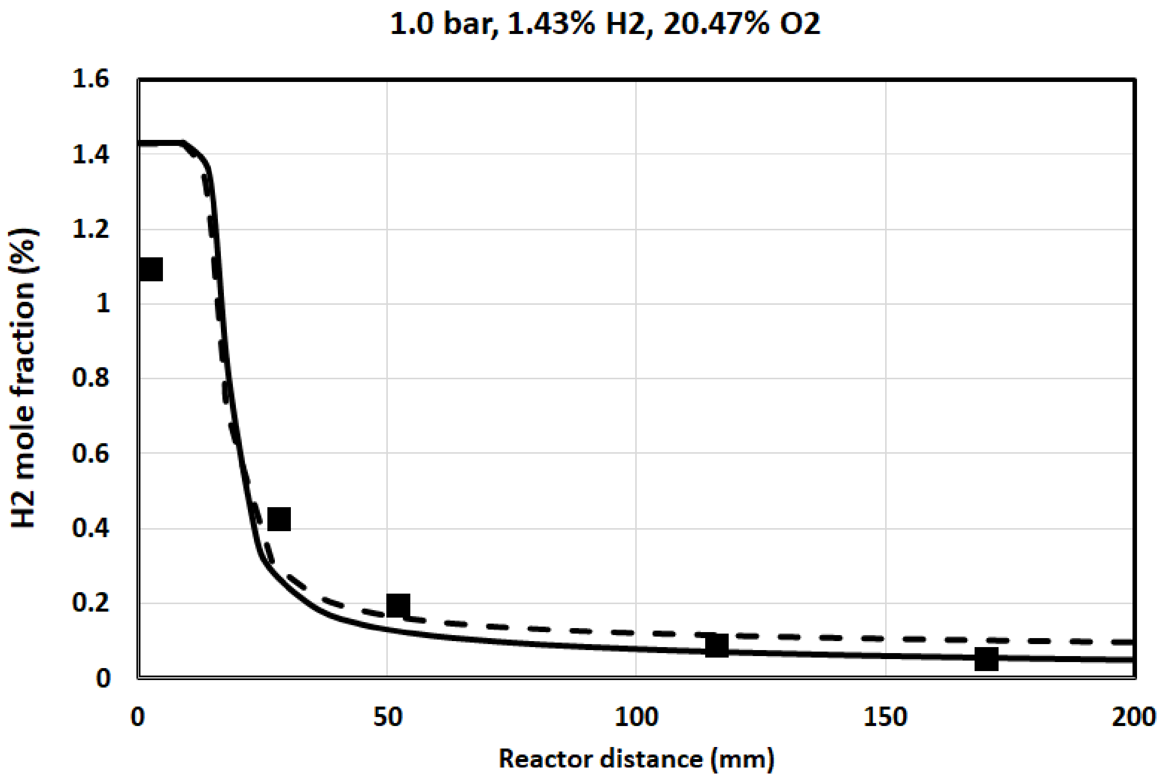

T = 880 K, p = 0.3 atm, 0.5% H2, 0.5% O2
H2 [%]
O2 [%]
H2O [%]
AramcoMech3.0
NUIGMech1.1
Mole fraction
time (s)
0.006
0.005
0.004
0.003
0.002
0.001
0
0
0.005
0.01
0.015
0.02
0.025
0.03



1.11) Lu, Zhewen, Junqiu Jiang, Yi Yang, Joshua Lacey, and Michael J. Brear., Proceedings of the Combustion Institute (2020).

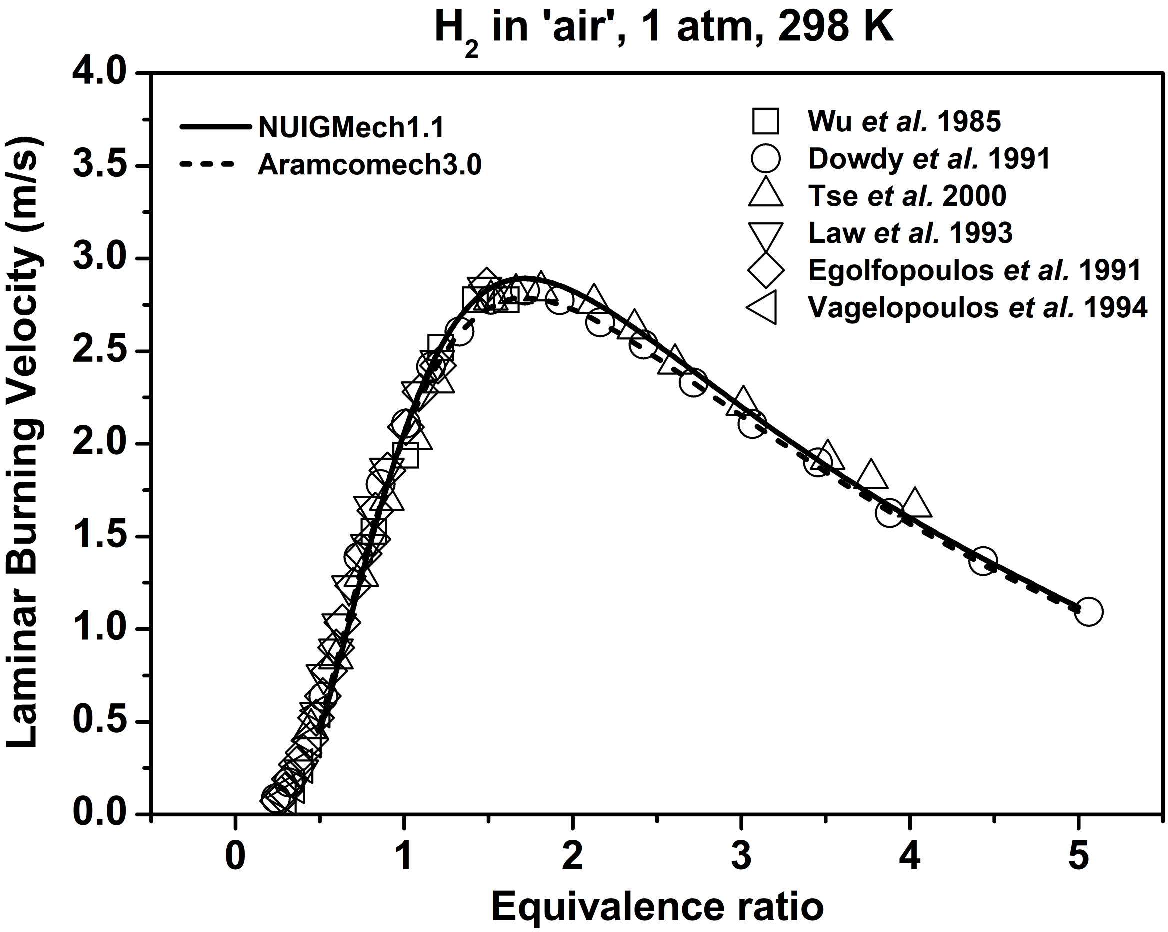


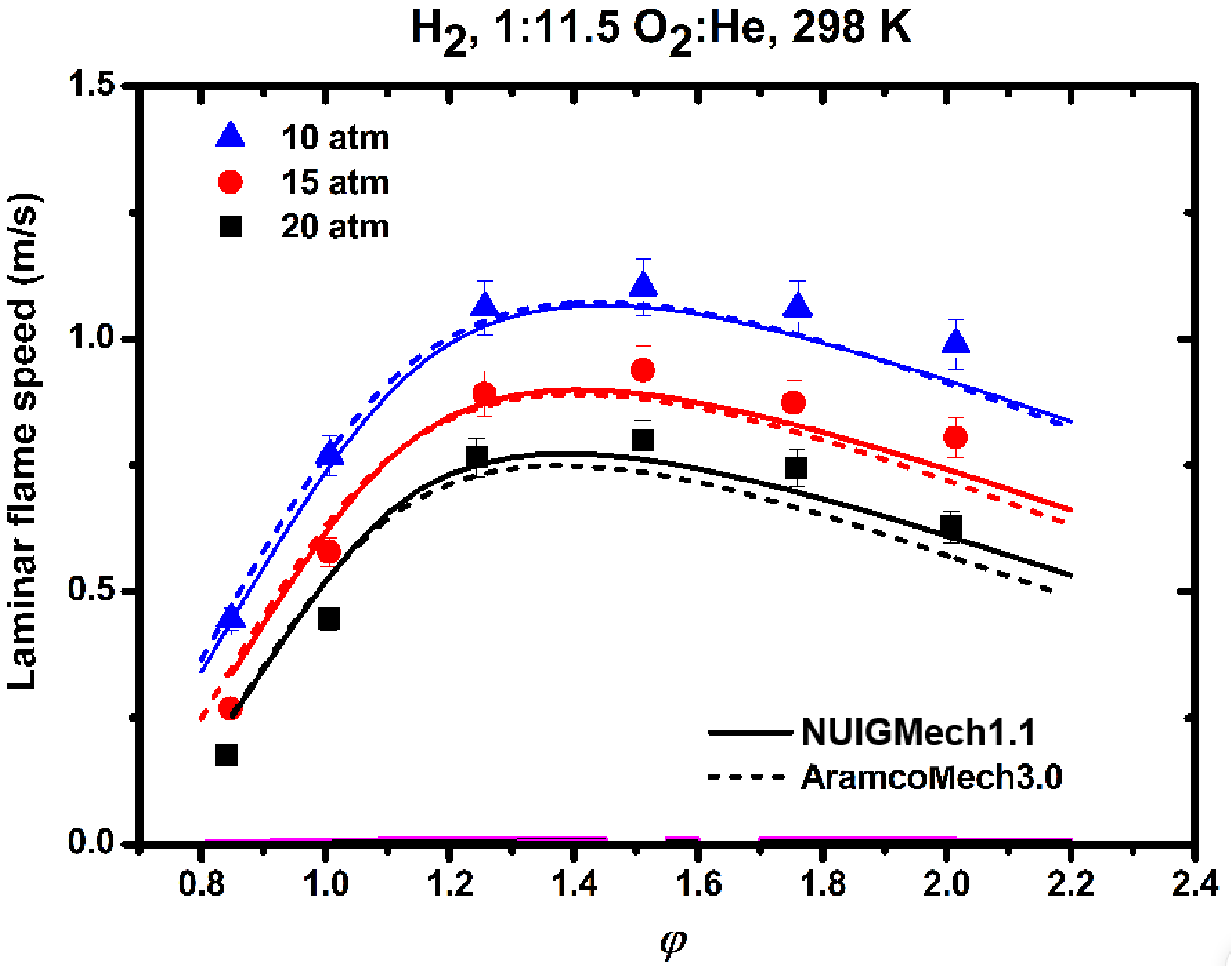

8.0 bar, 1.43% H2, 20.47% O2
H2 mole fraction (%)
Reactor distance (mm)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
0
200
400
600
800
1000


1.0 bar, 1.43% H2, 20.47% O2
H2 mole fraction (%)
Reactor distance (mm)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
0
50
100
150
200

Laminar flame speed

1.11) Tse, S. D., Zhu, D. L., & Law, C. K., Proceedings of the combustion institute, 28 (2) (2000) 1793-1800.
1.12) Wu, C., & Law, C. K., Symposium (International) on Combustion, 20 (1985, January) 1941-1949
1.13) Dowdy, D. R., Smith, D. B., Taylor, S. C., & Williams, A., In Symposium (International) on Combustion, 23 (1991, January) 325-332
1.14)Egolfopoulos, F. N., & Law, C. K., In Symposium (international) on combustion, 23, (1991, January) 333-340
1.15)Vagelopoulos, C. M., Egolfopoulos, F. N., & Law, C. K., In Symposium (international) on combustion, 25 (1994, January) 1341-1347



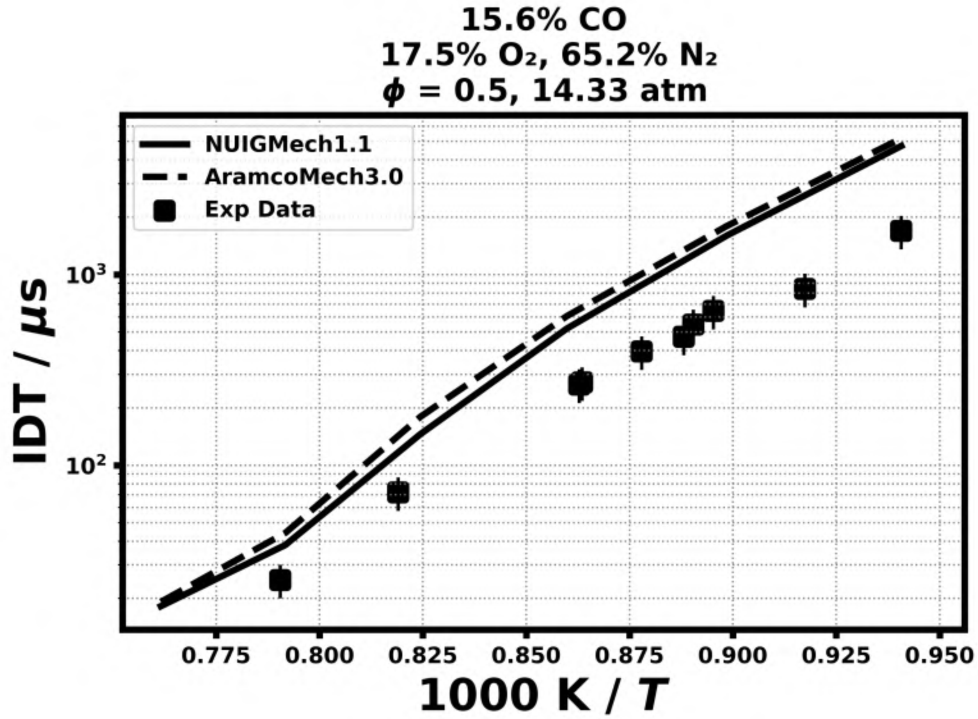


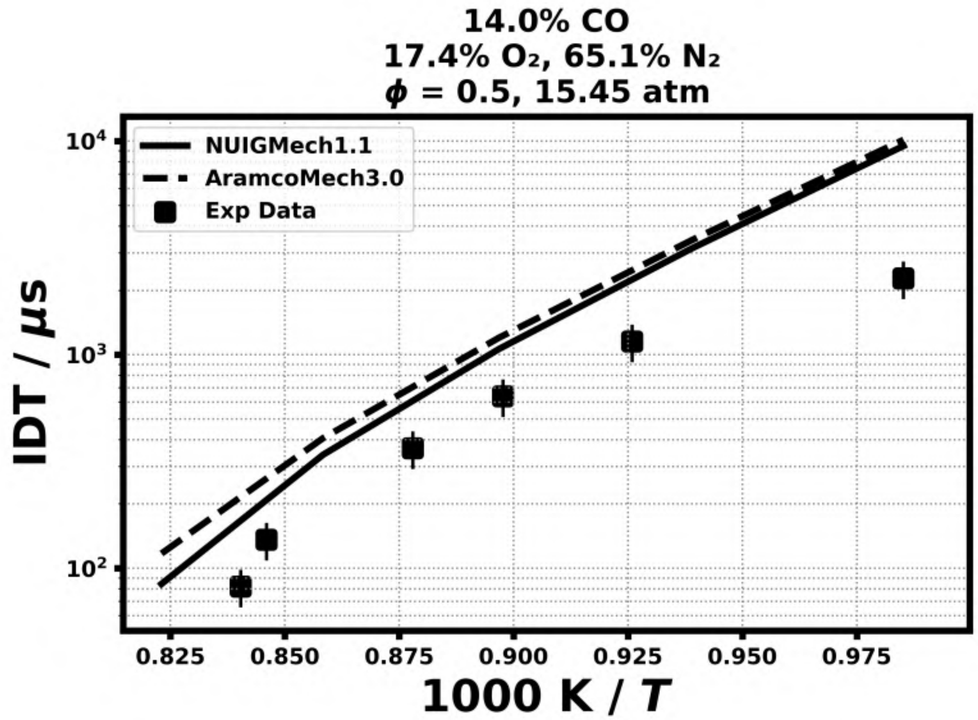
H2, 1:11.5 O2:He, 298 K
Laminar flame speed (m/s)
φ
10 atm
15 atm
20 atm
NUIGMech1.1
AramcoMech3.0
1.5
1.0
0.5
0.0
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4

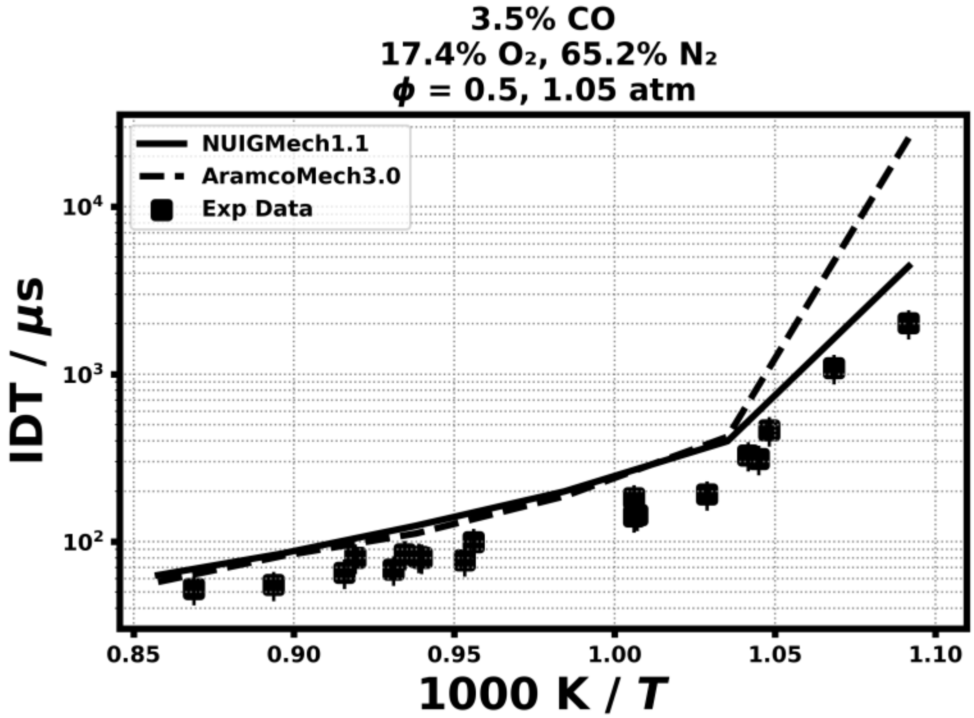
2. Validation for H_2/CO:

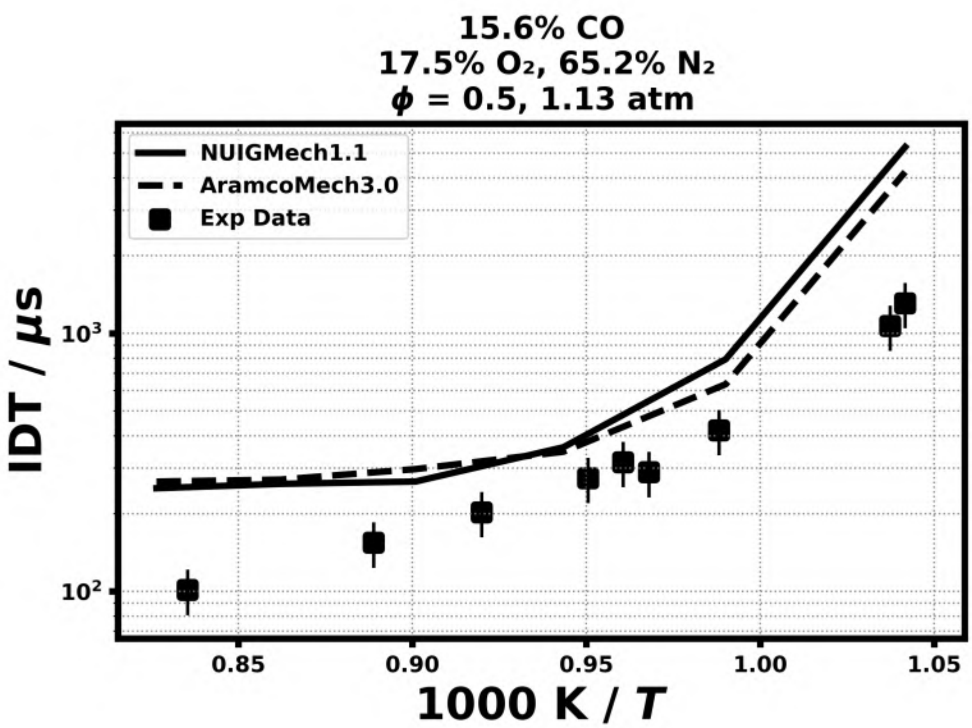
Shock tube ignition delay time

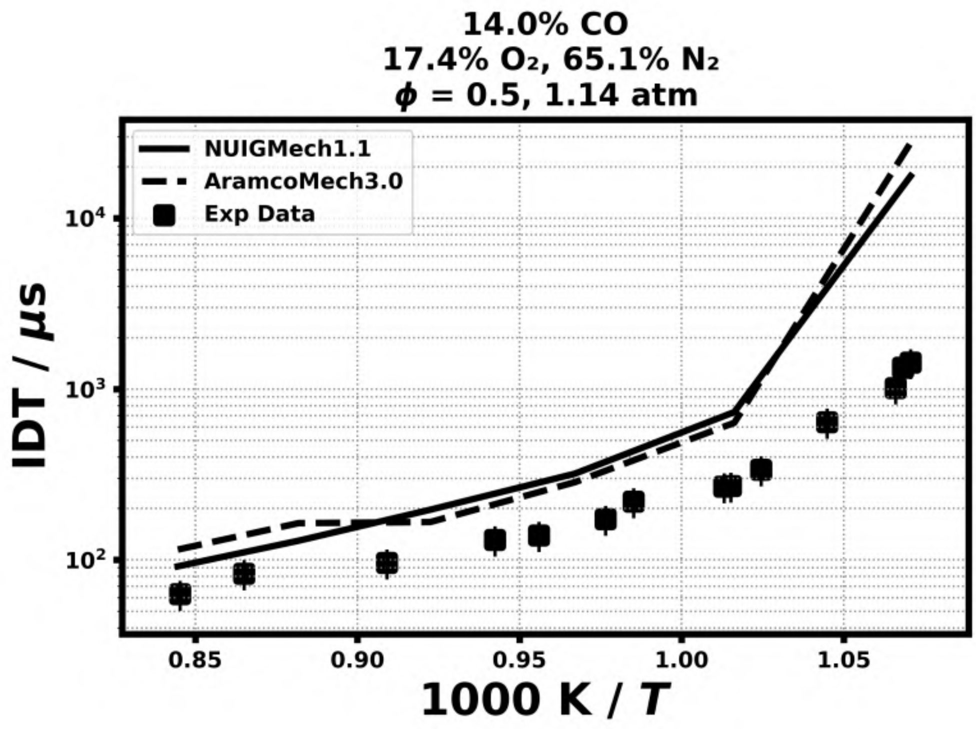
2.1) Kalitan, D. M., Mertens, J. D., Crofton, M. W., & Petersen, E. L., Journal of propulsion and power, 23(6) (2007) 1291-1301.





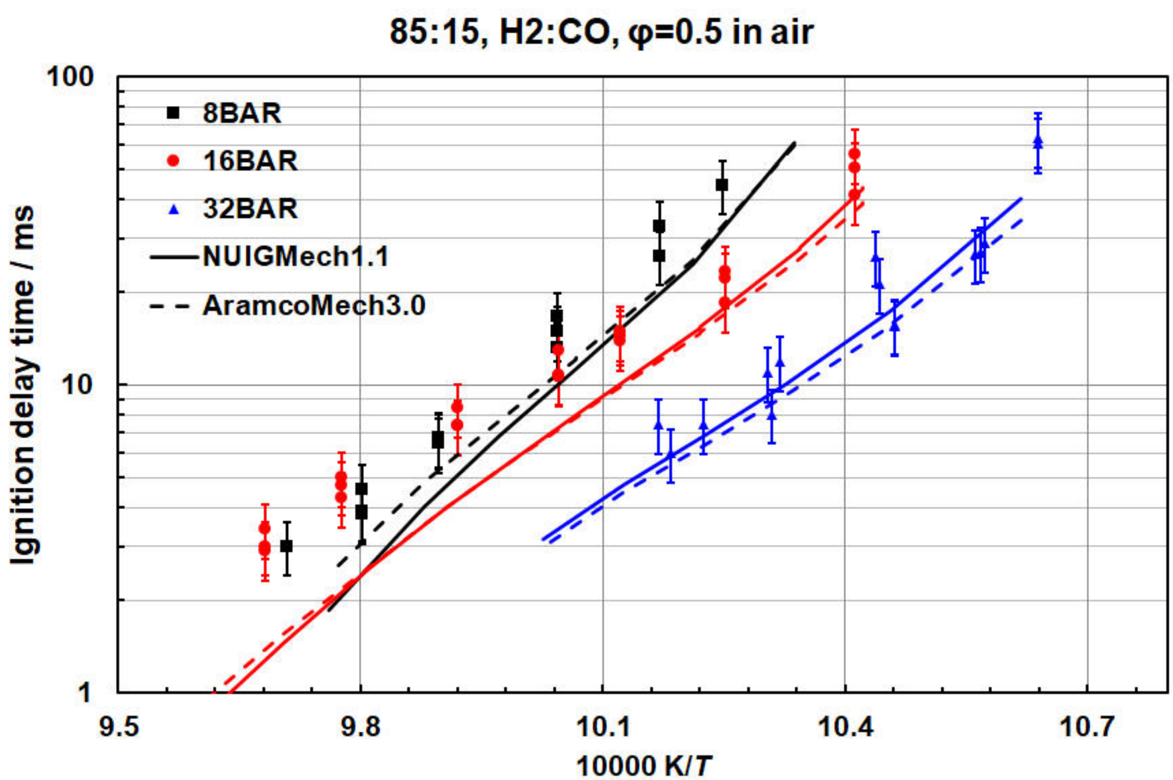

3.5% CO
17.4% O₂, 65.2% N₂
φ = 0.5, 1.05 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T

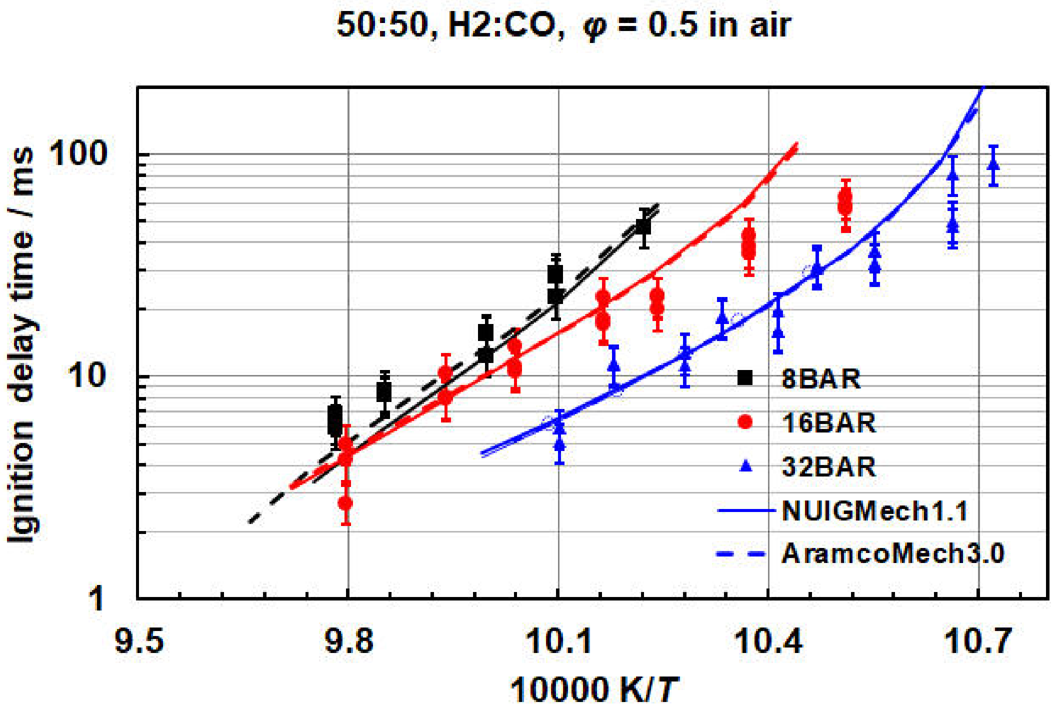

15.6% CO
17.5% O₂, 65.2% N₂
φ = 0.5, 1.13 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T



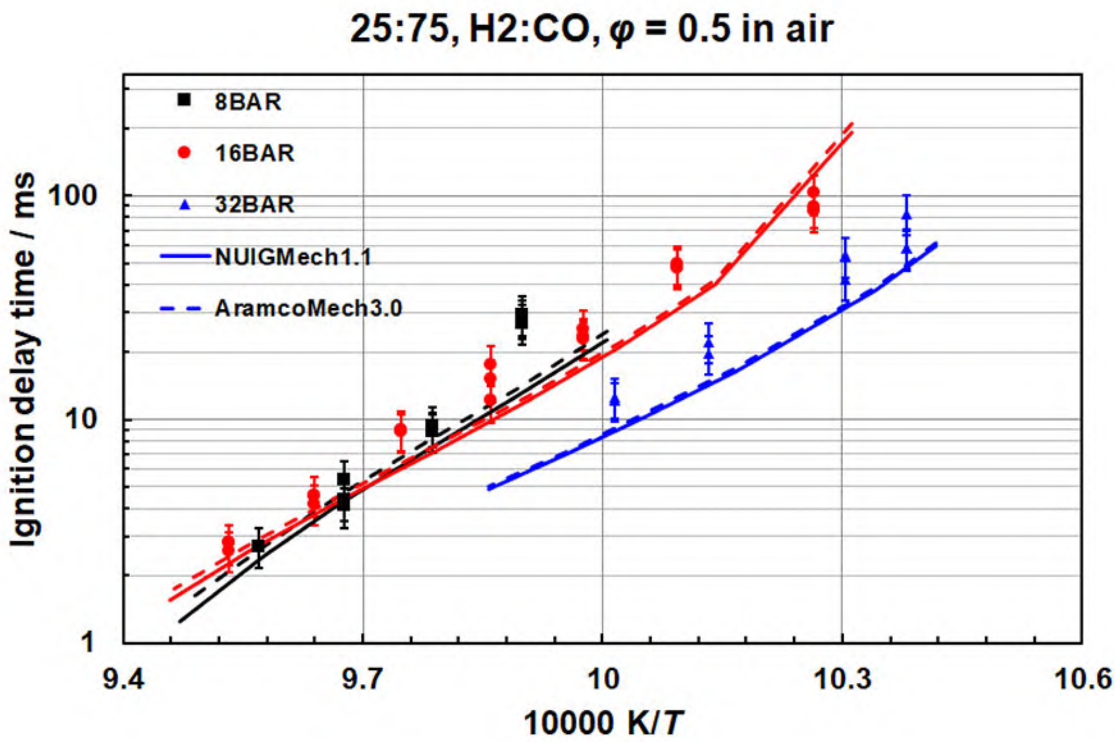
RCM Ignition delay time

2.1) Kéromnès, A., Metcalfe, W. K., Heufer, K. A., Donohoe, N., Das, A. K., Sung, C. J., & Krejci, M. C., Combustion and Flame, 160(6), (2013) 995-1011.





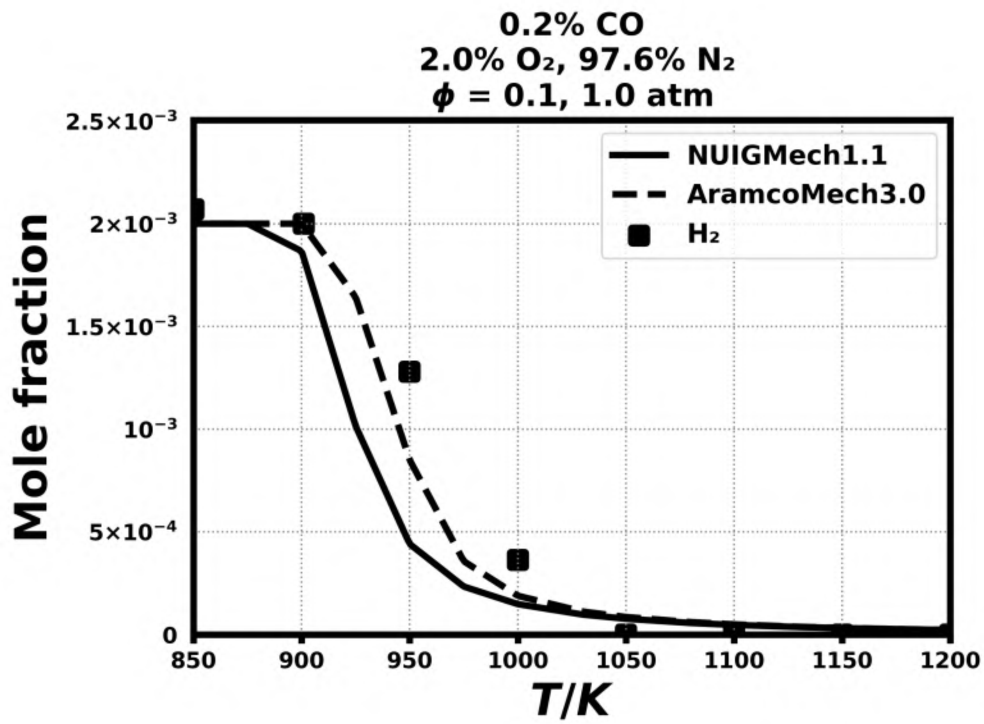
50:50, H2:CO, φ = 0.5 in air
Ignition delay time / ms
10000 K/T
8BAR
16BAR
32BAR
NUIGMech1.1
AramcoMech3.0
1
10
100
9.5
9.8
10.1
10.4
10.7

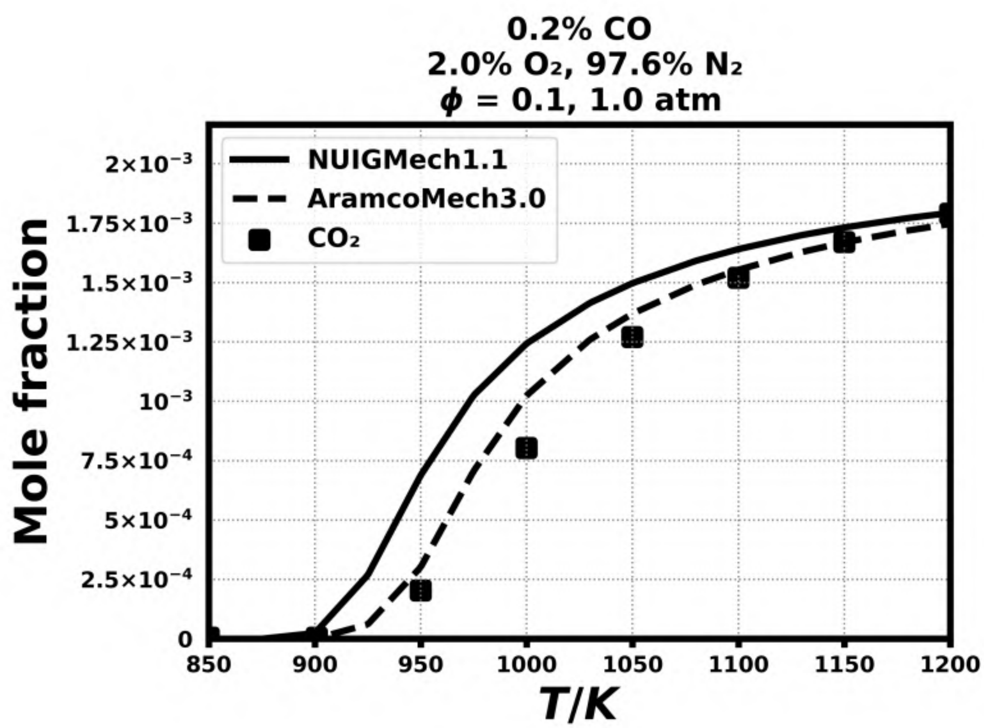


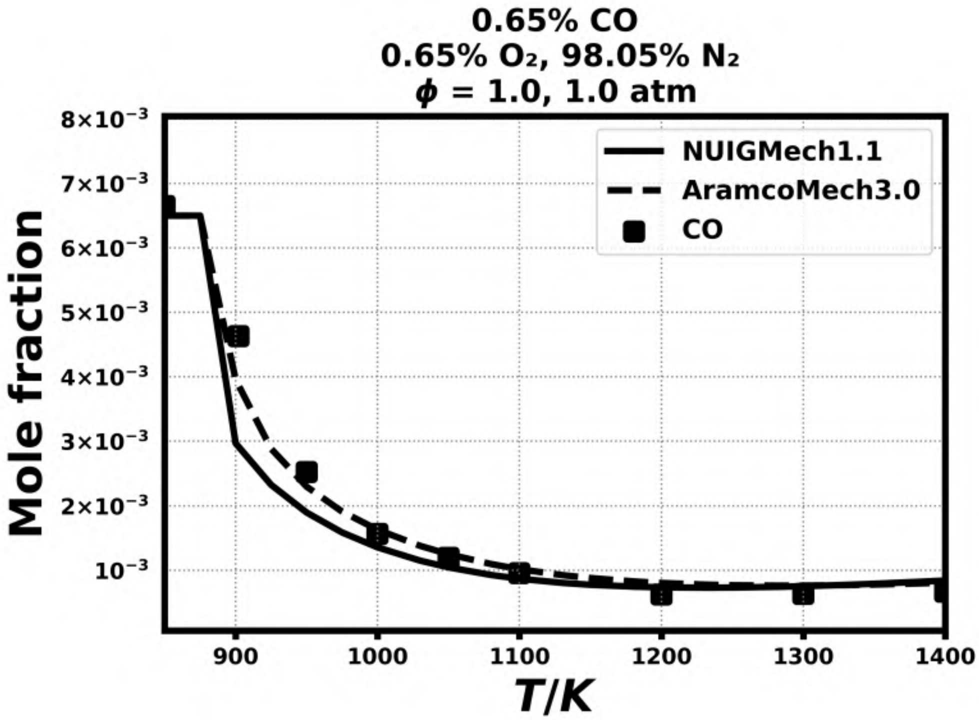
25:75, H2:CO, φ = 0.5 in air
Ignition delay time / ms
10000 K/T
8BAR
16BAR
32BAR
NUIGMech1.1
AramcoMech3.0
1
10
100
9.4
9.7
10
10.3
10.6

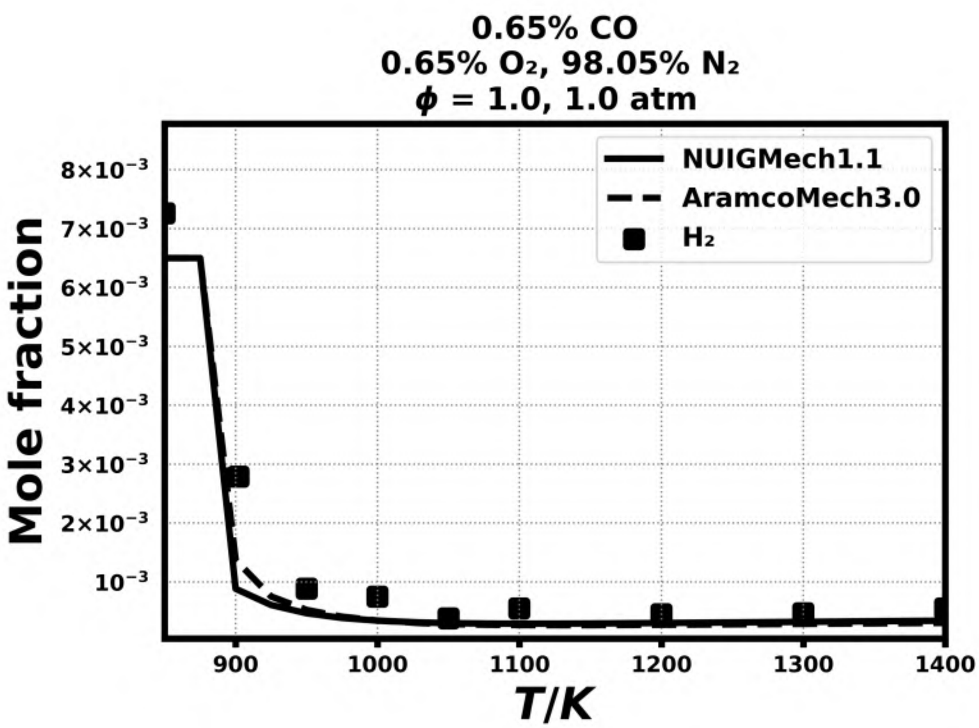
Speciation in Jet-stirred reactor

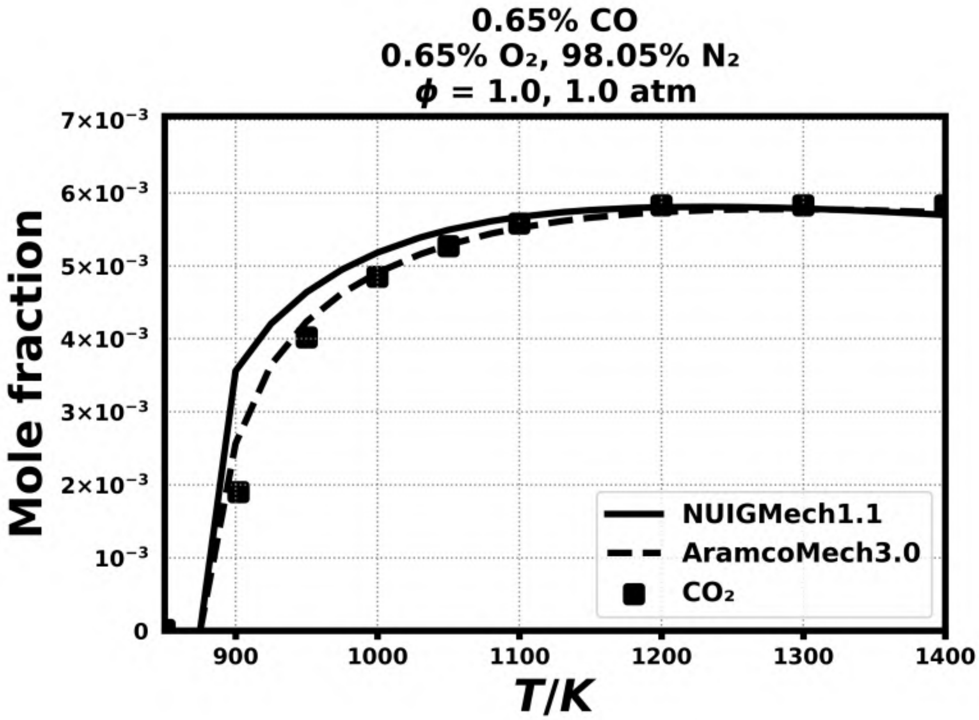
2.2) Le Cong, T., & Dagaut, P., Energy & Fuels, 23(2) (2009) 725-734.

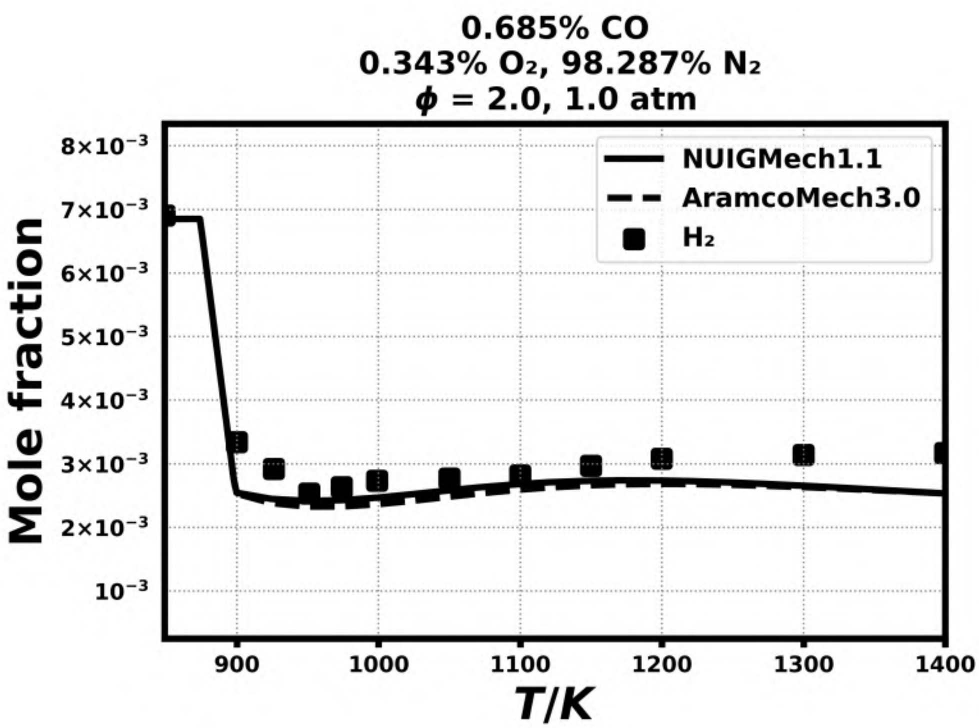


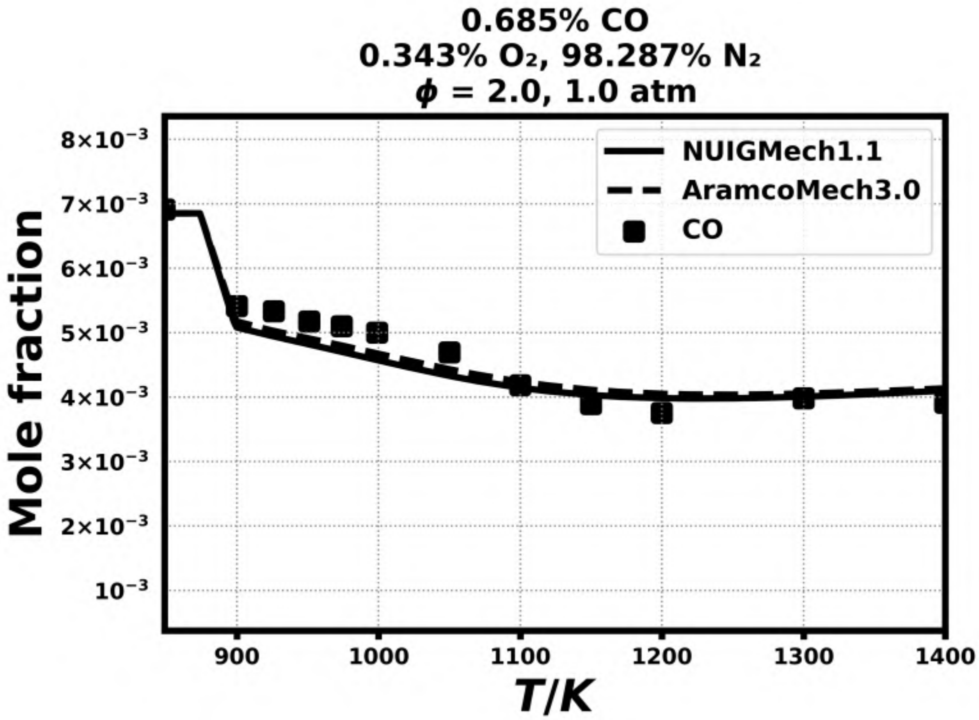



0.65% CO
0.65% O₂, 98.05% N₂
ϕ = 1.0, 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
8×10⁻³
7×10⁻³
6×10⁻³
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
900
1000
1100
1200
1300
1400
T/K

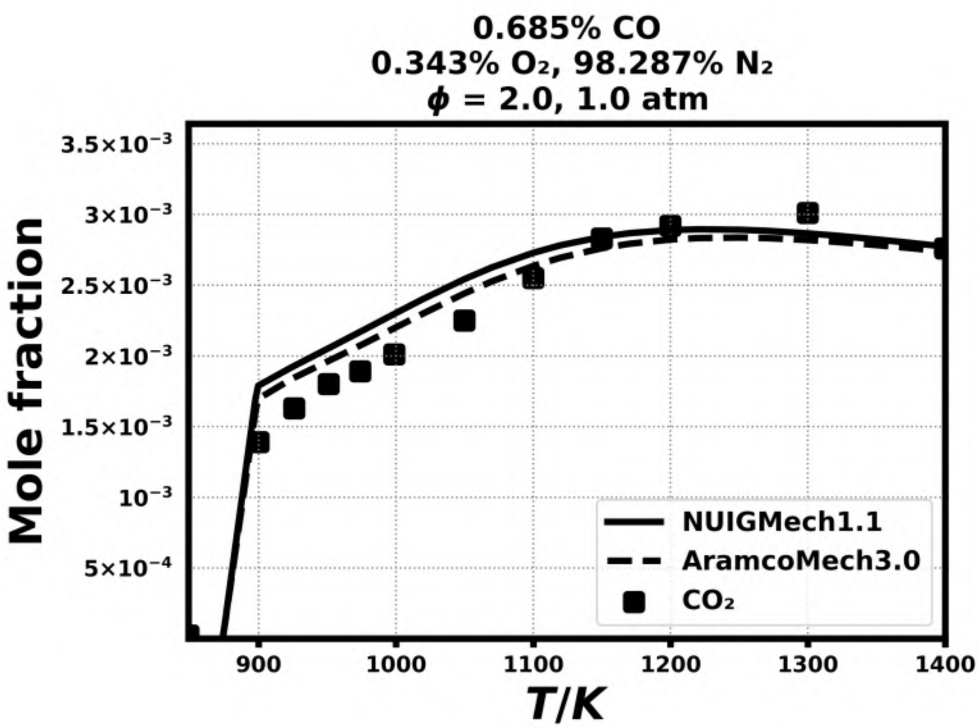

0.65% CO
0.65% O₂, 98.05% N₂
ϕ = 1.0, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
8×10⁻³
7×10⁻³
6×10⁻³
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
900
1000
1100
1200
1300
1400
T/K


0.65% CO
0.65% O₂, 98.05% N₂
ϕ = 1.0, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CO₂


0.685% CO
0.343% O₂, 98.287% N₂
ϕ = 2.0, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
H₂



0.685% CO
0.343% O₂, 98.287% N₂
ϕ = 2.0, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CO
8×10⁻³
7×10⁻³
6×10⁻³
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
900
1000
1100
1200
1300
1400

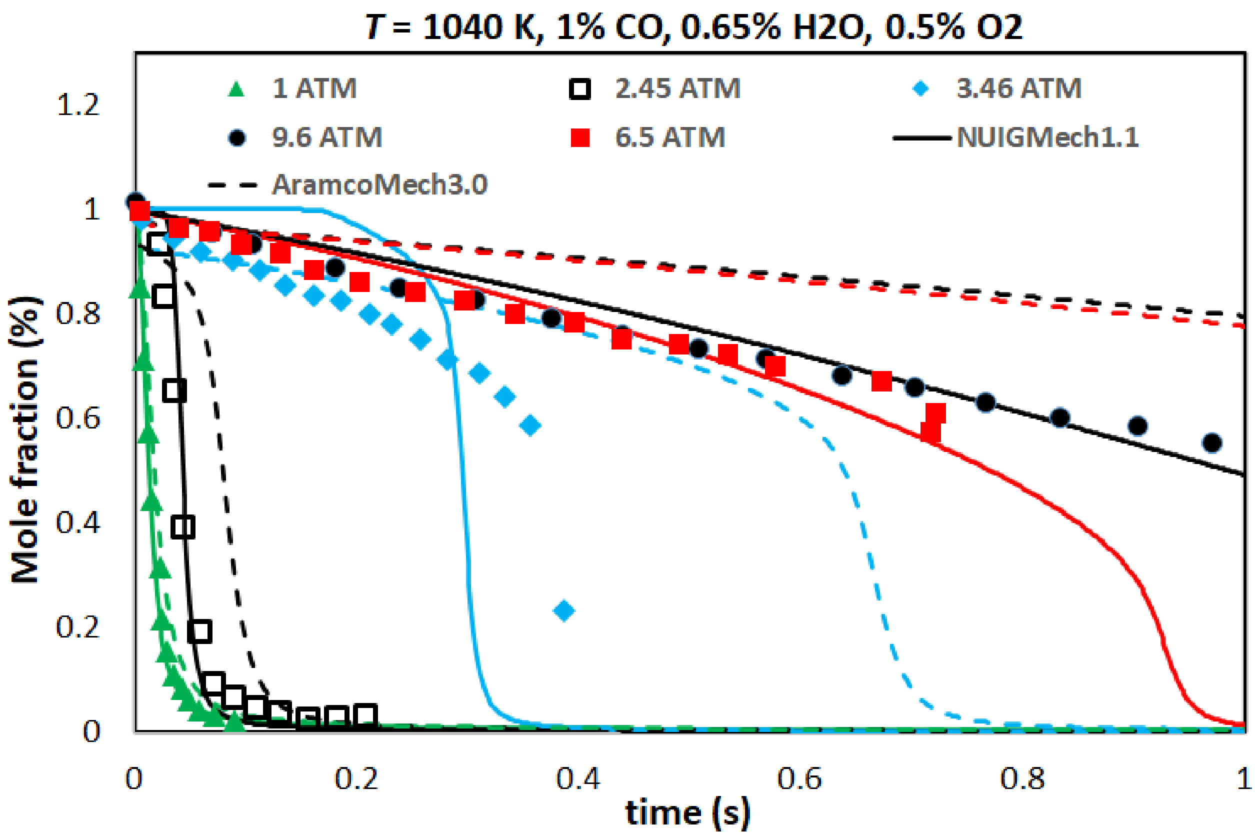


0.685% CO
0.343% O₂, 98.287% N₂
ϕ = 2.0, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CO₂
3.5×10⁻³
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
900
1000
1100
1200
1300
1400

Speciation in Flow reactor

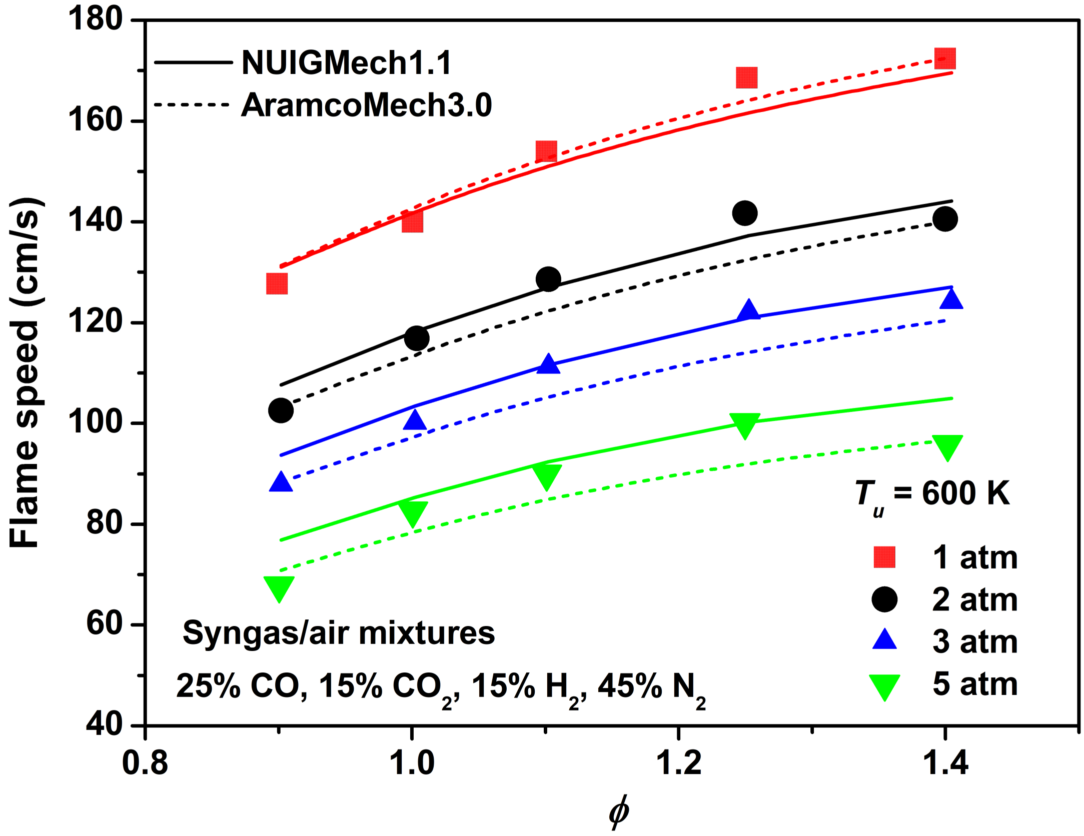
T.J. Kim, R.A. Yetter, F.L. Dryer, Twenty-FifthSymposium(International)on Combust. (1994) 759–766.

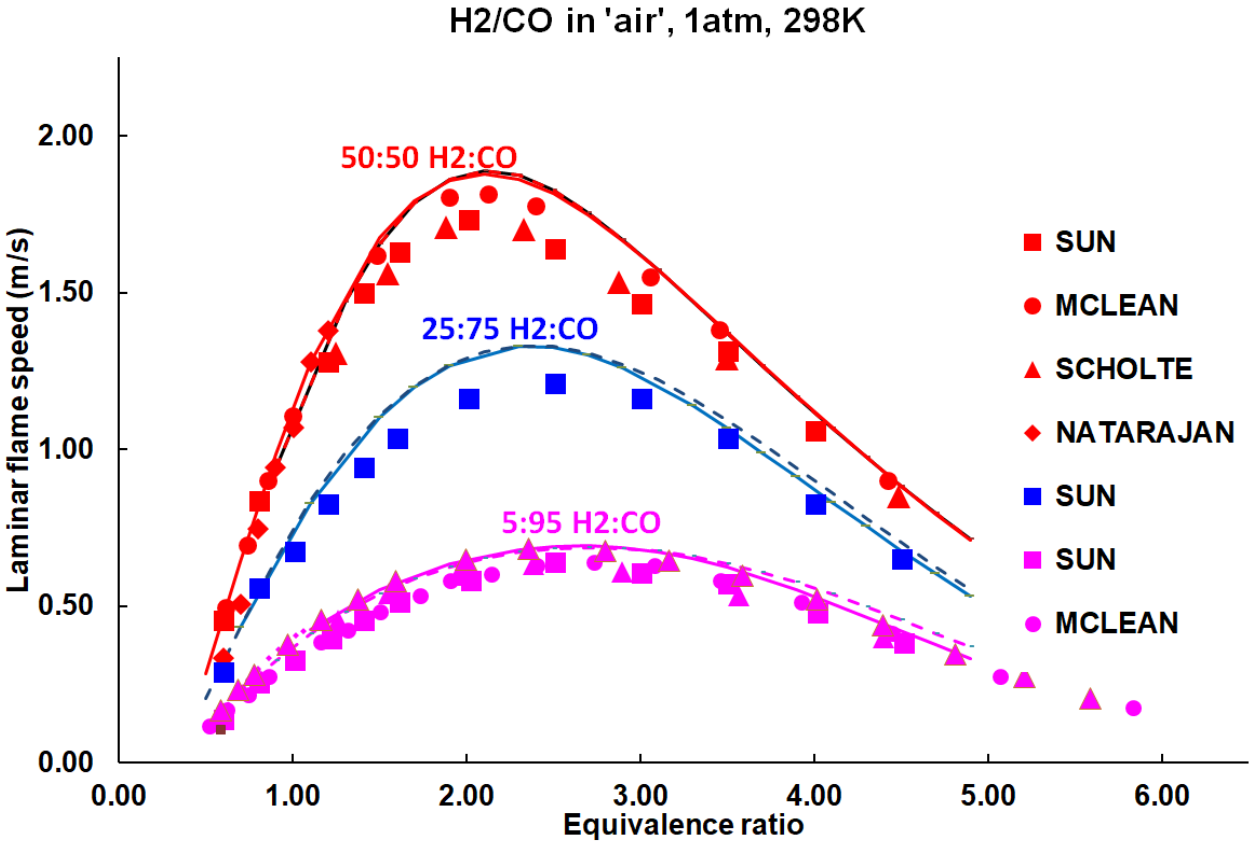
CO mole raction



Laminar flame speed

2.4) Varghese, Robin John, and Sudarshan Kumar., Fuel 279 (2020) 118475.
2.5) H. Sun, S.I. Yang, G. Jomaas, C.K. Law, Proc. Combust. Inst. 31 (2007) 439–446

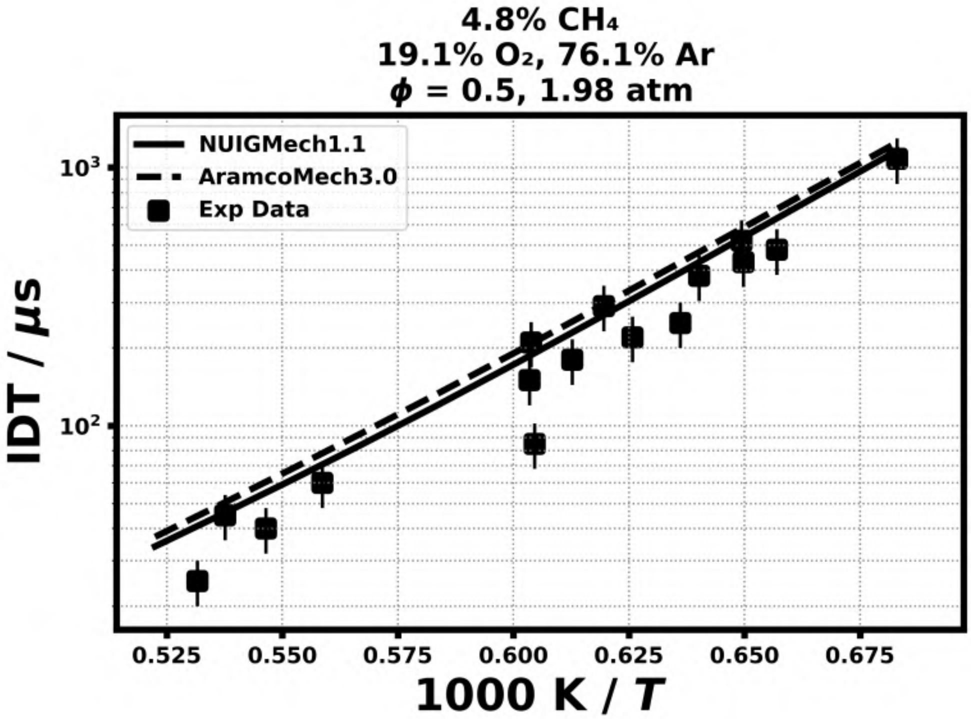


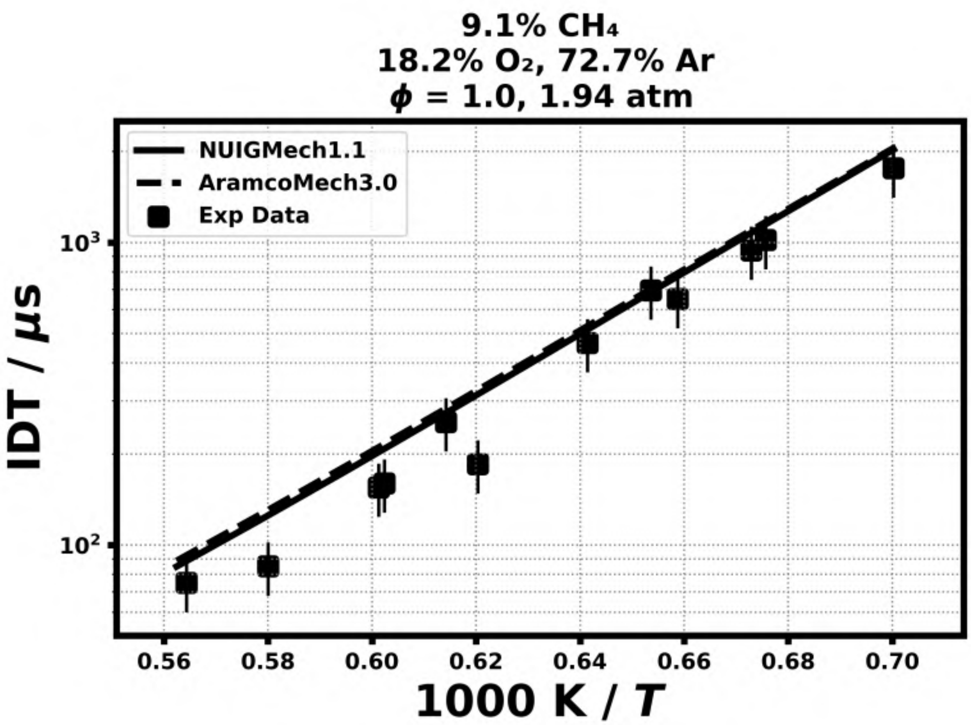


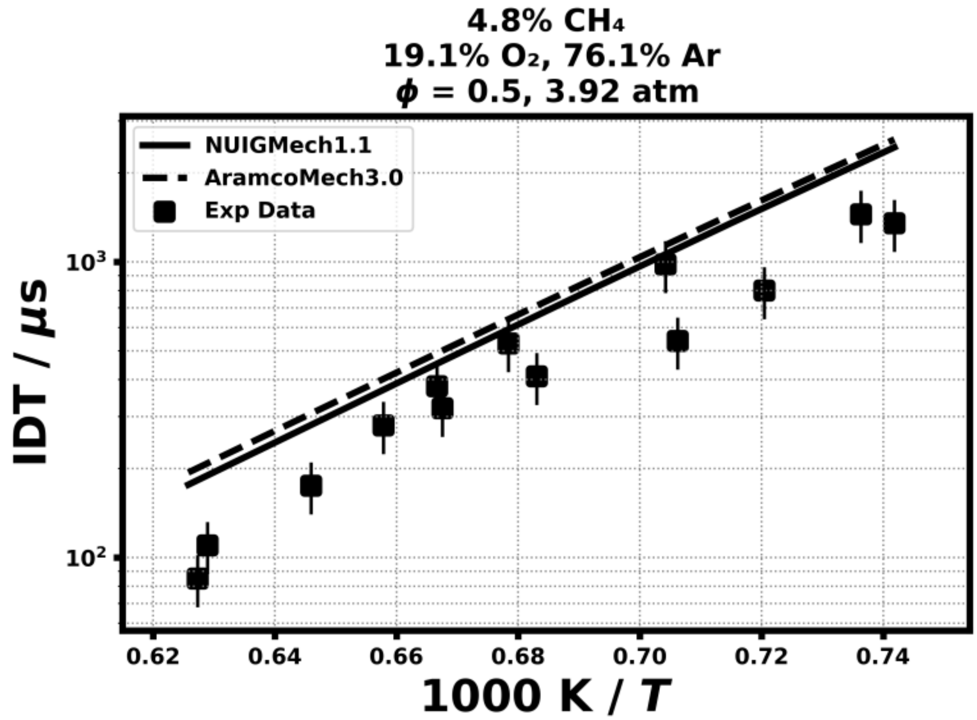
3. Validation for CH_4

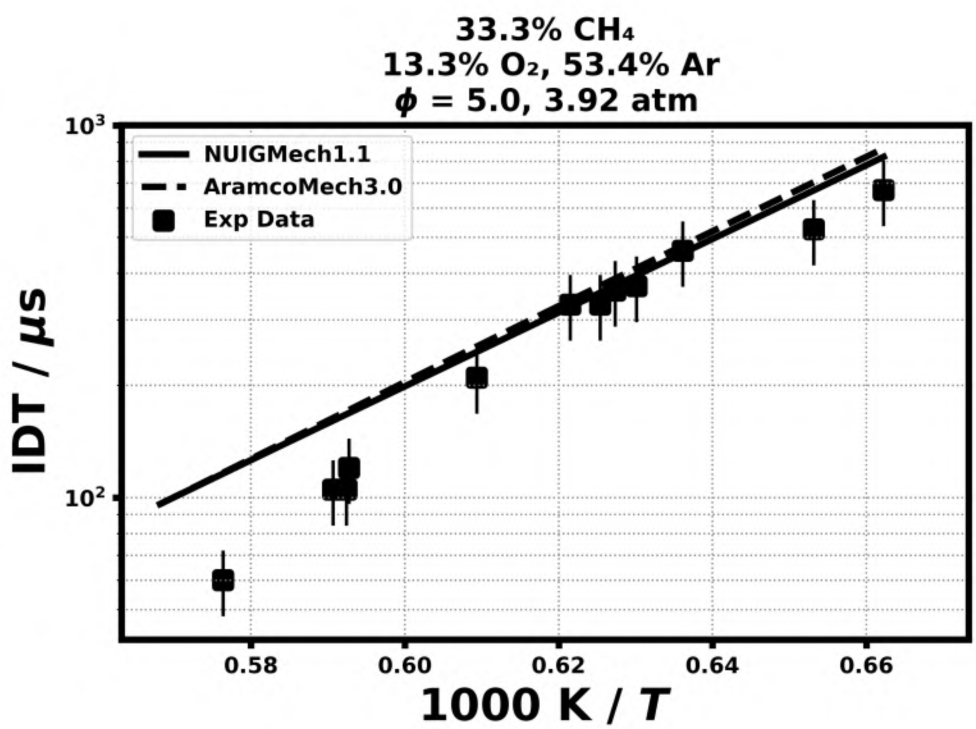
Shock tube ignition delay time

3.1) D.J. Seery. and C.T. Bowman., Combustion and Flame, 14 1 (1970) 37-47.

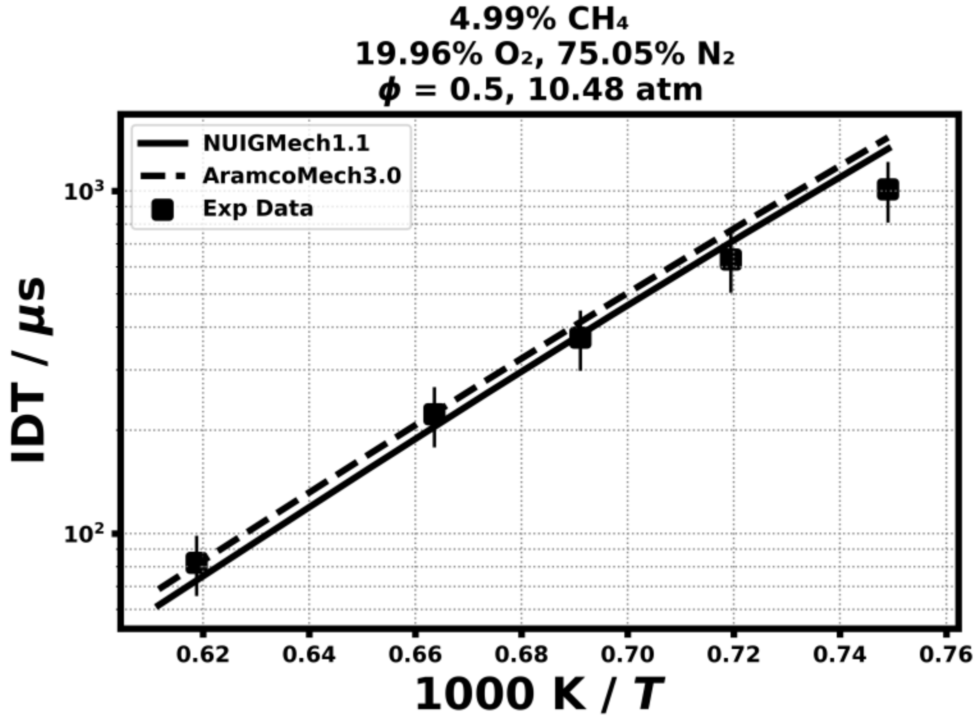


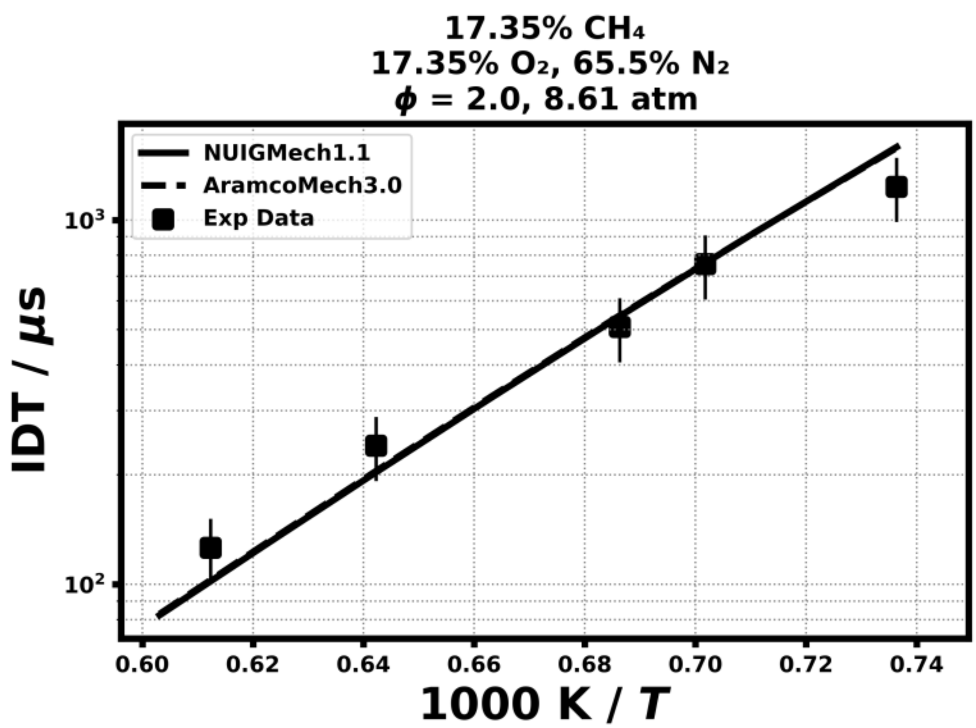


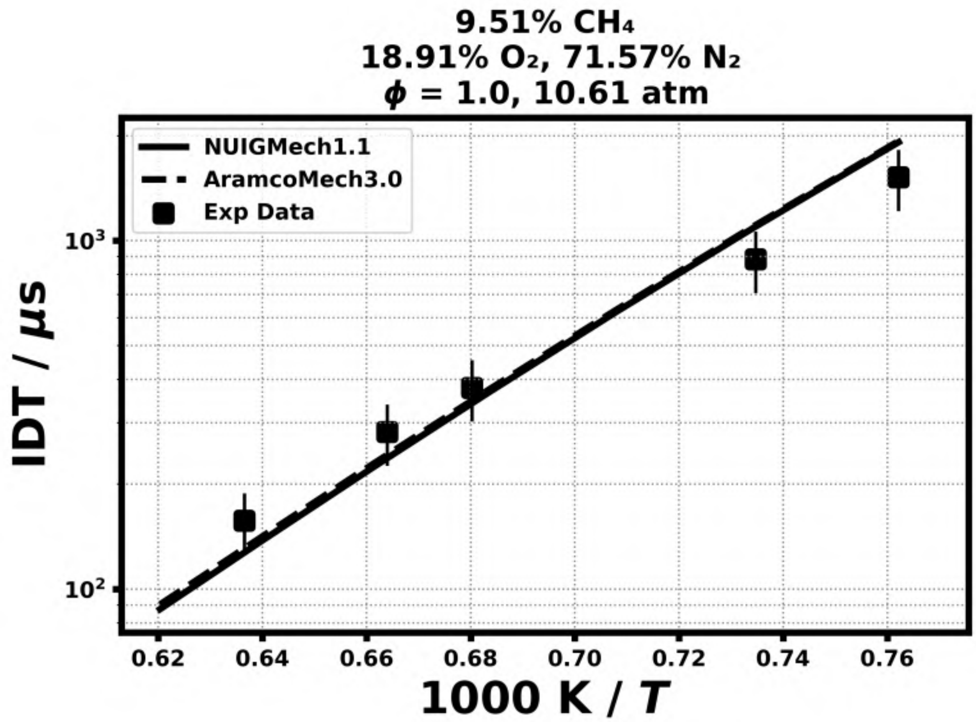

4.8% CH4
19.1% O2, 76.1% Ar
ϕ = 0.5, 3.92 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T

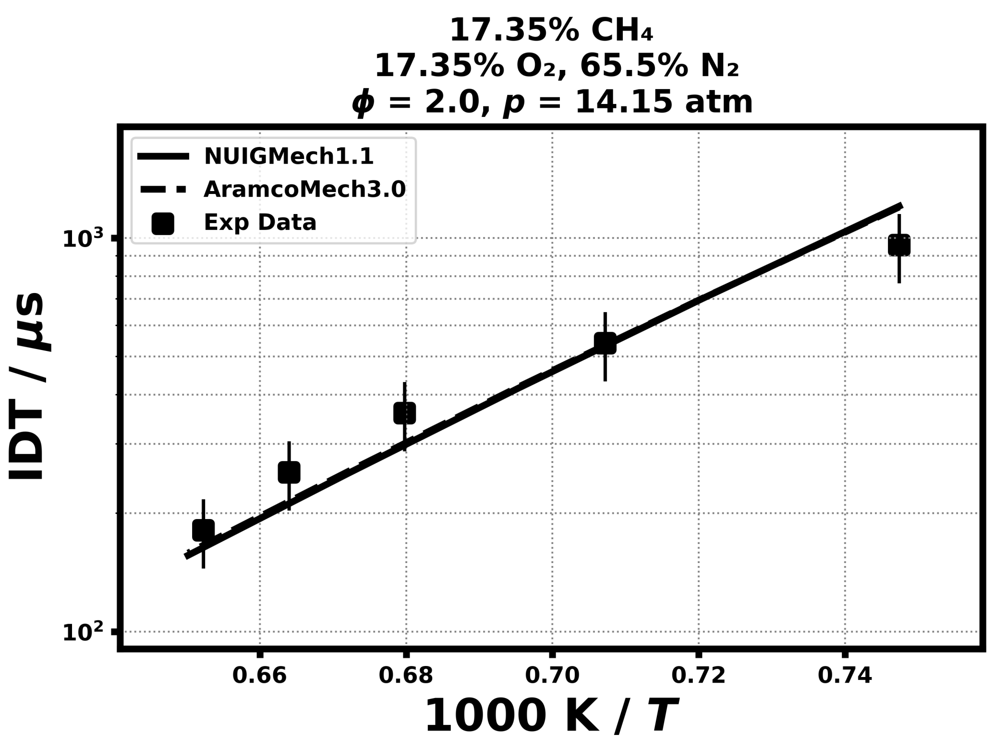

33.3% CH4
13.3% O2, 53.4% Ar
ϕ = 5.0, 3.92 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T

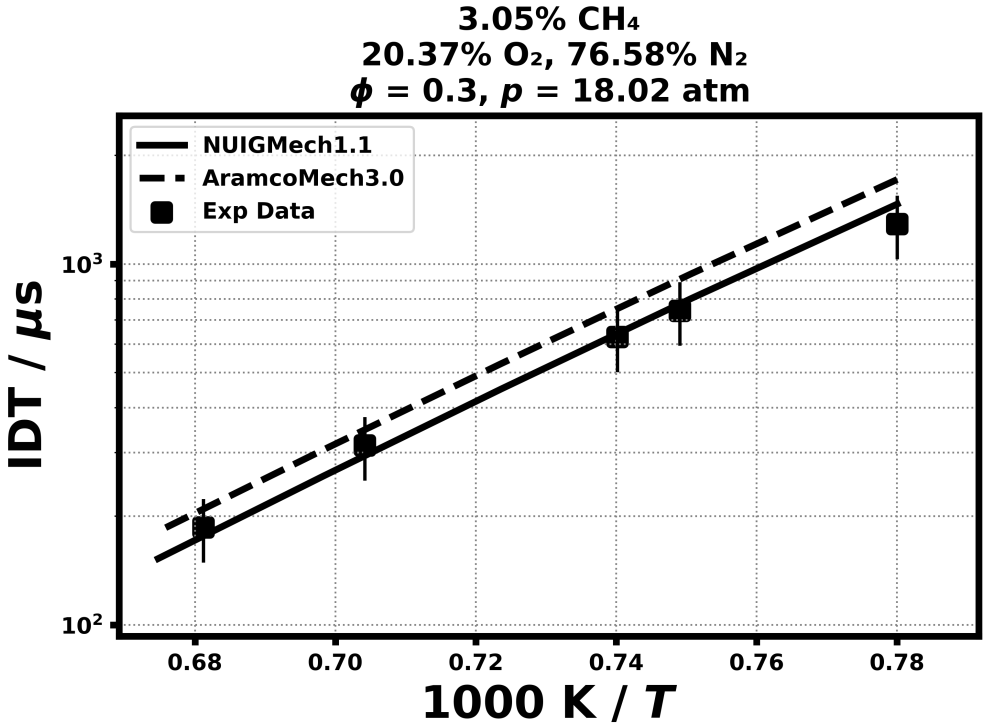
3.2) Burke, U., Somers, K. P., O'Toole, P., Zinner, C. M., Marquet, N., Bourque, G., ... & Curran, H. J., Combustion and flame, 162(2) (2015) 315-330.

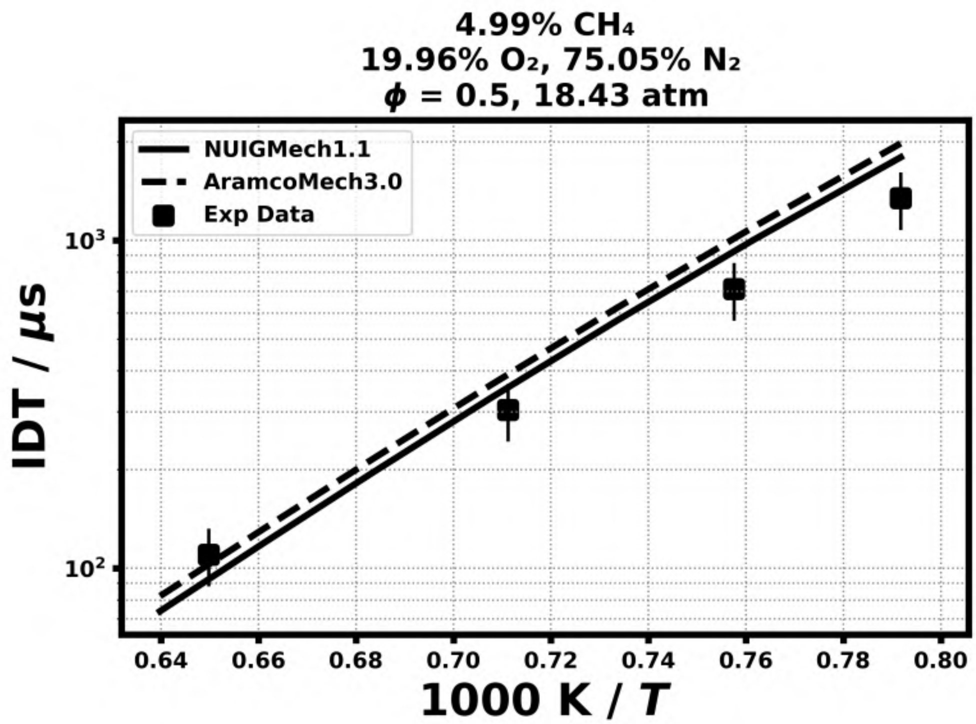


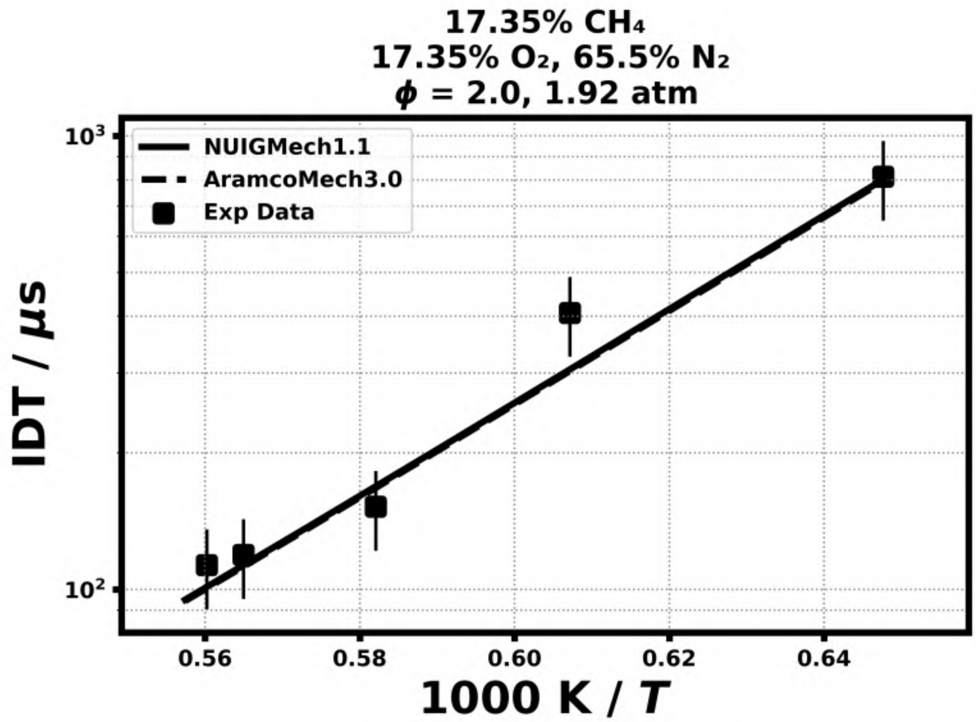


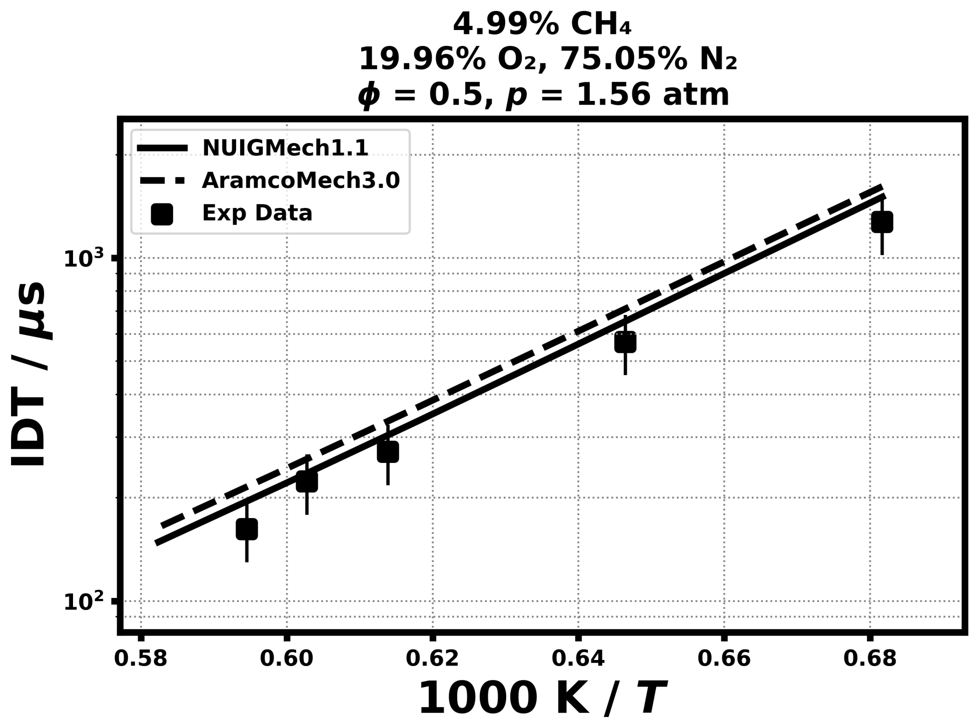

9.51% CH4
18.91% O2, 71.57% N2
ϕ = 1.0, 10.61 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.62
0.64
0.66
0.68
0.70
0.72
0.74
0.76
1000 K / T

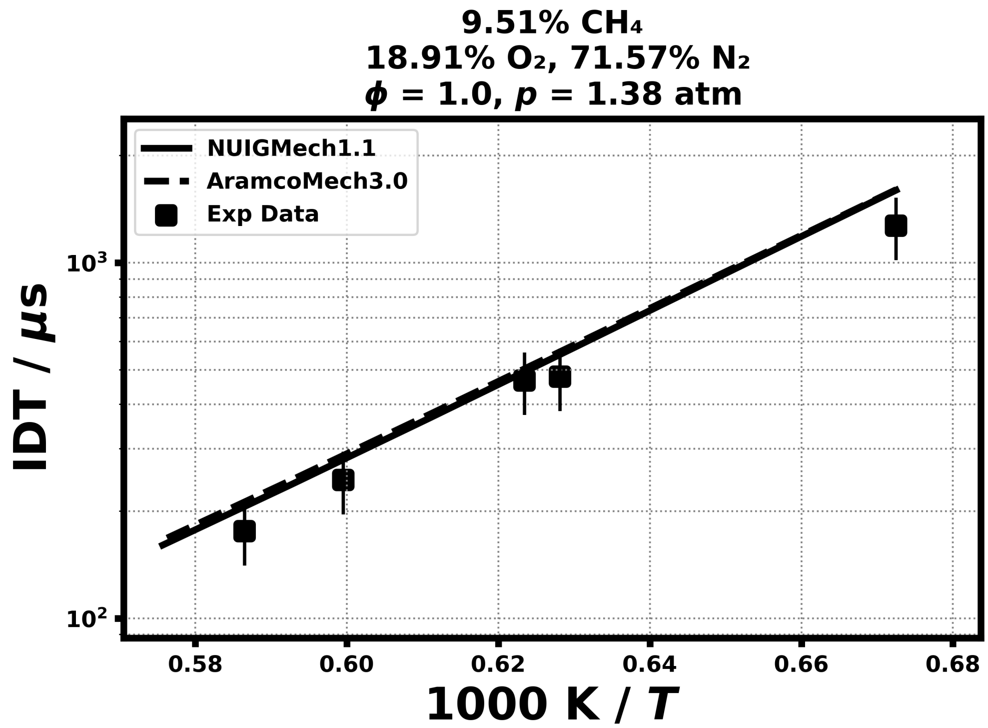

17.35% CH4
17.35% O2, 65.5% N2
ϕ = 2.0, p = 14.15 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.66
0.68
0.70
0.72
0.74
1000 K / T

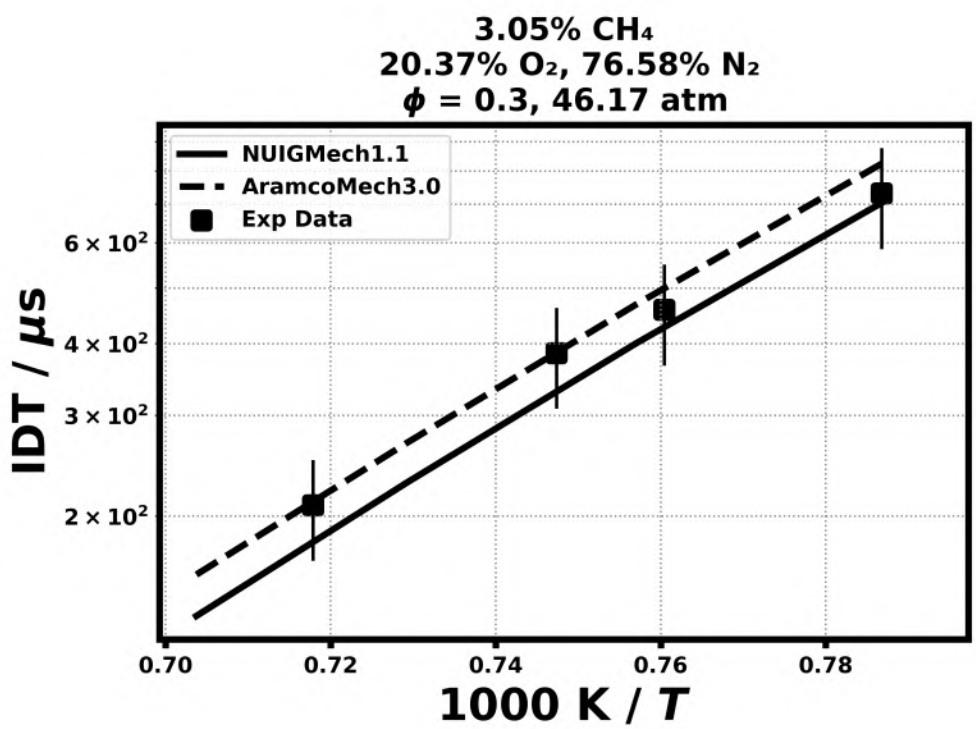

3.05% CH₄
20.37% O₂, 76.58% N₂
ϕ = 0.3, p = 18.02 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.68
0.70
0.72
0.74
0.76
0.78
1000 K / T

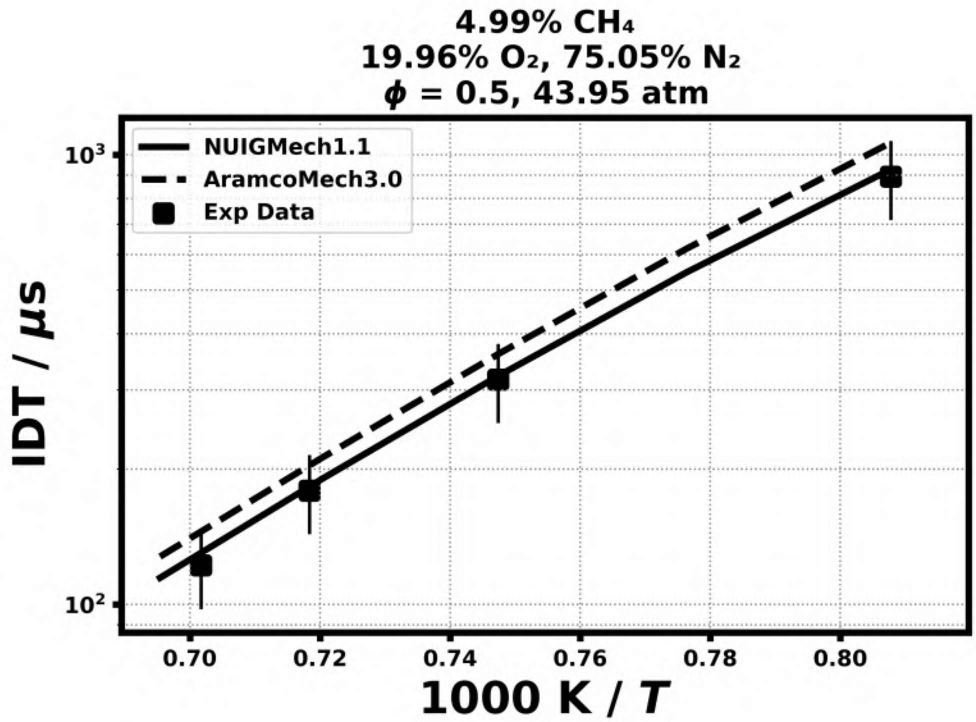

4.99% CH₄
19.96% O₂, 75.05% N₂
ϕ = 0.5, 18.43 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.64
0.66
0.68
0.70
0.72
0.74
0.76
0.78
0.80
1000 K / T

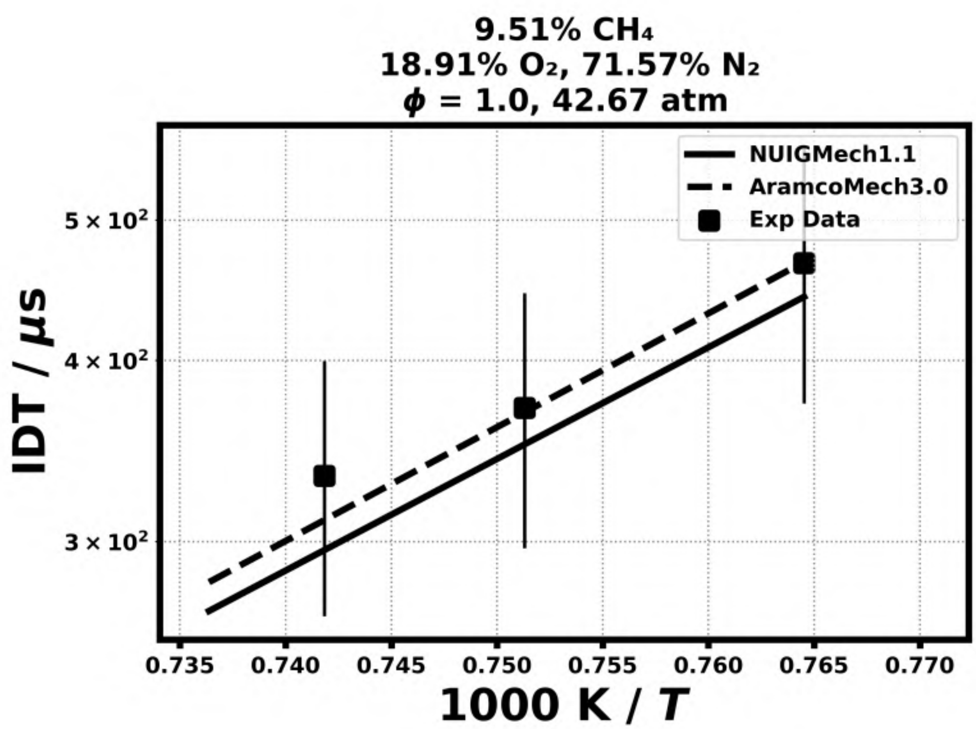

17.35% CH₄
17.35% O₂, 65.5% N₂
ϕ = 2.0, 1.92 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.56
0.58
0.60
0.62
0.64
1000 K / T

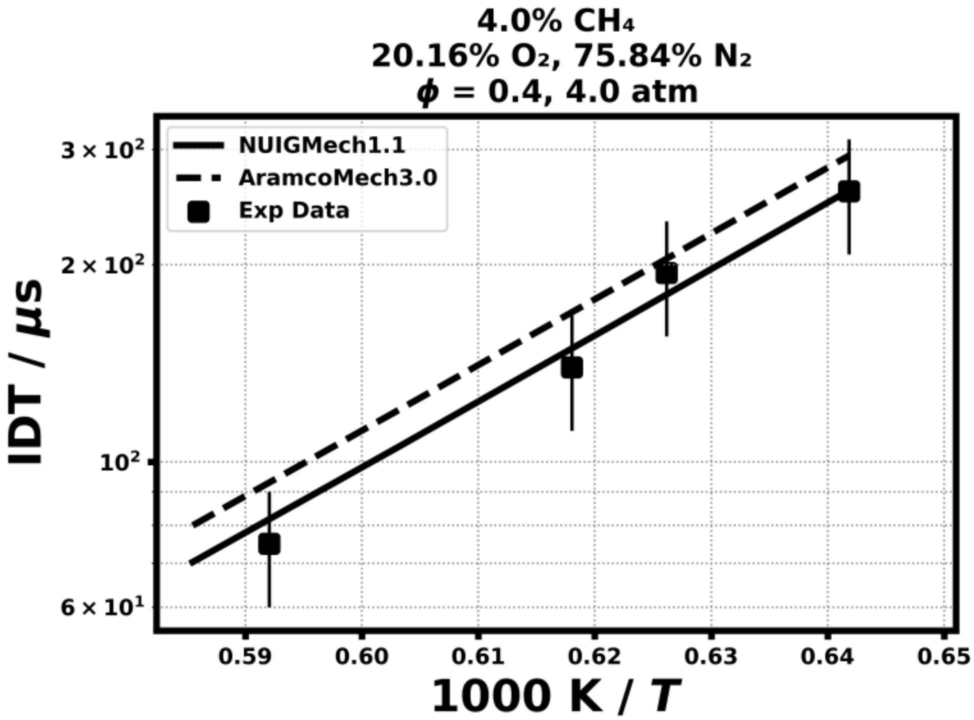

4.99% CH₄
19.96% O₂, 75.05% N₂
ϕ = 0.5, p = 1.56 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.58
0.60
0.62
0.64
0.66
0.68
1000 K / T


9.51% CH_4
18.91% O_2, 71.57% N_2
ϕ = 1.0, p = 1.38 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10^3
10^2
0.58
0.60
0.62
0.64
0.66
0.68
1000 K / T

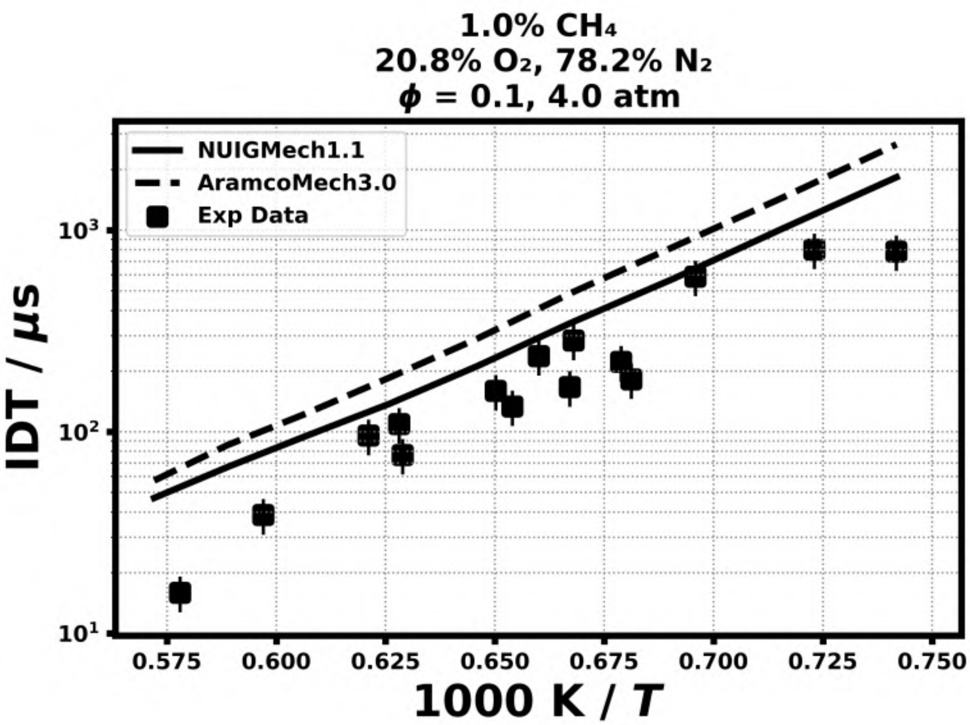

3.05% CH_4
20.37% O_2, 76.58% N_2
ϕ = 0.3, 46.17 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
6×10^2
4×10^2
3×10^2
2×10^2
0.70
0.72
0.74
0.76
0.78
1000 K / T

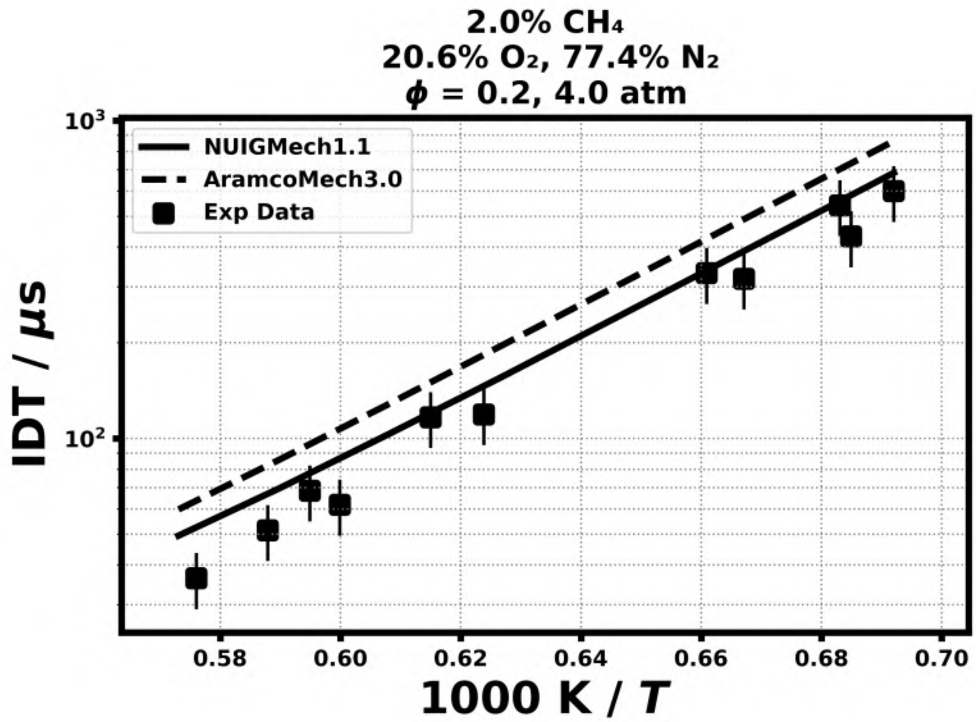

4.99% CH4
19.96% O2, 75.05% N2
ϕ = 0.5, 43.95 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.70
0.72
0.74
0.76
0.78
0.80
1000 K / T

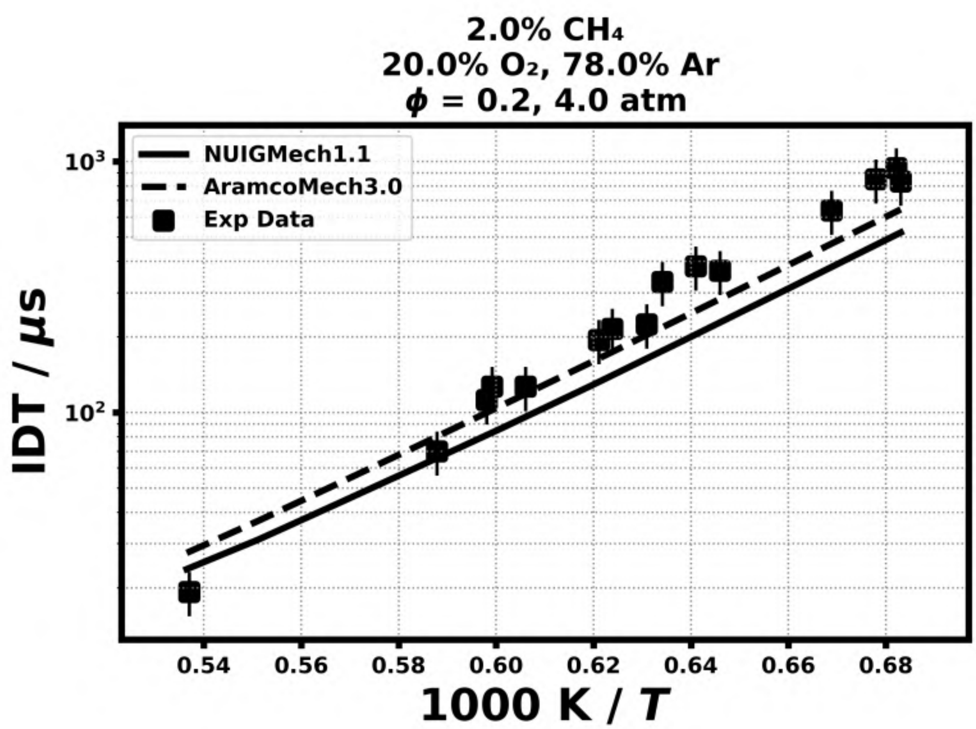

9.51% CH4
18.91% O2, 71.57% N2
ϕ = 1.0, 42.67 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
5 × 10²
4 × 10²
3 × 10²
0.735
0.740
0.745
0.750
0.755
0.760
0.765
0.770
1000 K / T



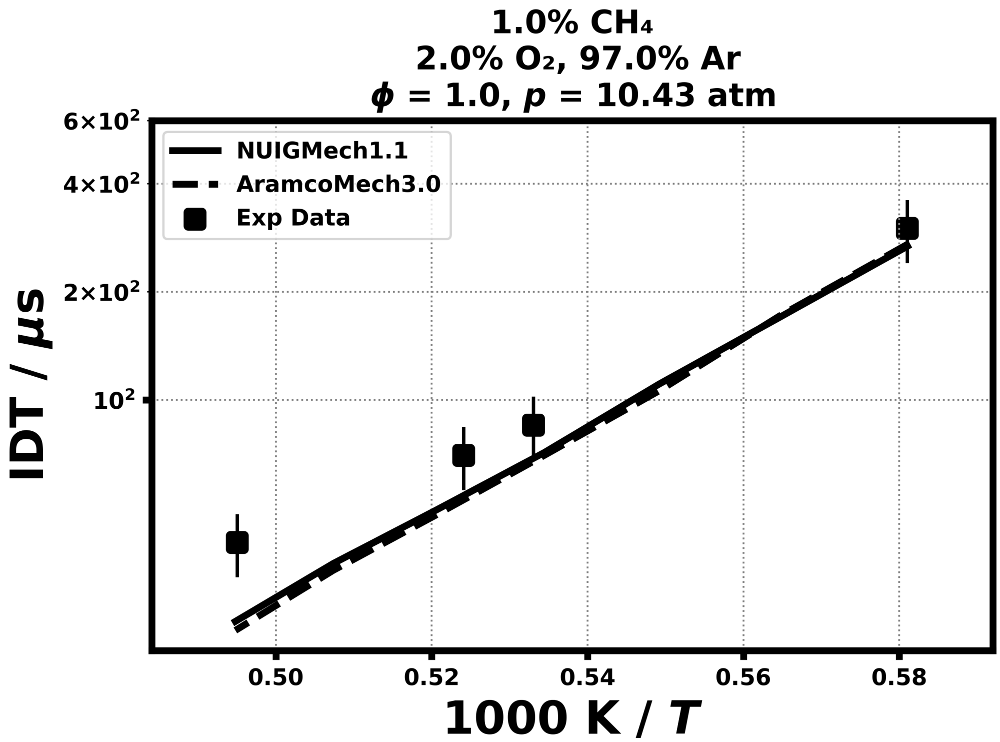
3.3) Eubank, C. S., M. J. Rabinowitz, W. C. Gardiner Jr, and R. E. Zellner, In Symposium (International) on Combustion, 18 (1981) 1767-1774.

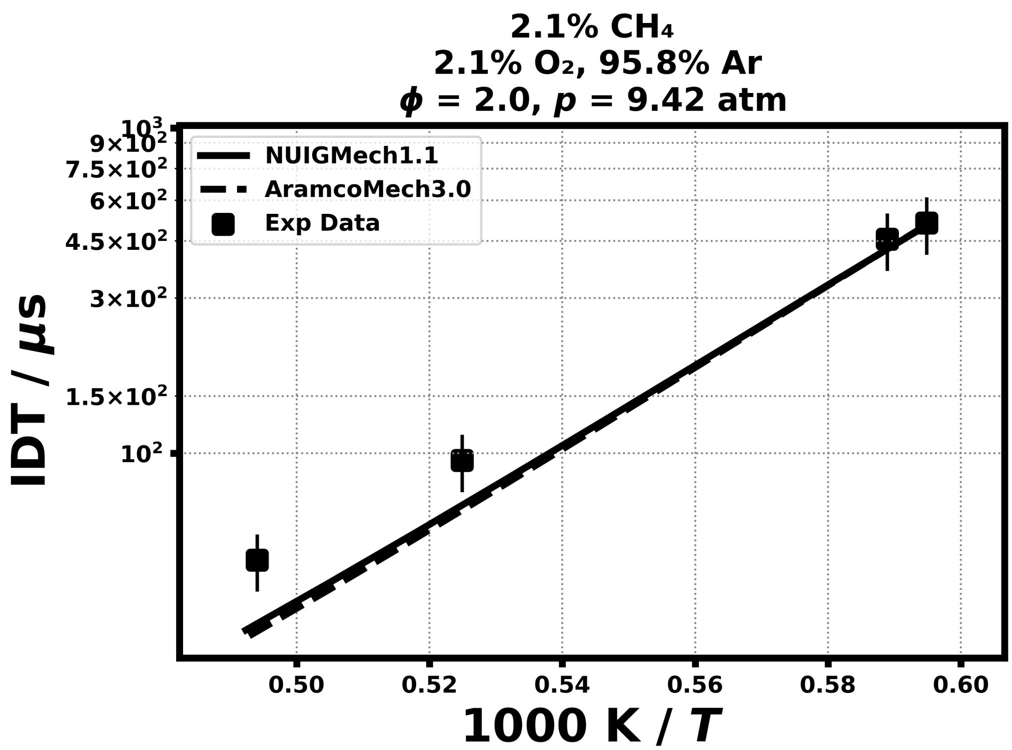


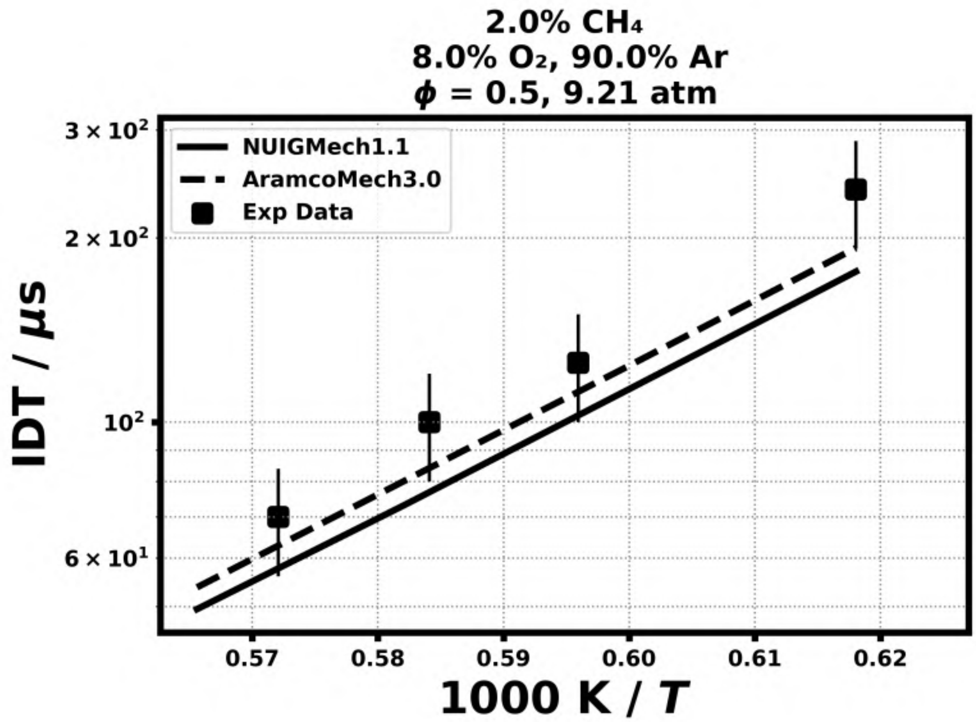

2.0% CH₄
20.6% O₂, 77.4% N₂
ϕ = 0.2, 4.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.58
0.60
0.62
0.64
0.66
0.68
0.70
1000 K / T

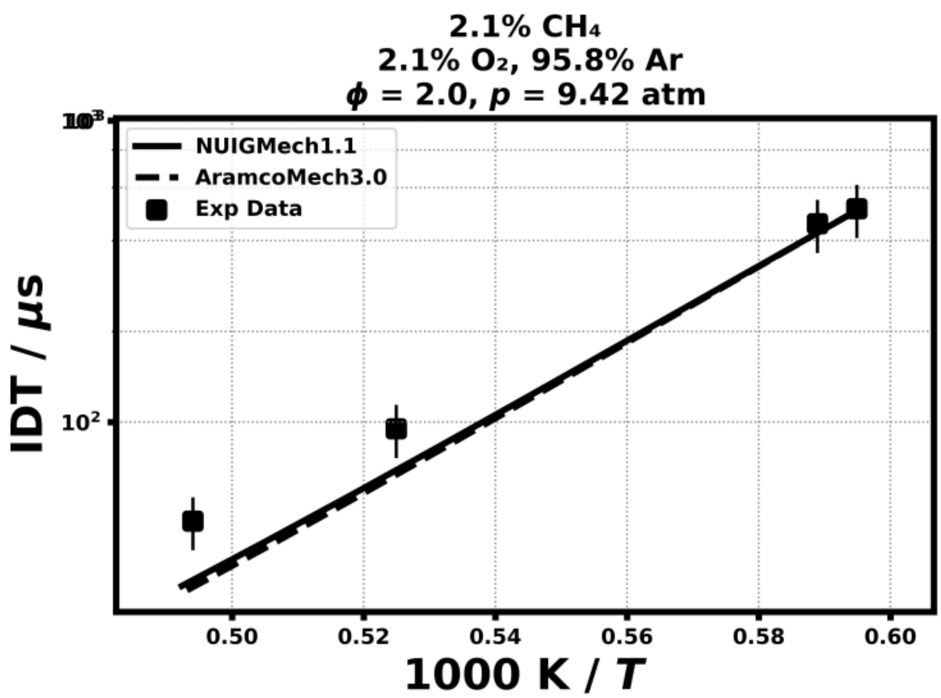

2.0% CH₄
20.0% O₂, 78.0% Ar
ϕ = 0.2, 4.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.54
0.56
0.58
0.60
0.62
0.64
0.66
0.68
1000 K / T

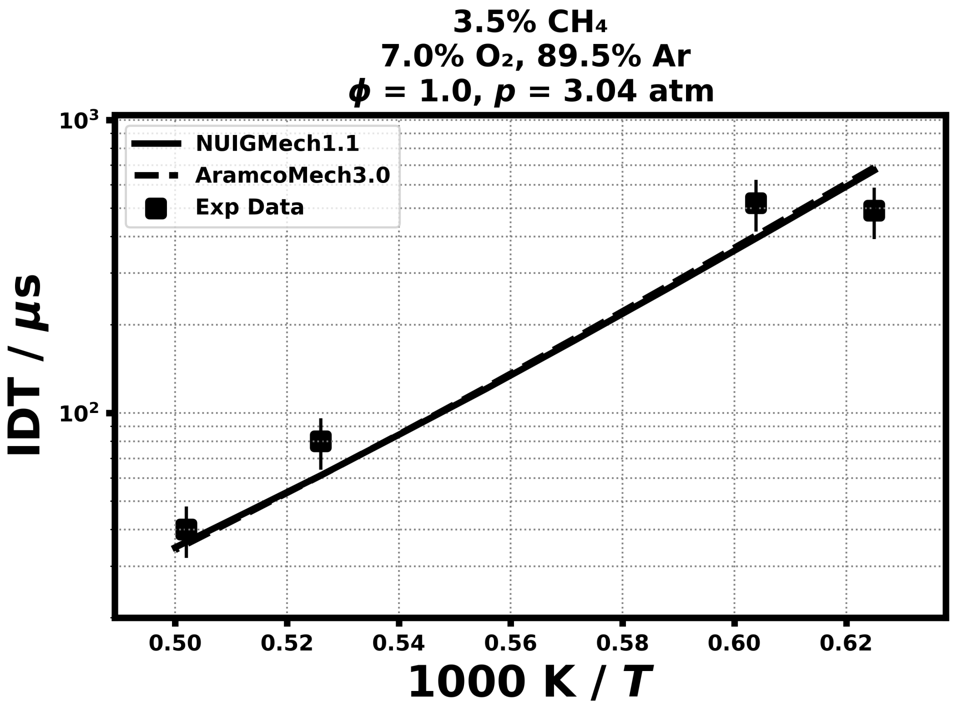
3.4) Lifshitz, A., Scheller, K., Burcat, A., & Skinner, G. B. Combustion and Flame, 16(3) (1971) 311-321.

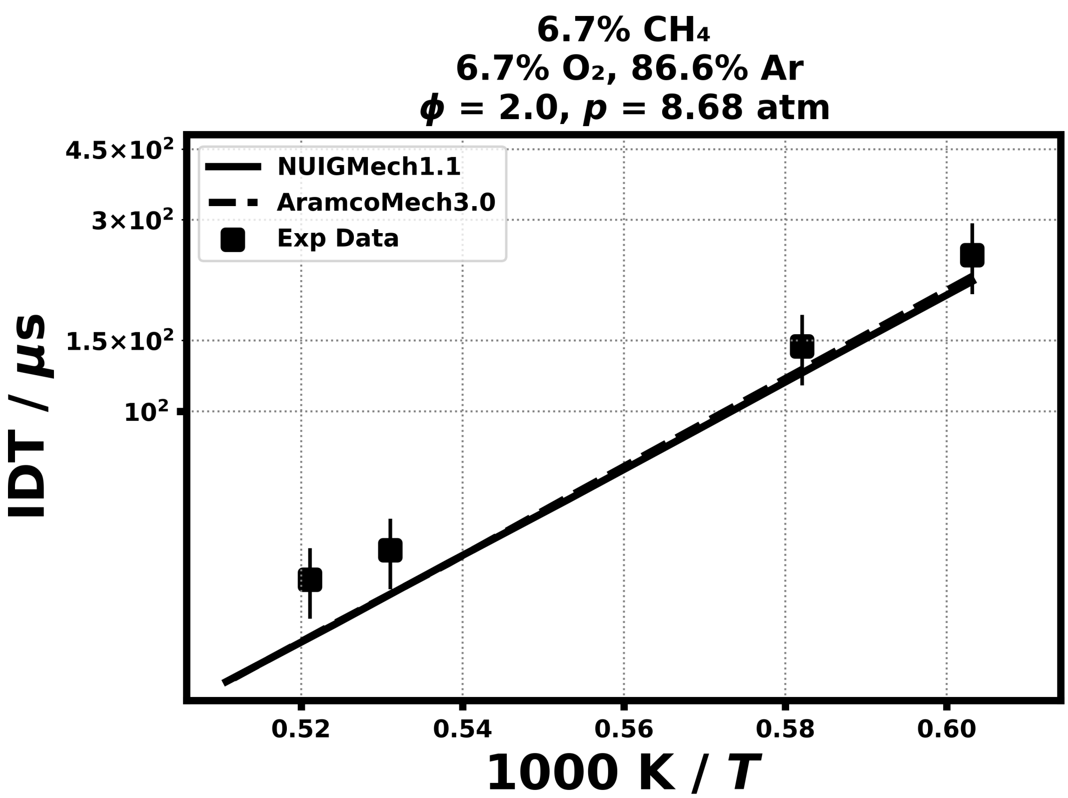




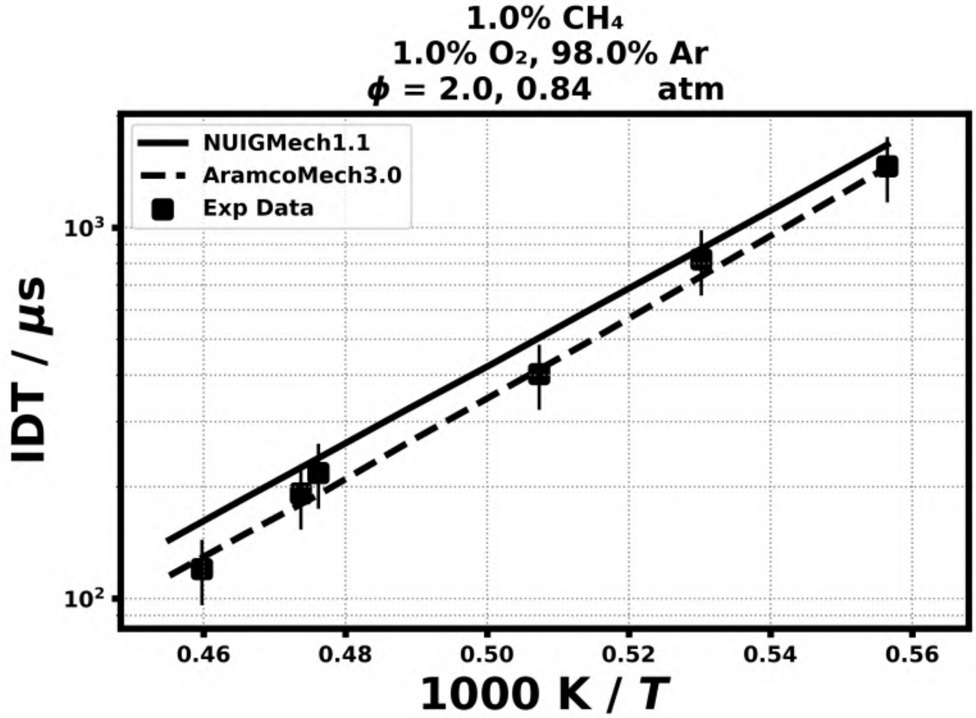

2.0% CH4
8.0% O2, 90.0% Ar
ϕ = 0.5, 9.21 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
0.57
0.58
0.59
0.60
0.61
0.62

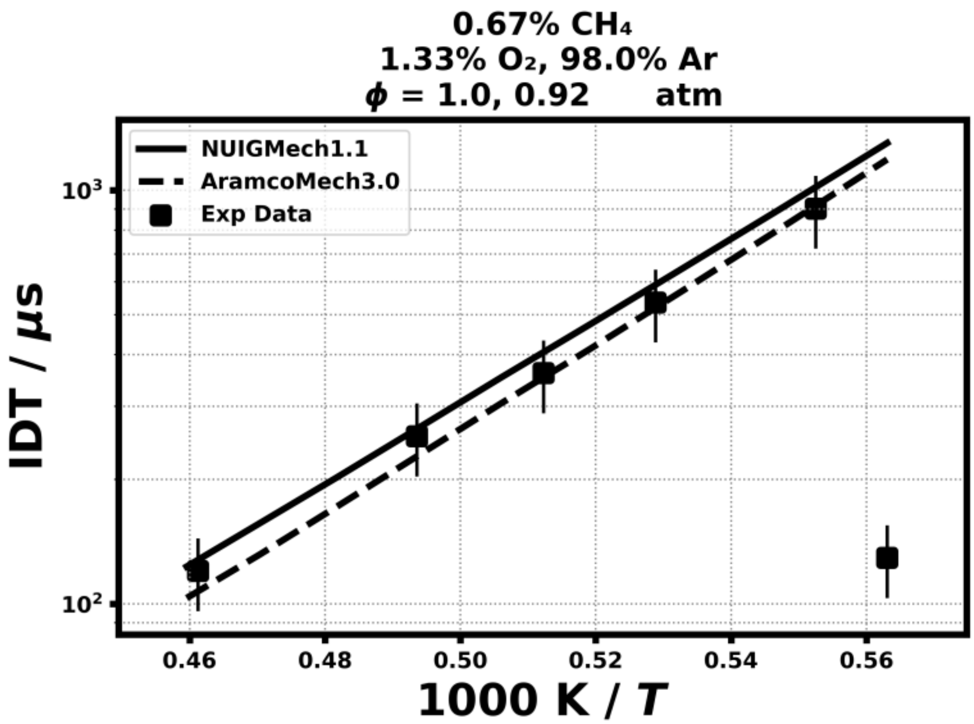

2.1% CH4
2.1% O2, 95.8% Ar
ϕ = 2.0, p = 9.42 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
0.50
0.52
0.54
0.56
0.58
0.60


3.5% CH₄
7.0% O₂, 89.5% Ar
ϕ = 1.0, p = 3.04 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
10³
10²
0.50
0.52
0.54
0.56
0.58
0.60
0.62

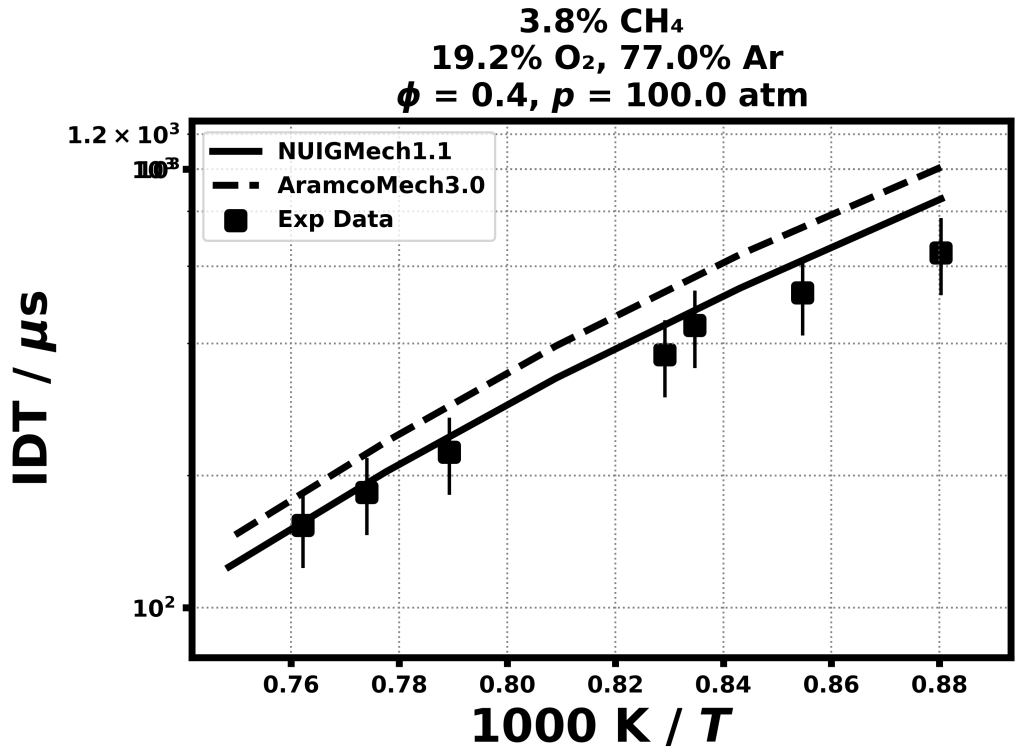

6.7% CH₄
6.7% O₂, 86.6% Ar
ϕ = 2.0, p = 8.68 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
4.5×10²
3×10²
1.5×10²
10²
0.52
0.54
0.56
0.58
0.60

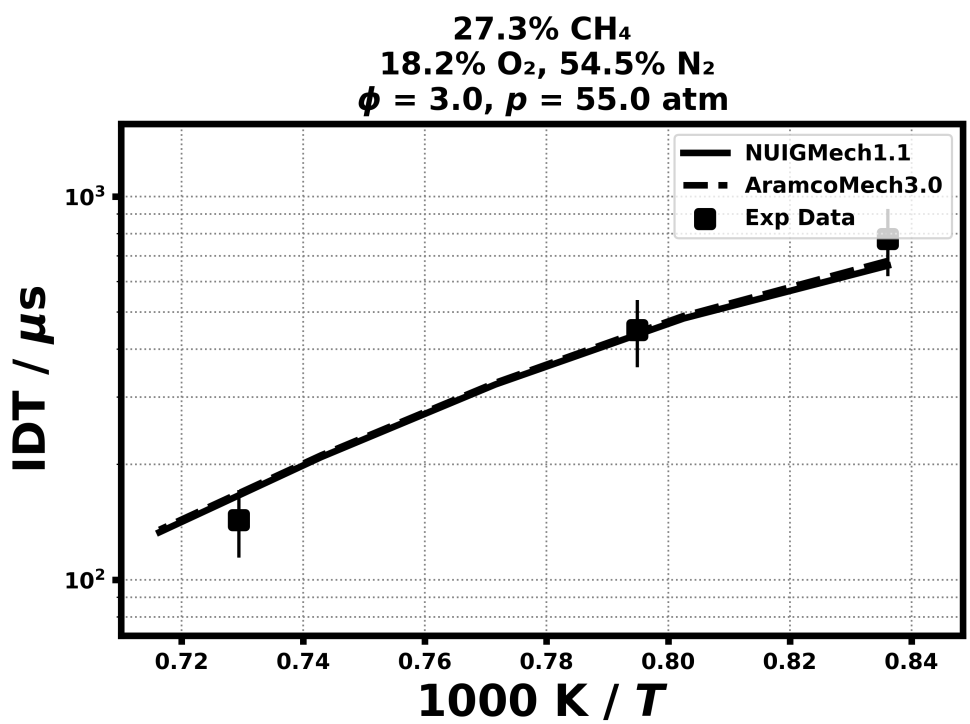
3.5) Mathieu, O., Goulier, J., Gourmel, F., Mannan, M. S., Chaumeix, N., & Petersen, E. L., Proceedings of the Combustion Institute, 35(3) (2015) 2731-2739.

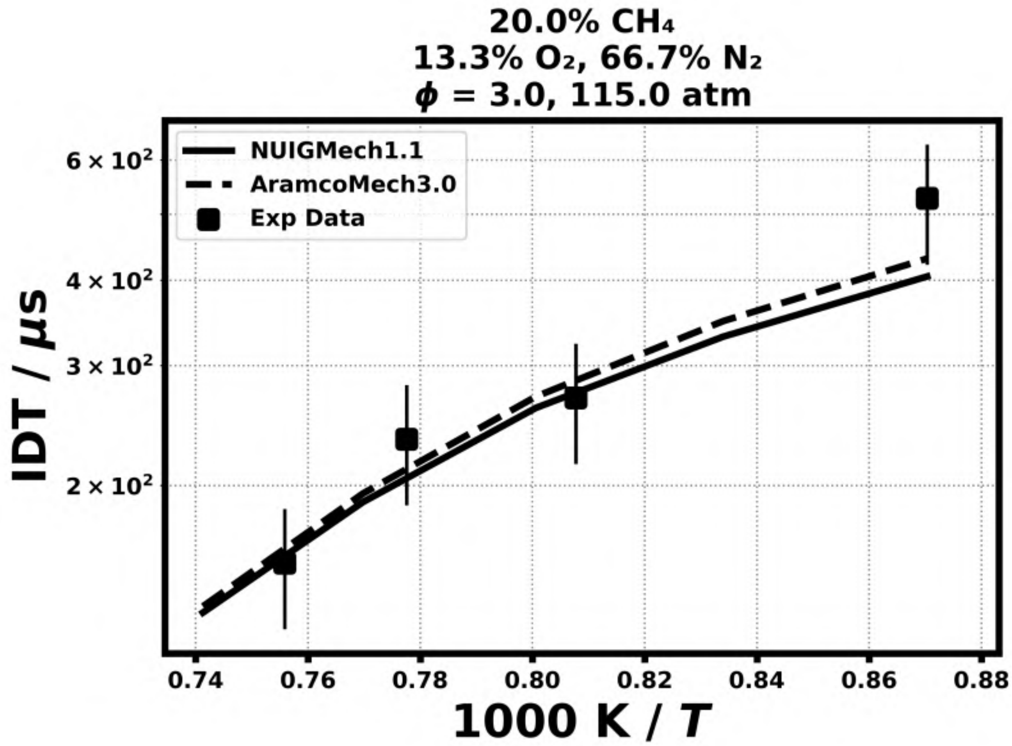


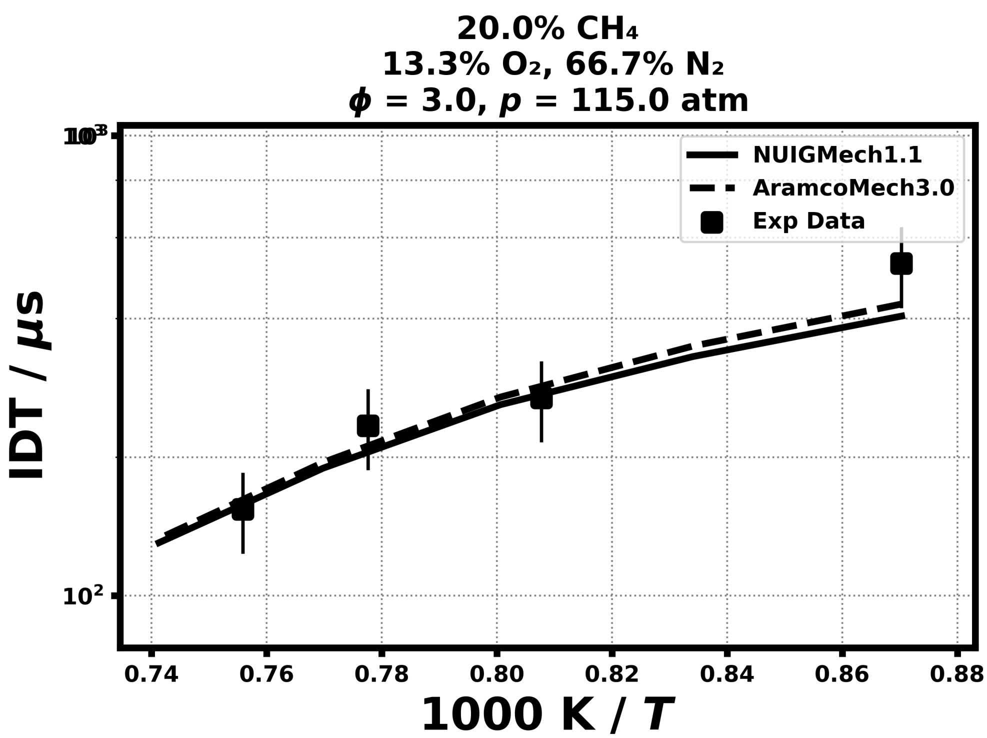


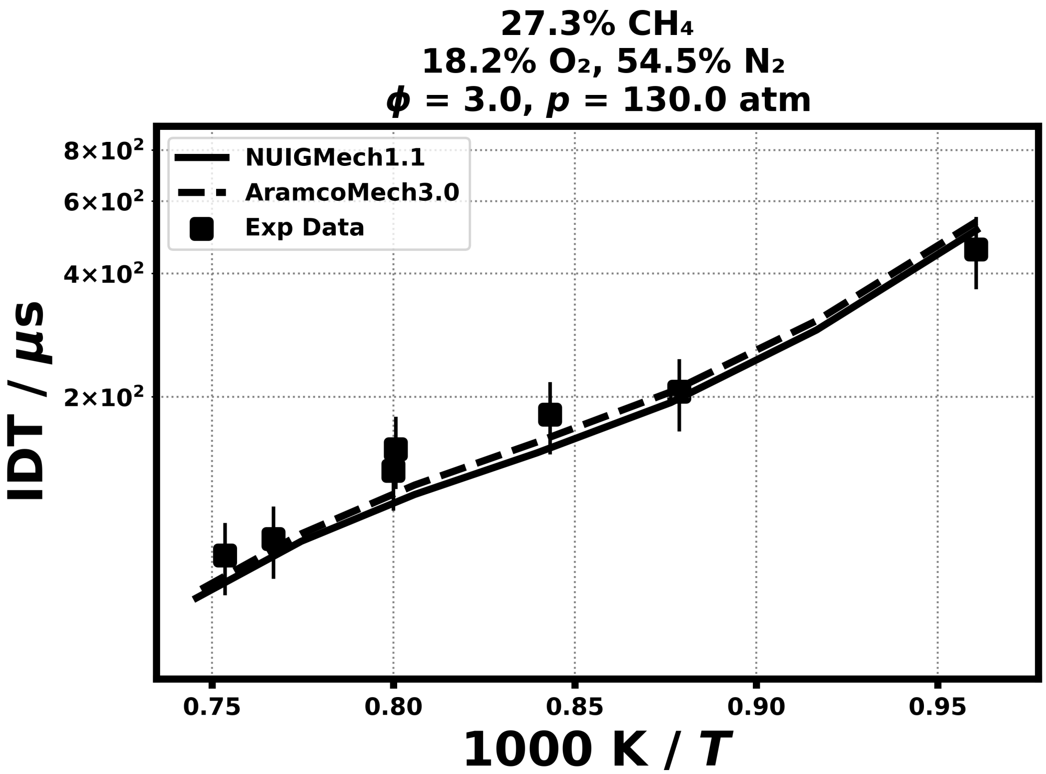
3.6) Petersen, E. L., Davidson, D. F., & Hanson, R. K. Journal of Propulsion and Power, 15(1) (1999) 82-91.

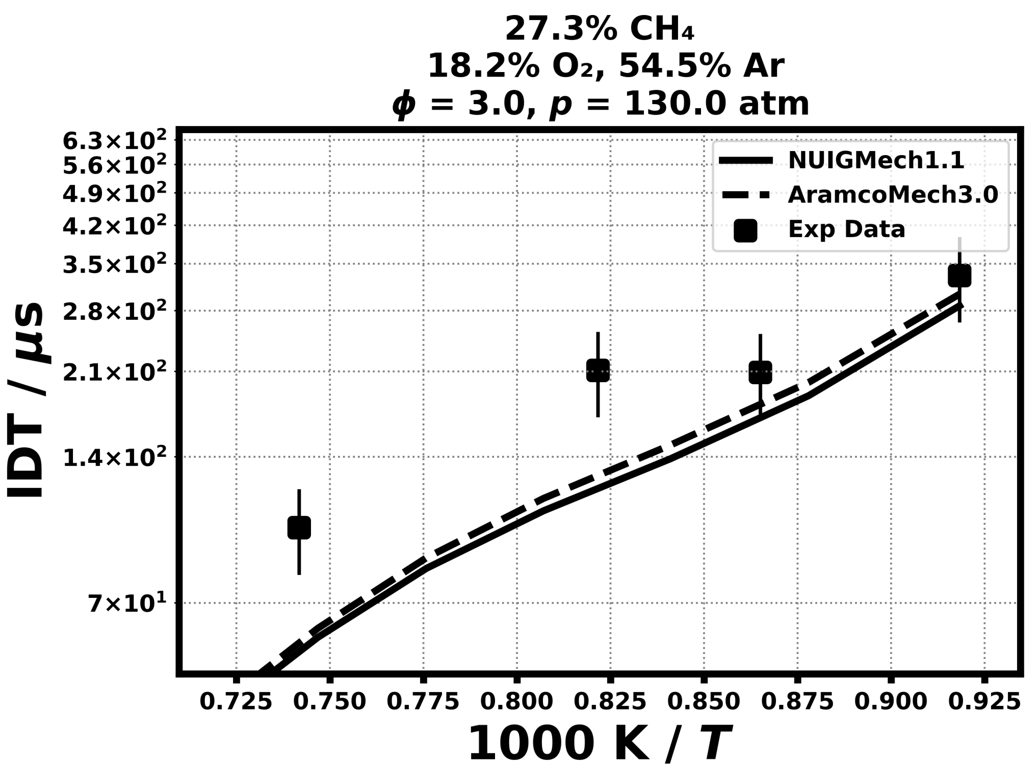


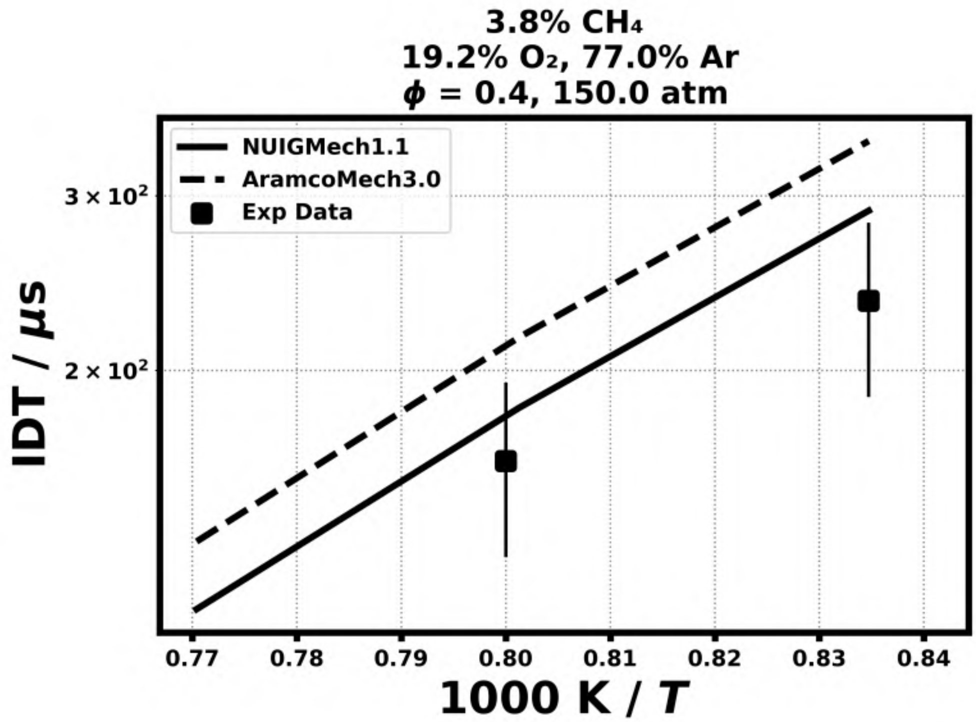


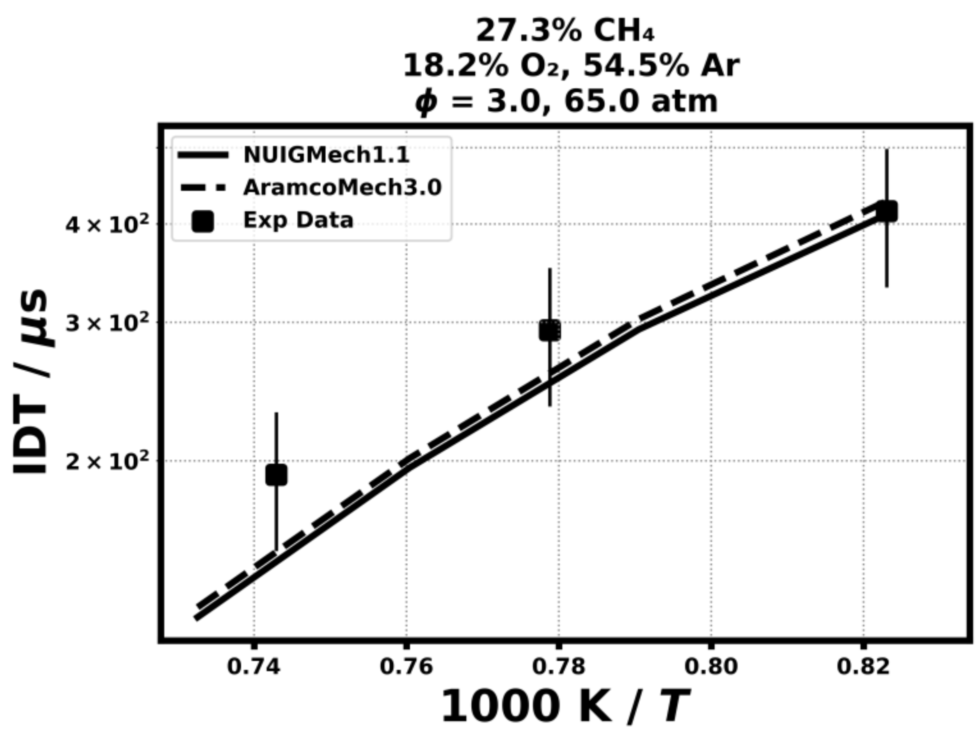

20.0% CH₄
13.3% O₂, 66.7% N₂
ϕ = 3.0, 115.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T

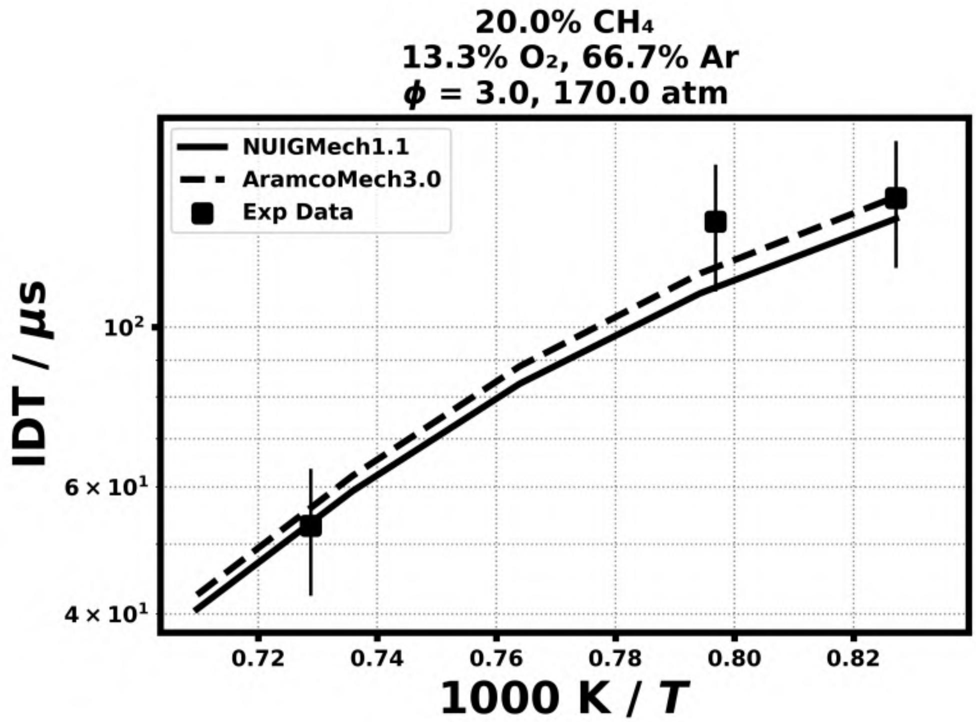

20.0% CH₄
13.3% O₂, 66.7% N₂
ϕ = 3.0, p = 115.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T

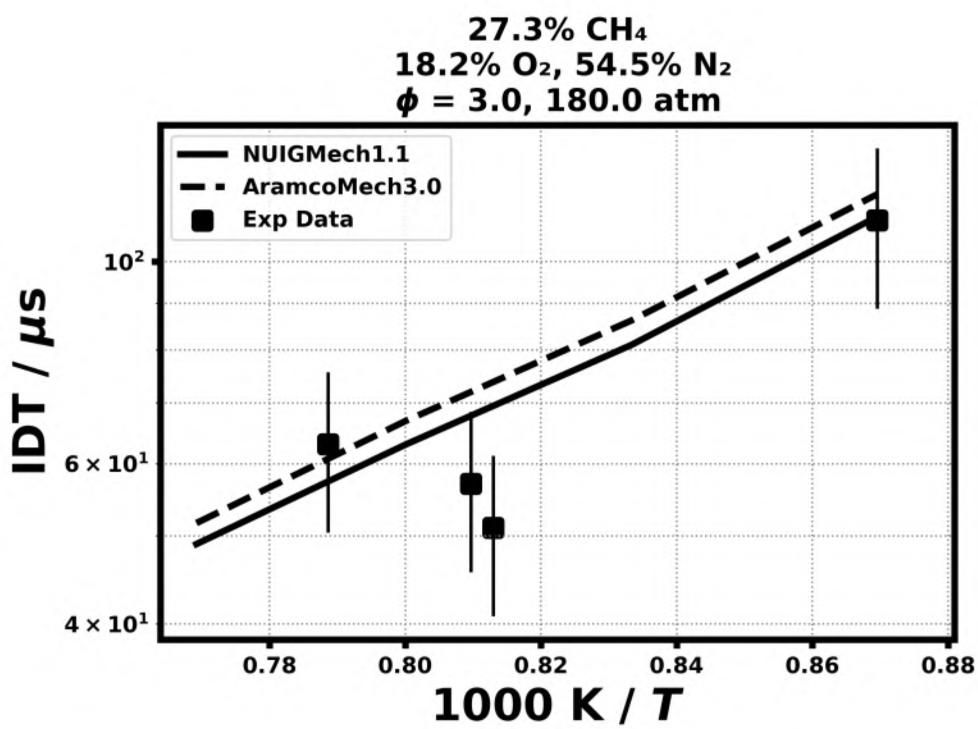

27.3% CH₄
18.2% O₂, 54.5% N₂
ϕ = 3.0, p = 130.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
8×10²
6×10²
4×10²
2×10²
IDT / μs
0.75
0.80
0.85
0.90
0.95
1000 K / T

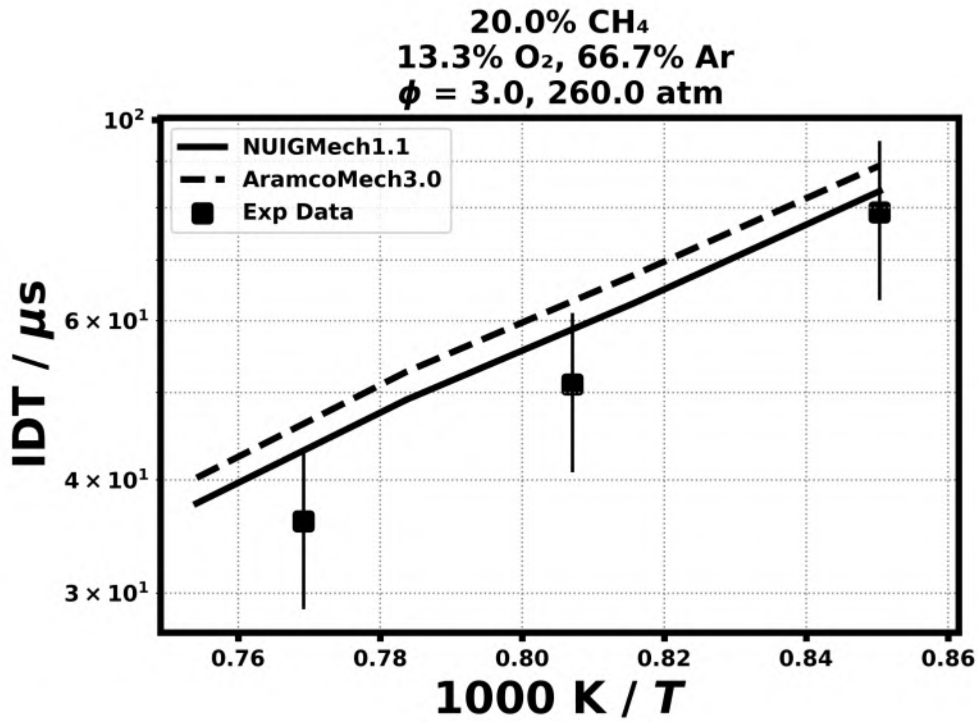

27.3% CH₄
18.2% O₂, 54.5% Ar
ϕ = 3.0, p = 130.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
6.3×10²
5.6×10²
4.9×10²
4.2×10²
3.5×10²
2.8×10²
2.1×10²
1.4×10²
7×10¹
IDT / μs
0.725
0.750
0.775
0.800
0.825
0.850
0.875
0.900
0.925
1000 K / T


3.8% CH4
19.2% O2, 77.0% Ar
ϕ = 0.4, 150.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
3 × 10²
2 × 10²
0.77
0.78
0.79
0.80
0.81
0.82
0.83
0.84
1000 K / T

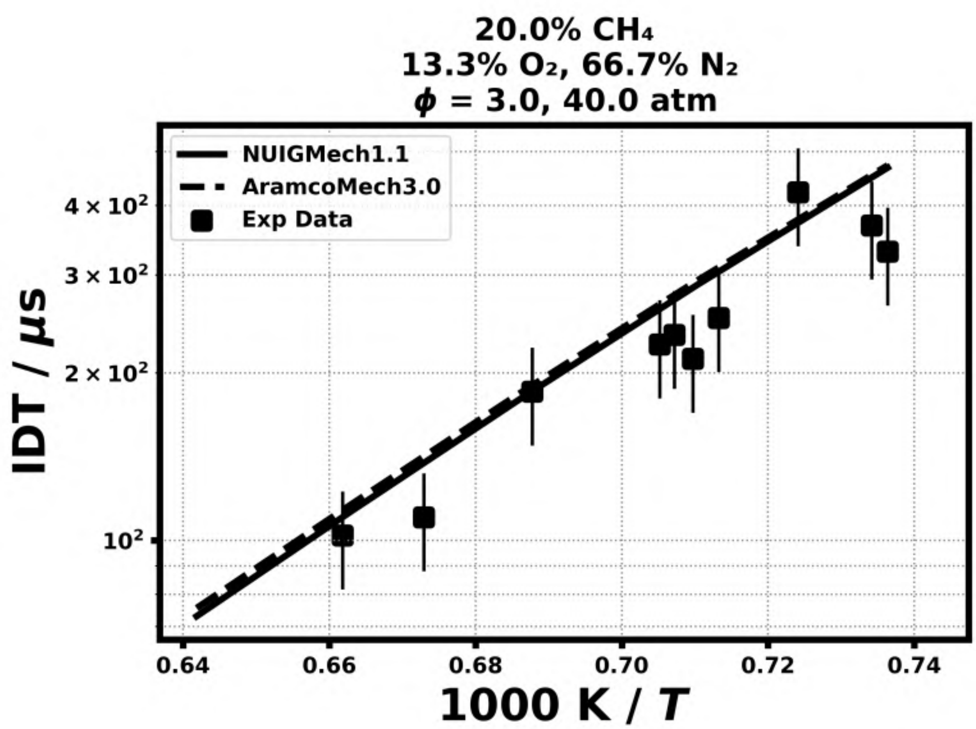

27.3% CH4
18.2% O2, 54.5% Ar
ϕ = 3.0, 65.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
4 × 10²
3 × 10²
2 × 10²
0.74
0.76
0.78
0.80
0.82
1000 K / T


20.0% CH4
13.3% O2, 66.7% Ar
ϕ = 3.0, 170.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10^2
6 × 10^1
4 × 10^1
0.72
0.74
0.76
0.78
0.80
0.82
1000 K / T

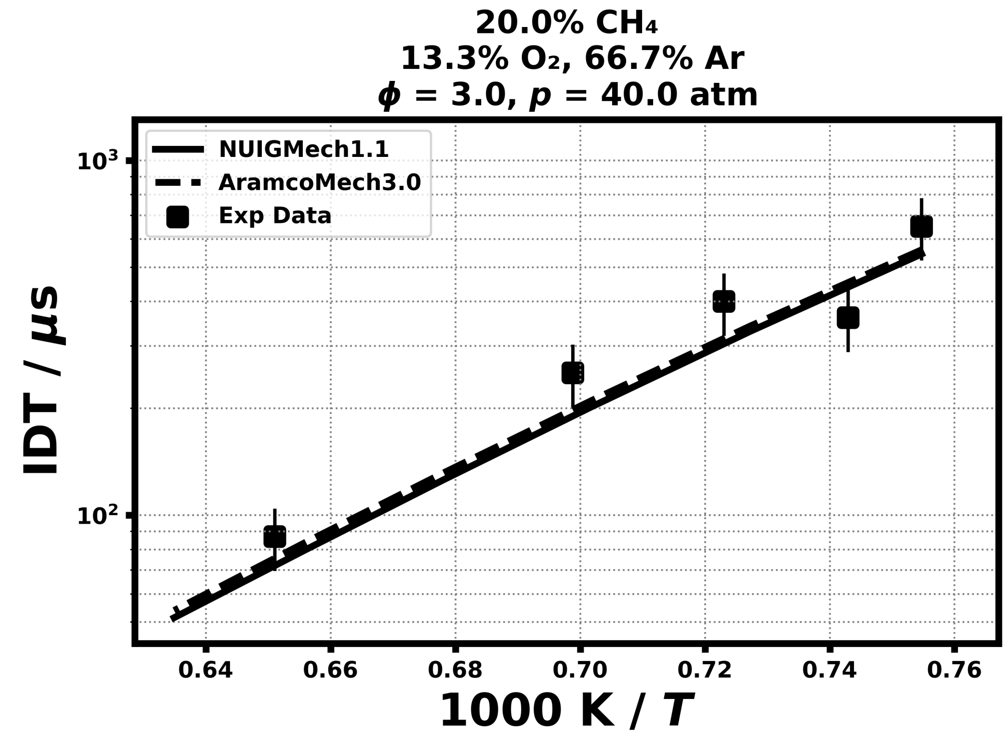

27.3% CH4
18.2% O2, 54.5% N2
ϕ = 3.0, 180.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10^2
6 × 10^1
4 × 10^1
0.78
0.80
0.82
0.84
0.86
0.88
1000 K / T

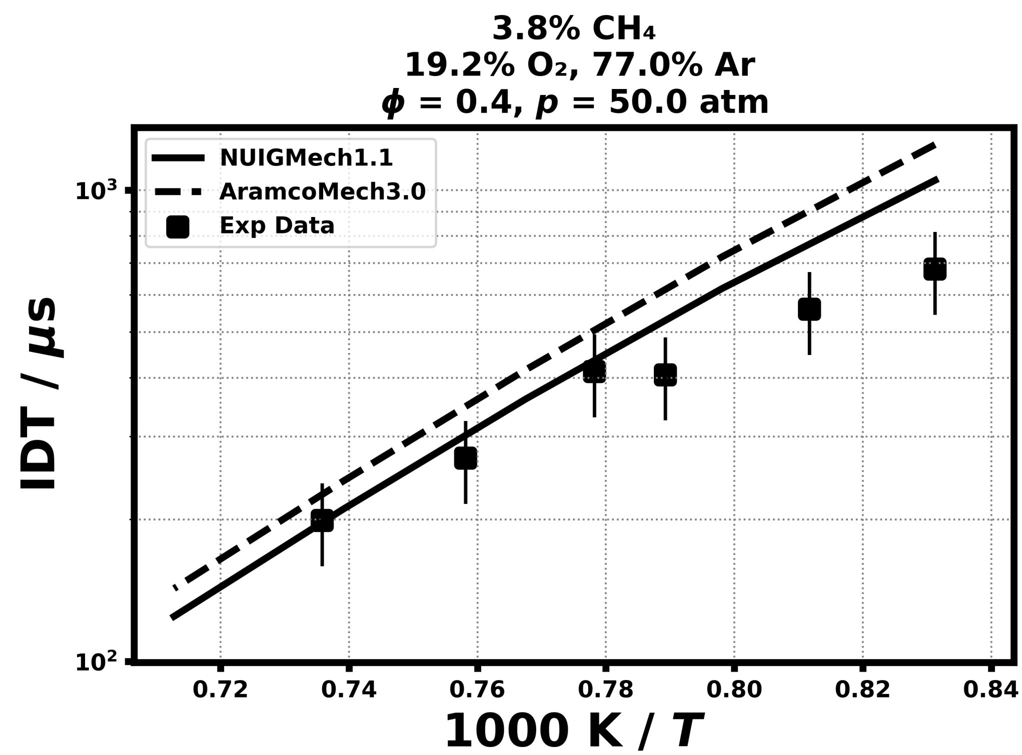


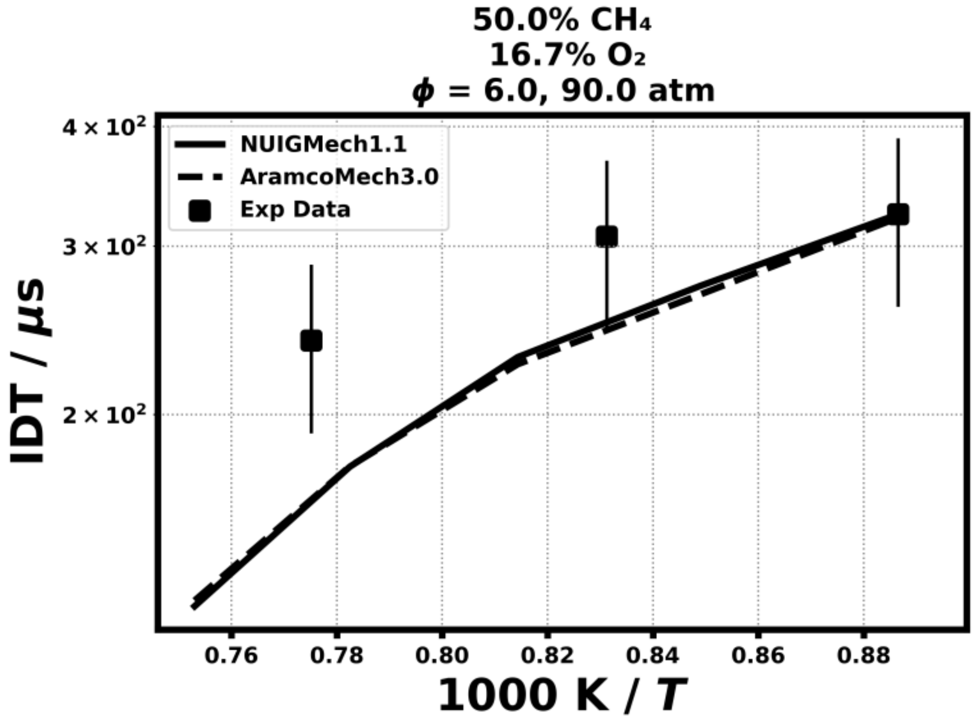
20.0% CH4
13.3% O2, 66.7% Ar
ϕ = 3.0, 260.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T

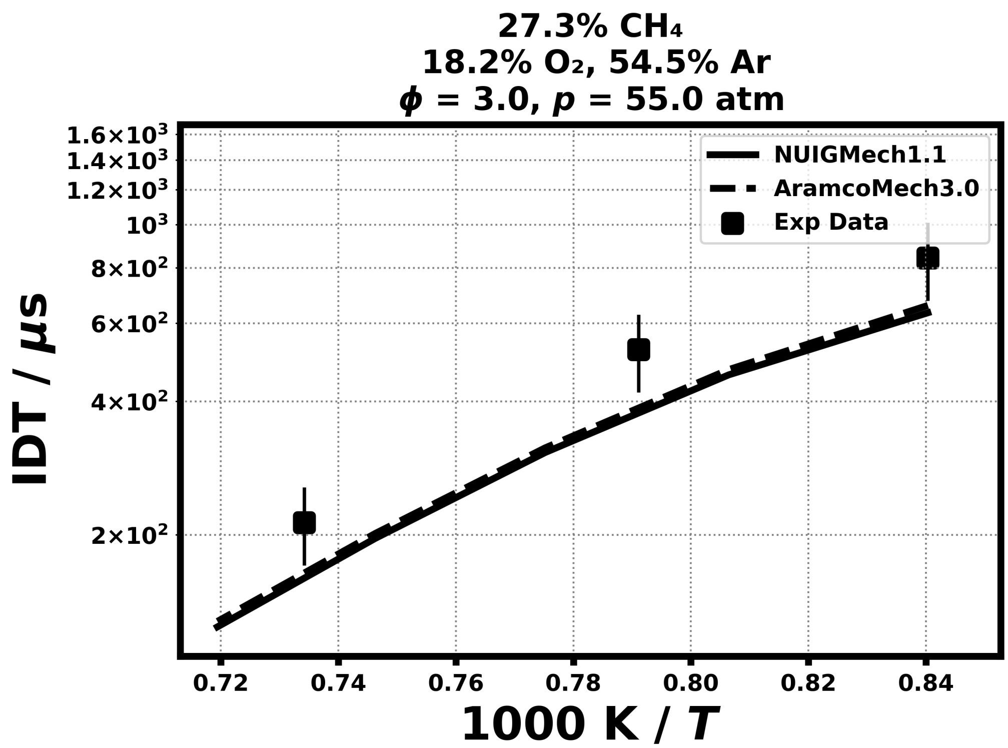


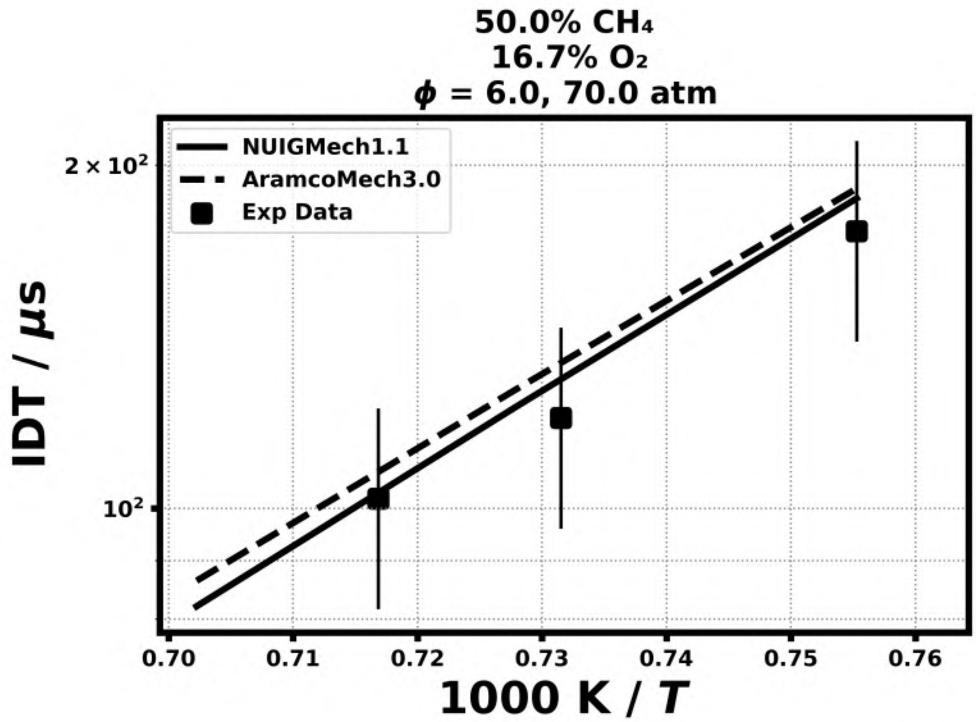
20.0% CH4
13.3% O2, 66.7% N2
ϕ = 3.0, 40.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T

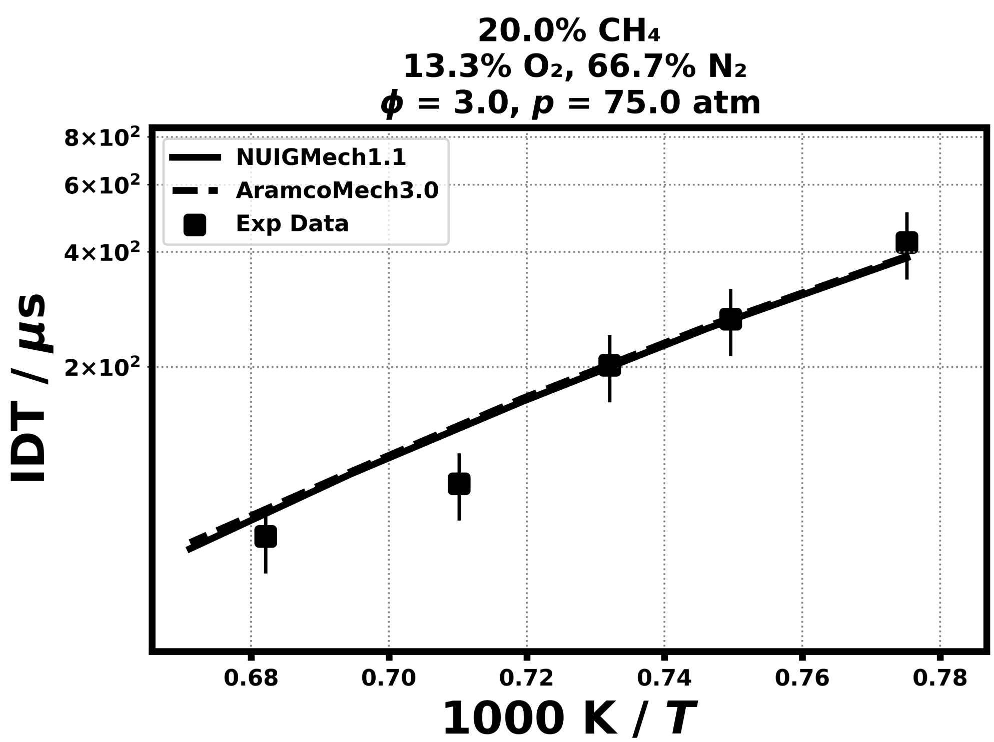

20.0% CH₄
13.3% O₂, 66.7% Ar
ϕ = 3.0, p = 40.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.64
0.66
0.68
0.70
0.72
0.74
0.76
1000 K / T

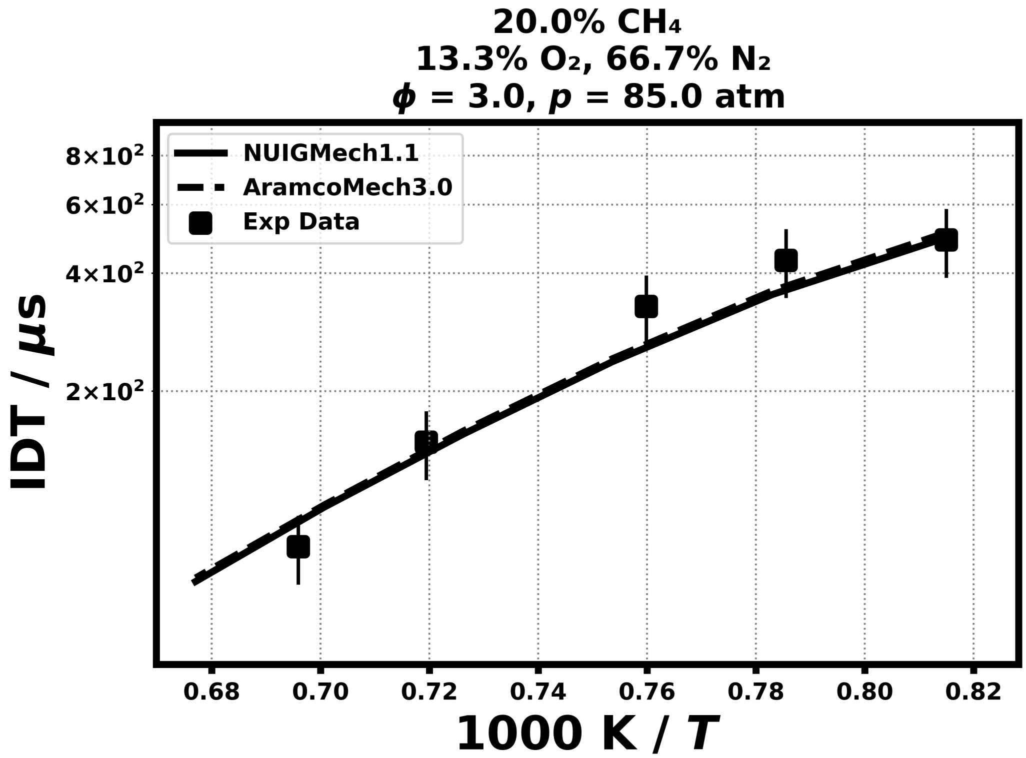

3.8% CH₄
19.2% O₂, 77.0% Ar
ϕ = 0.4, p = 50.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.72
0.74
0.76
0.78
0.80
0.82
0.84
1000 K / T

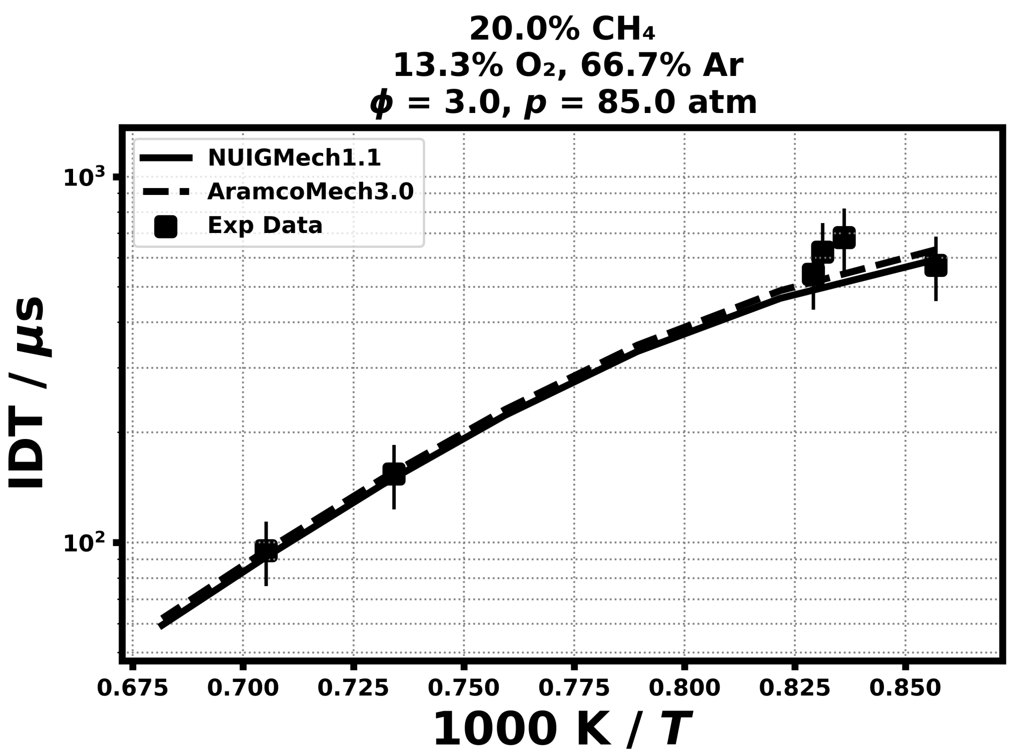

50.0% CH₄
16.7% O₂
ϕ = 6.0, 90.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
4 × 10²
3 × 10²
2 × 10²
IDT / μs
0.76
0.78
0.80
0.82
0.84
0.86
0.88
1000 K / T


27.3% CH₄
18.2% O₂, 54.5% Ar
ϕ = 3.0, p = 55.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
1.6×10³
1.4×10³
1.2×10³
10³
8×10²
6×10²
4×10²
2×10²
IDT / μs
0.72
0.74
0.76
0.78
0.80
0.82
0.84
1000 K / T

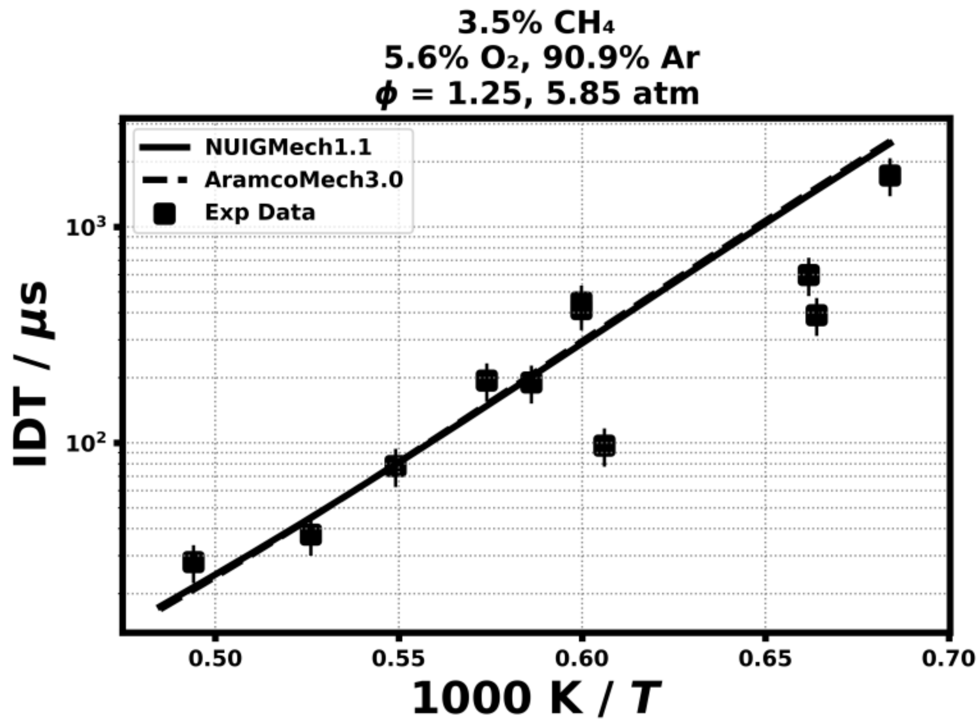

50.0% CH₄
16.7% O₂
ϕ = 6.0, 70.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
2 × 10²
10²
IDT / μs
0.70
0.71
0.72
0.73
0.74
0.75
0.76
1000 K / T

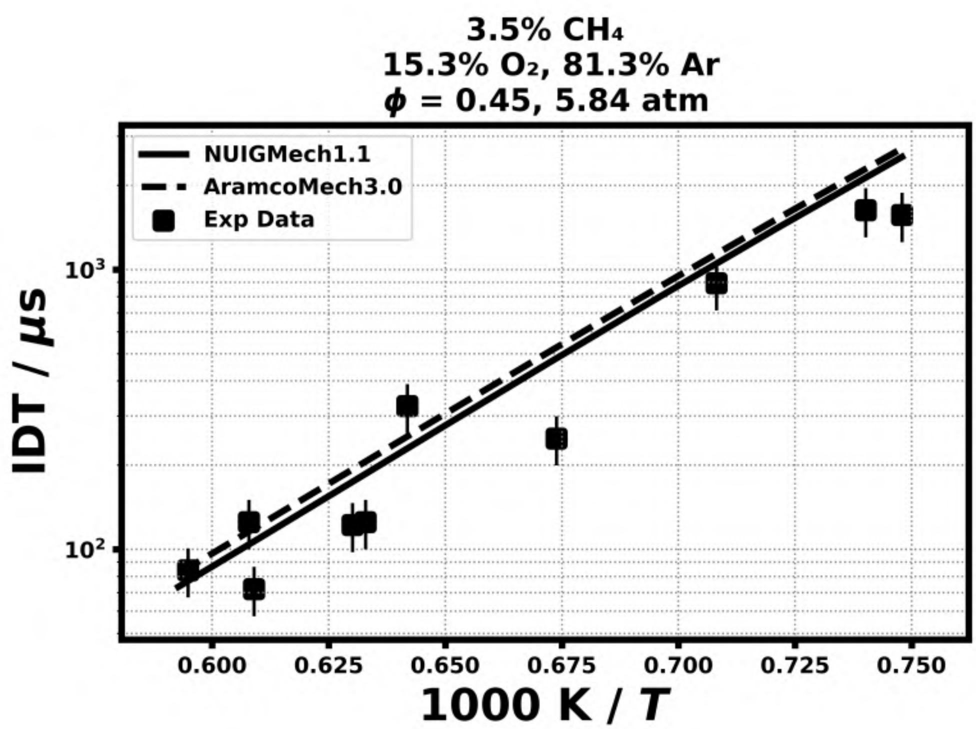

20.0% CH₄
13.3% O₂, 66.7% N₂
ϕ = 3.0, p = 75.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
8×10²
6×10²
4×10²
2×10²
IDT / μs
0.68
0.70
0.72
0.74
0.76
0.78
1000 K / T

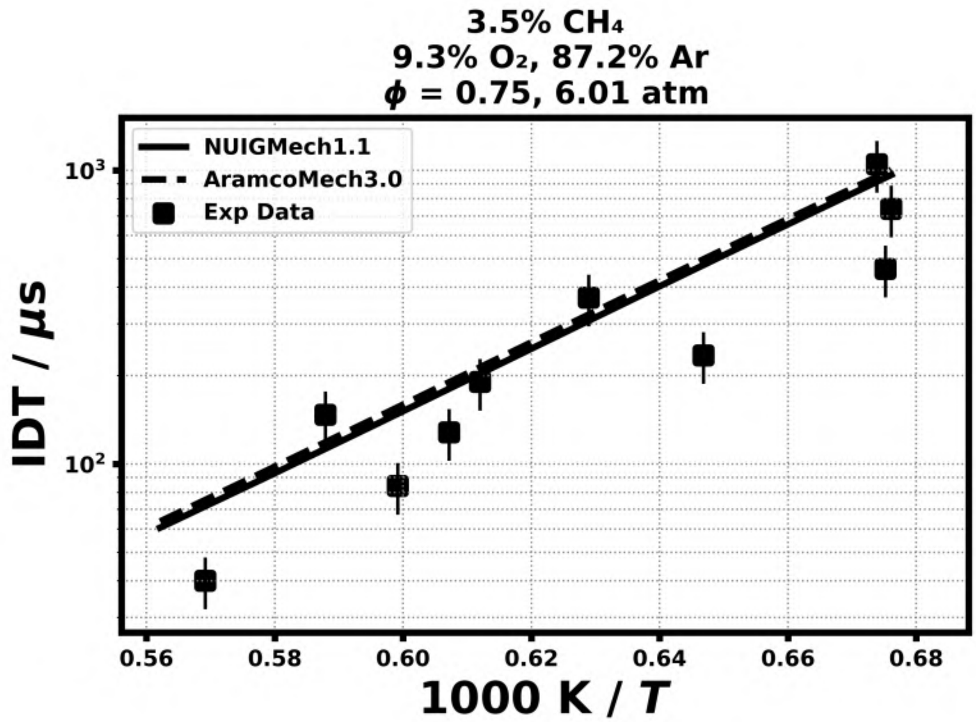

20.0% CH4
13.3% O2, 66.7% N2
ϕ = 3.0, p = 85.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
8×10²
6×10²
4×10²
2×10²
IDT / μs
0.68
0.70
0.72
0.74
0.76
0.78
0.80
0.82
1000 K / T

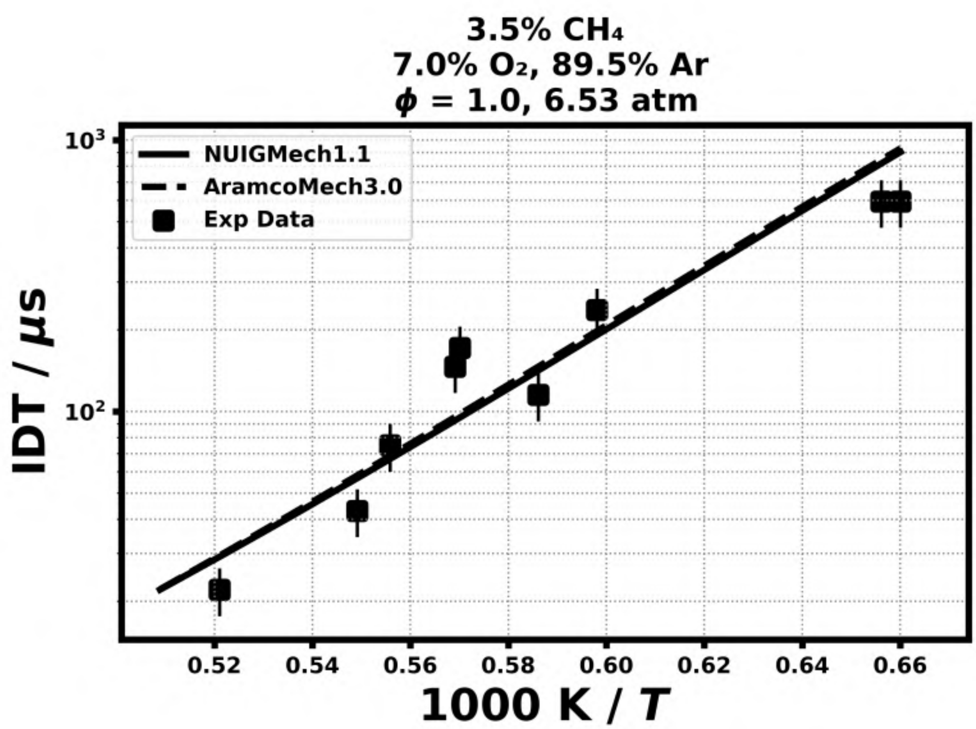

20.0% CH4
13.3% O2, 66.7% Ar
ϕ = 3.0, p = 85.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
10³
10²
IDT / μs
0.675
0.700
0.725
0.750
0.775
0.800
0.825
0.850
1000 K / T

3.8) Spadaccini, L. J., & Colket Iii, M. B., Progress in energy and combustion science, 20 (5) (1994) 431-460.



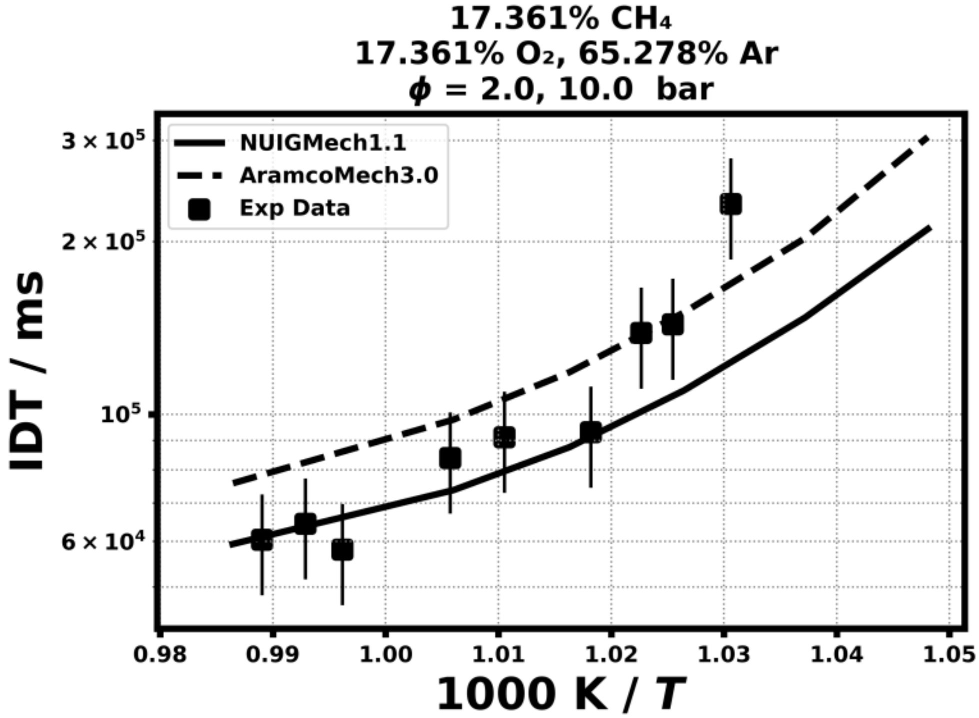


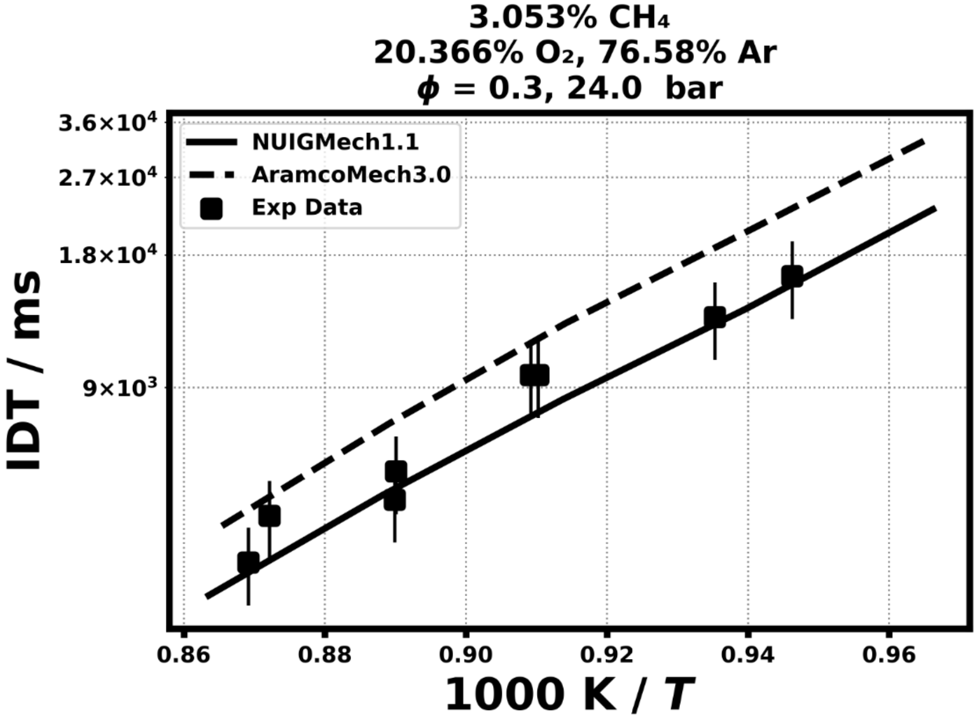

3.5% CH4
9.3% O2, 87.2% Ar
ϕ = 0.75, 6.01 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10^3
10^2
0.56
0.58
0.60
0.62
0.64
0.66
0.68
1000 K / T

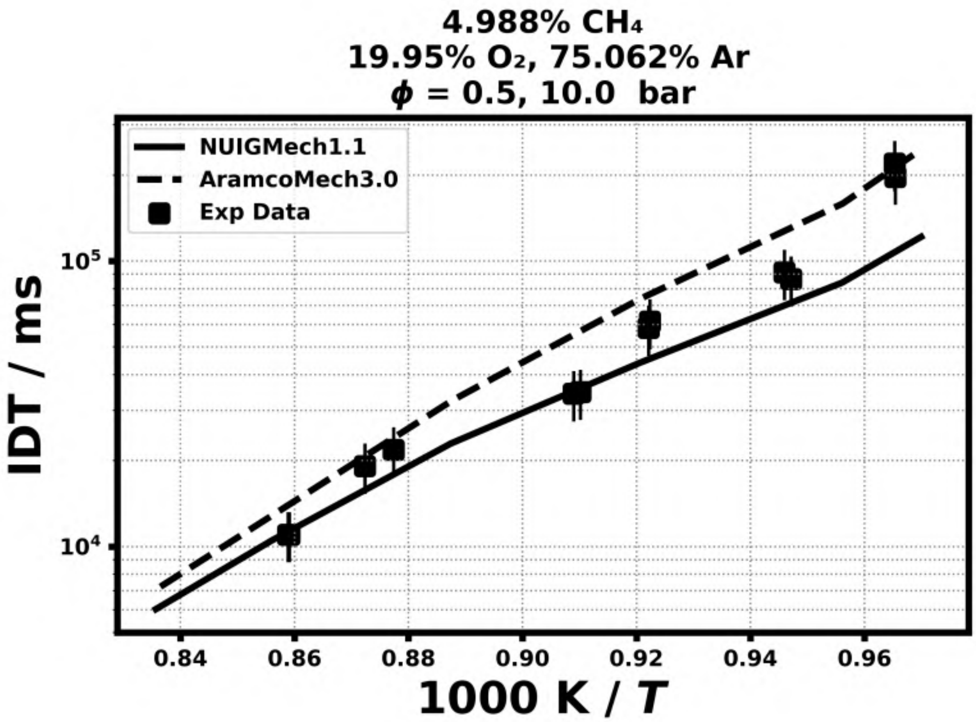

3.5% CH4
7.0% O2, 89.5% Ar
ϕ = 1.0, 6.53 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10^3
10^2
0.52
0.54
0.56
0.58
0.60
0.62
0.64
0.66
1000 K / T

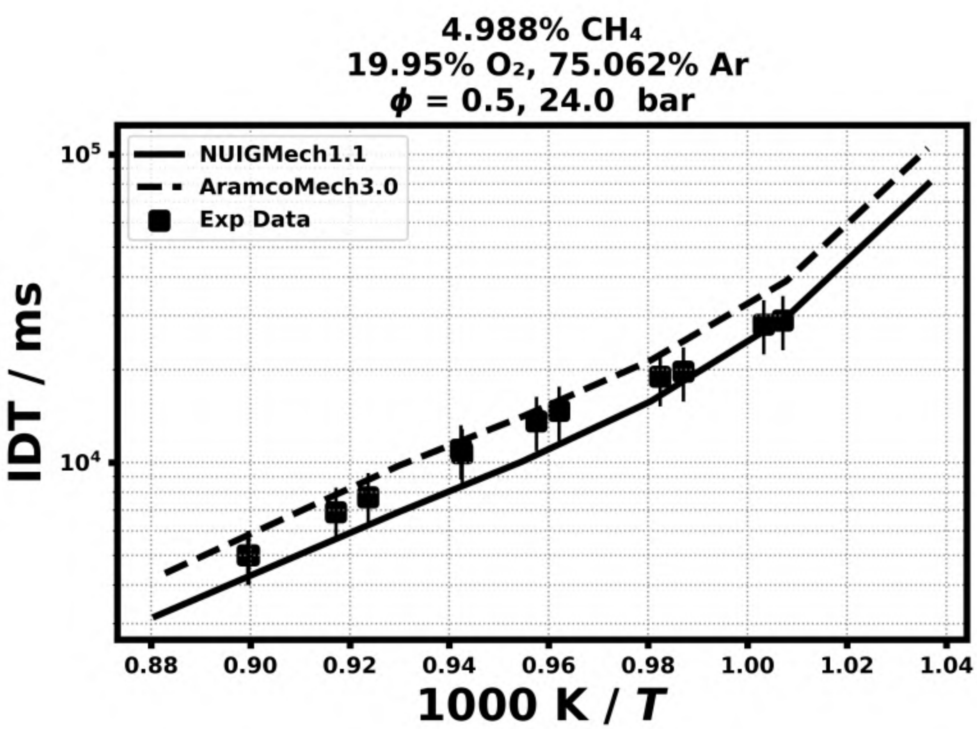
RCM Ignition delay time

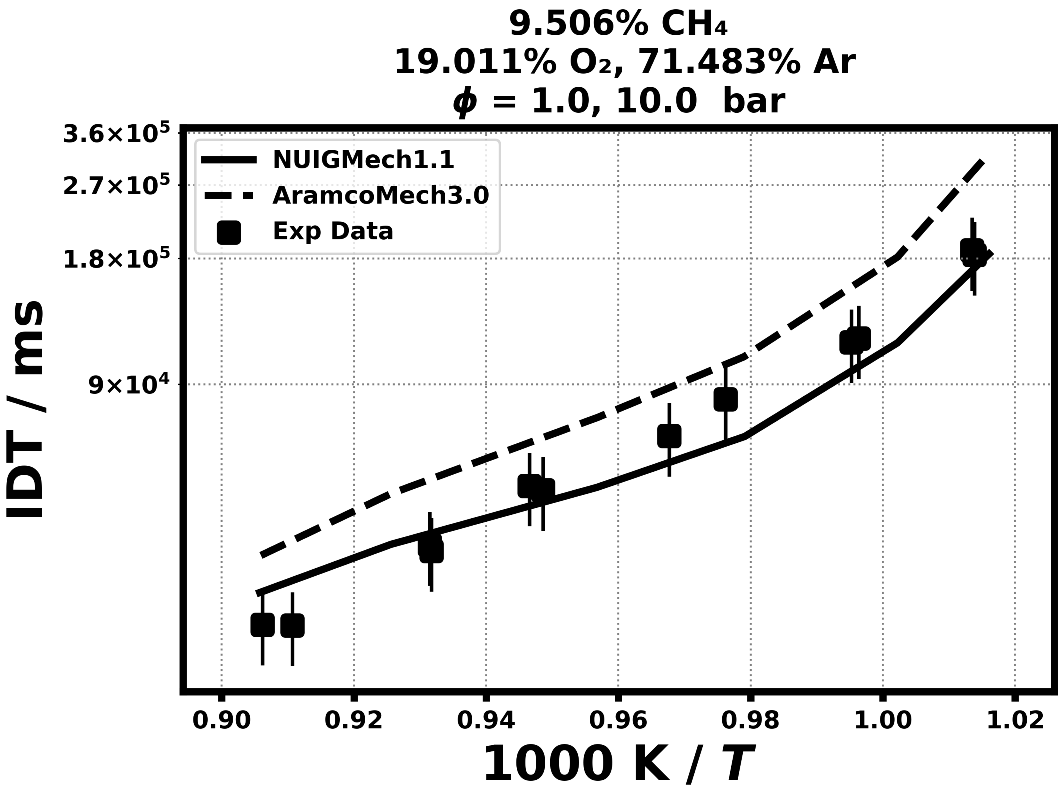
3.10) Burke, U., Somers, K. P., O'Toole, P., Zinner, C. M., Marquet, N., Bourque, G., & Curran, H. J., Combustion and flame, 162(2) (2015) 315-330.



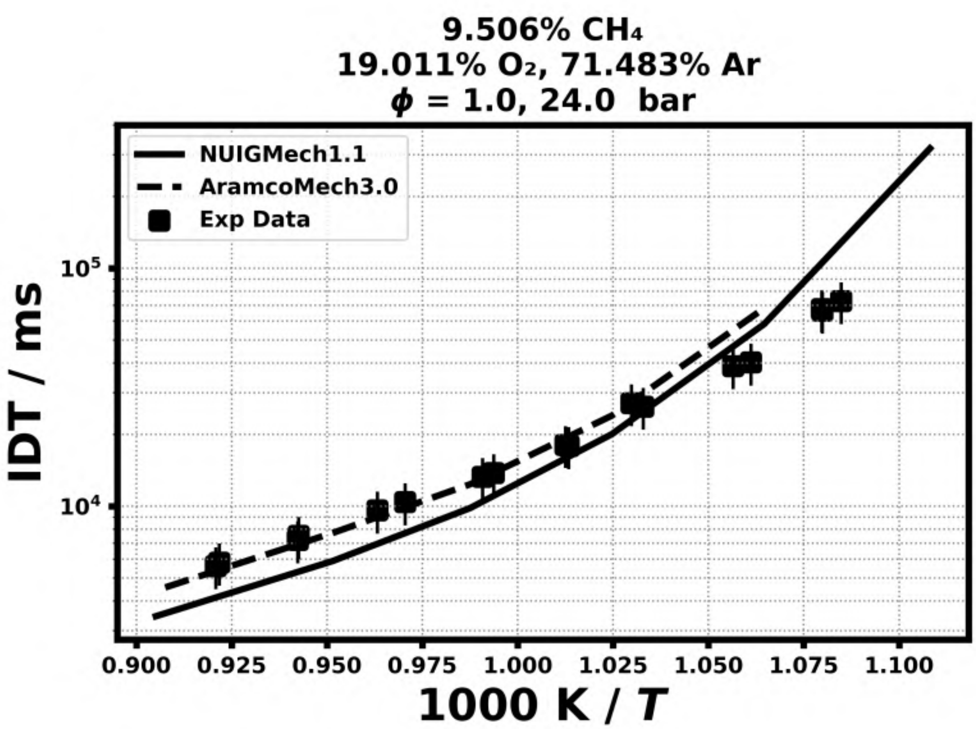



4.988% CH4
19.95% O2, 75.062% Ar
ϕ = 0.5, 10.0 bar
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / ms
1000 K / T


4.988% CH4
19.95% O2, 75.062% Ar
ϕ = 0.5, 24.0 bar
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / ms
1000 K / T



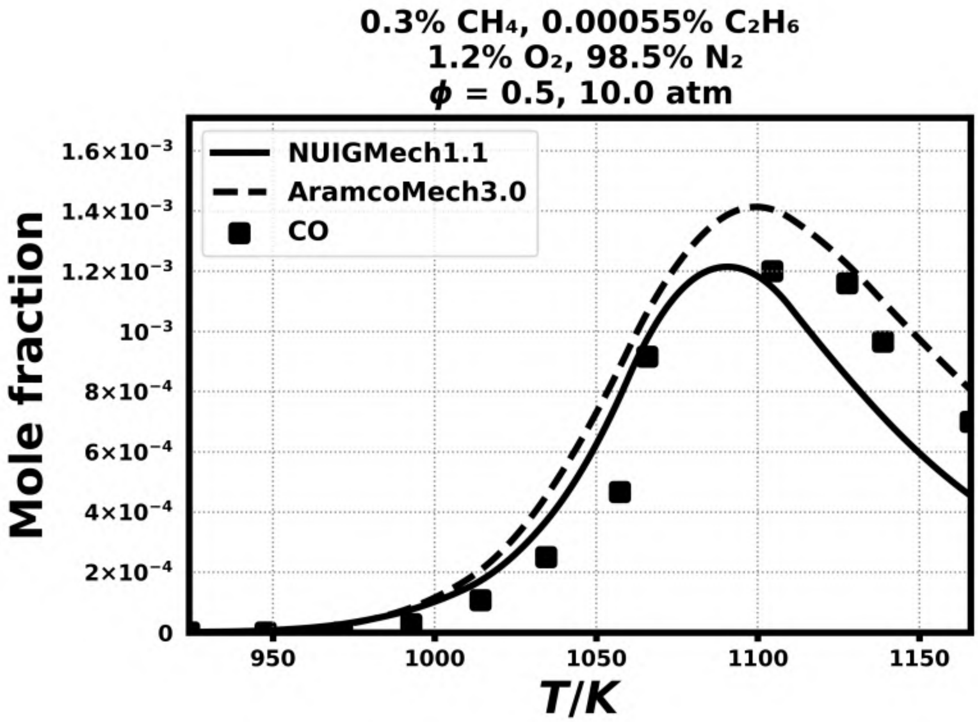
9.506% CH₄
19.011% O₂, 71.483% Ar
ϕ = 1.0, 10.0 bar
NUIGMech1.1
AramcoMech3.0
Exp Data
3.6×10^5
2.7×10^5
1.8×10^5
9×10^4
IDT / ms
0.90
0.92
0.94
0.96
0.98
1.00
1.02
1000 K / T

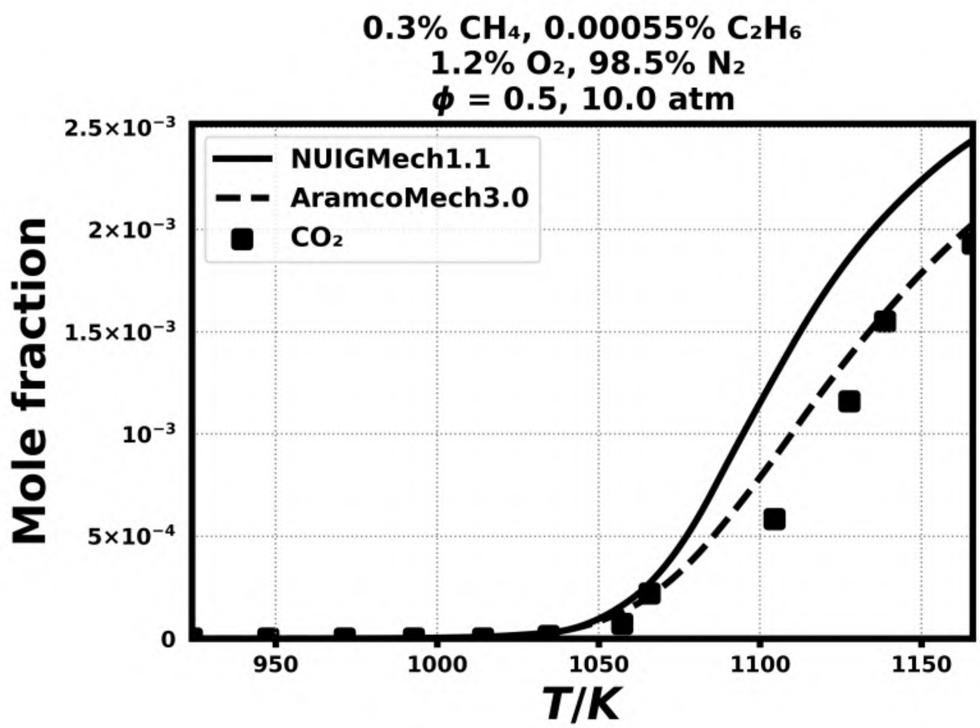


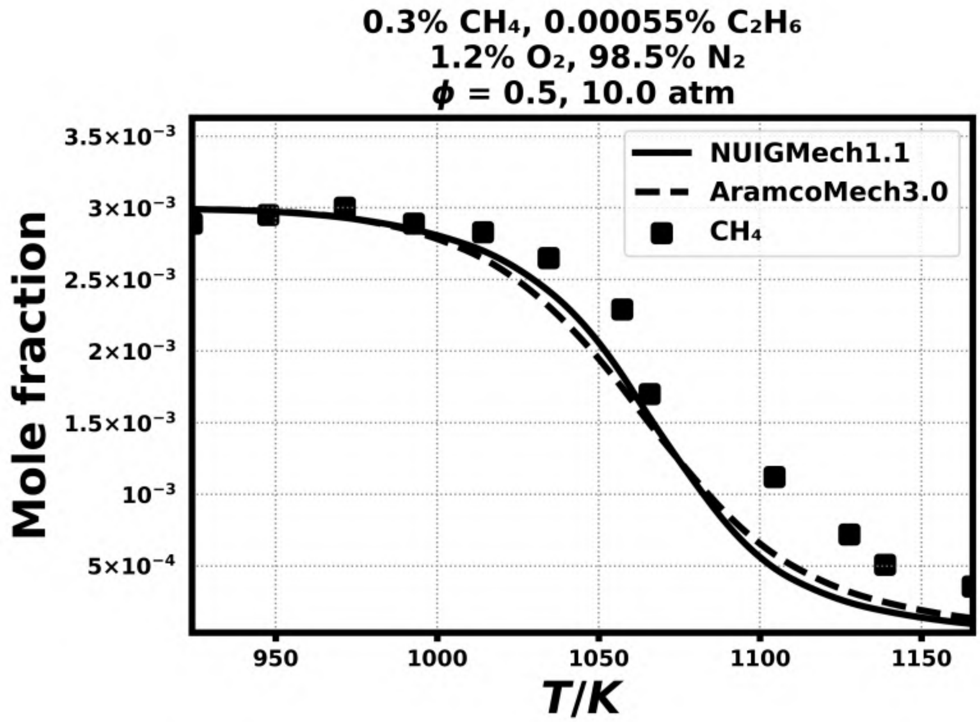
9.506% CH₄
19.011% O₂, 71.483% Ar
ϕ = 1.0, 24.0 bar
NUIGMech1.1
AramcoMech3.0
Exp Data
10^5
10^4
IDT / ms
0.900
0.925
0.950
0.975
1.000
1.025
1.050
1.075
1.100
1000 K / T

Speciation in Jet-stirred reactor

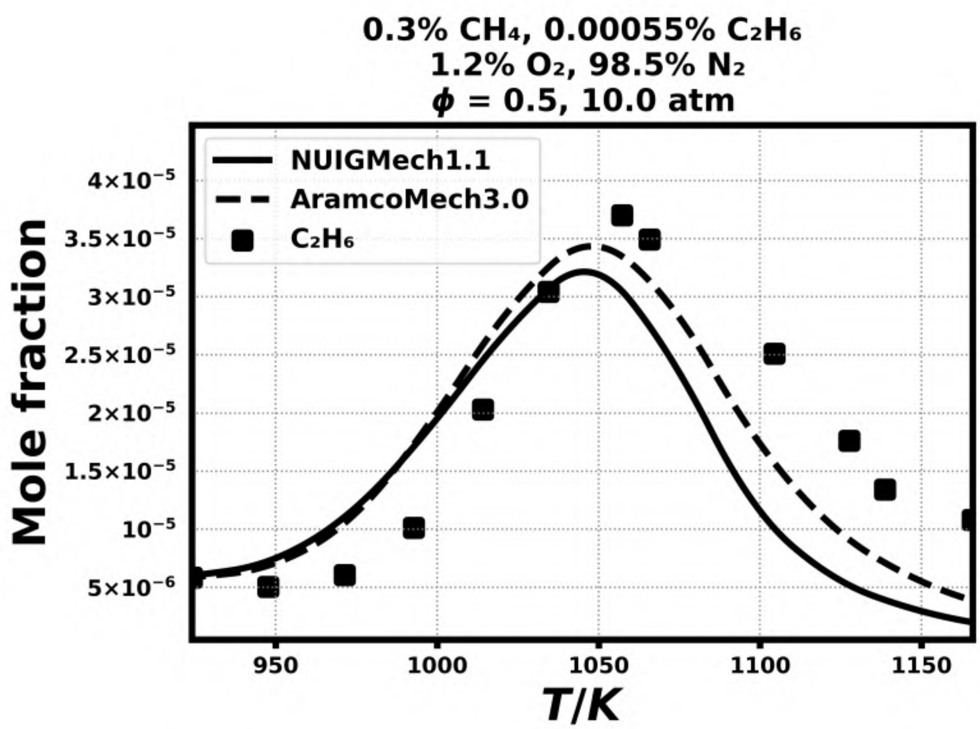
3.11) Dagaut, P., Boettner, J. C., & Cathonnet, M., Combustion science and technology, 77(1-3) (1991) 127-148.



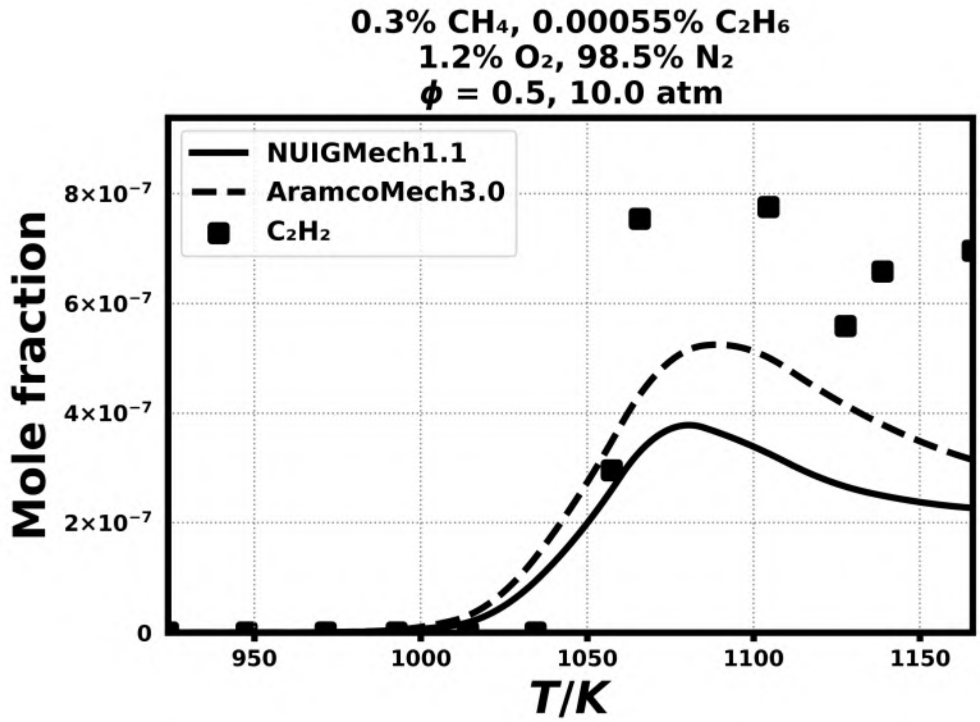


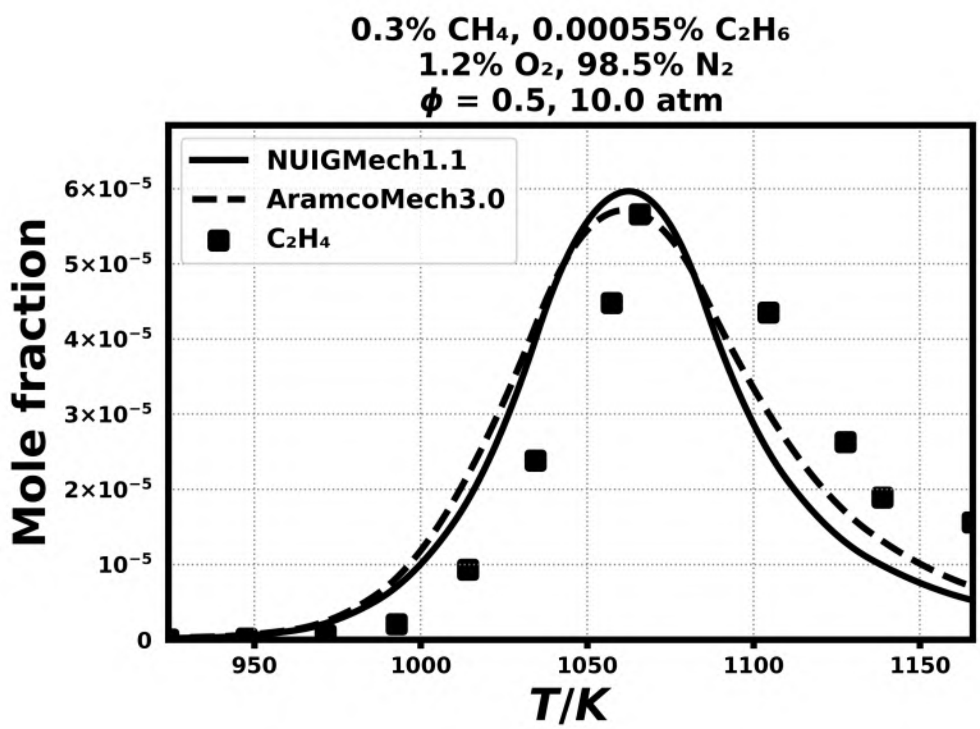


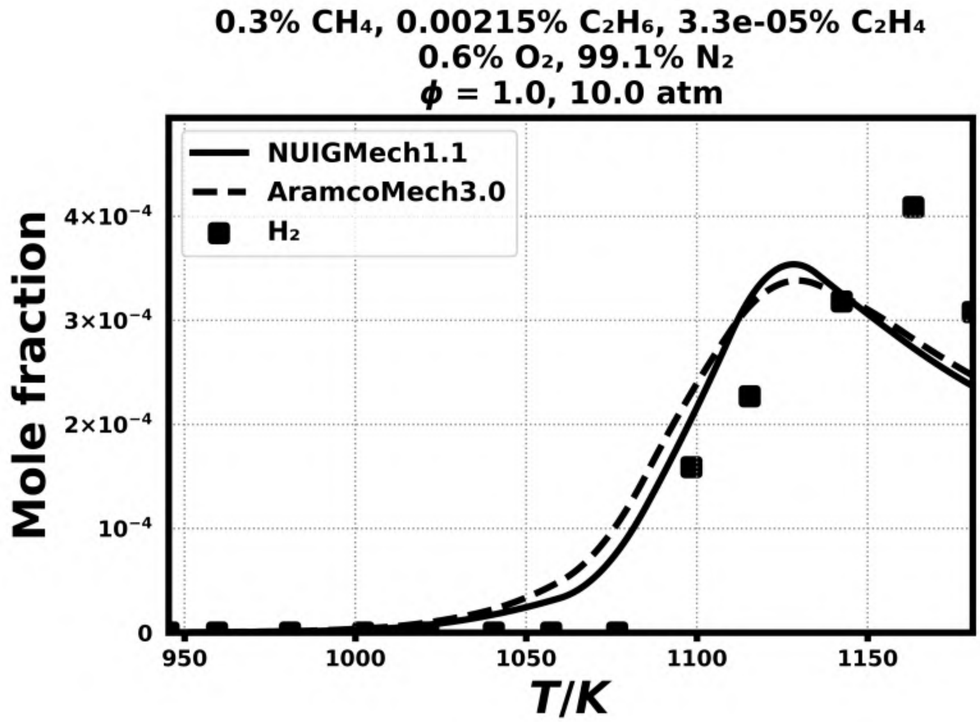
0.3% CH4, 0.00055% C2H6
1.2% O2, 98.5% N2
ϕ = 0.5, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH4

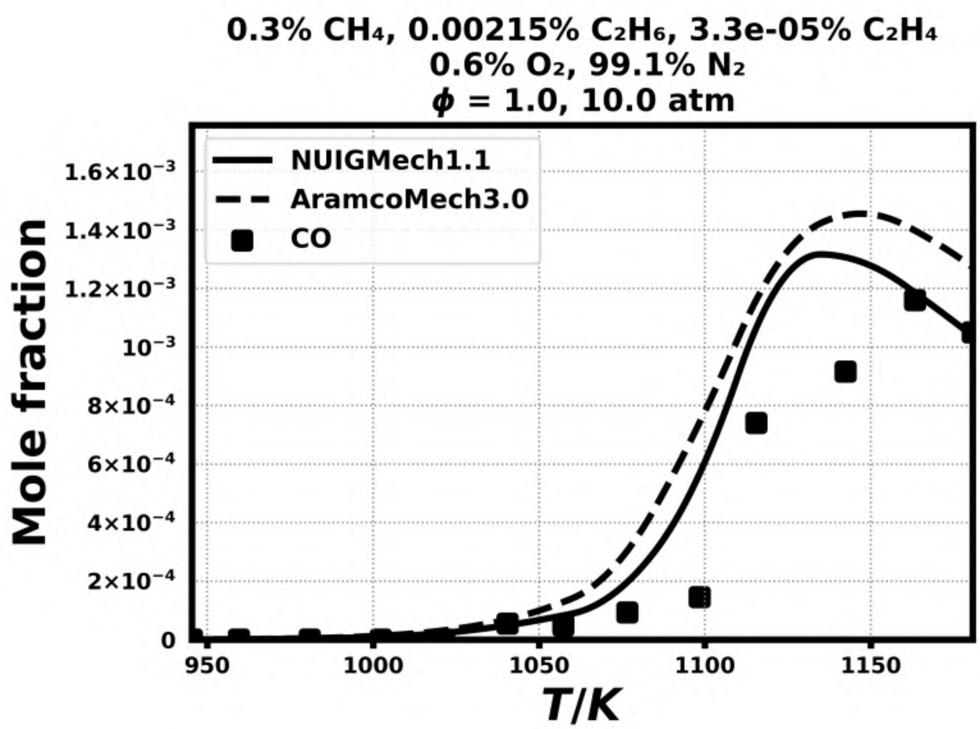


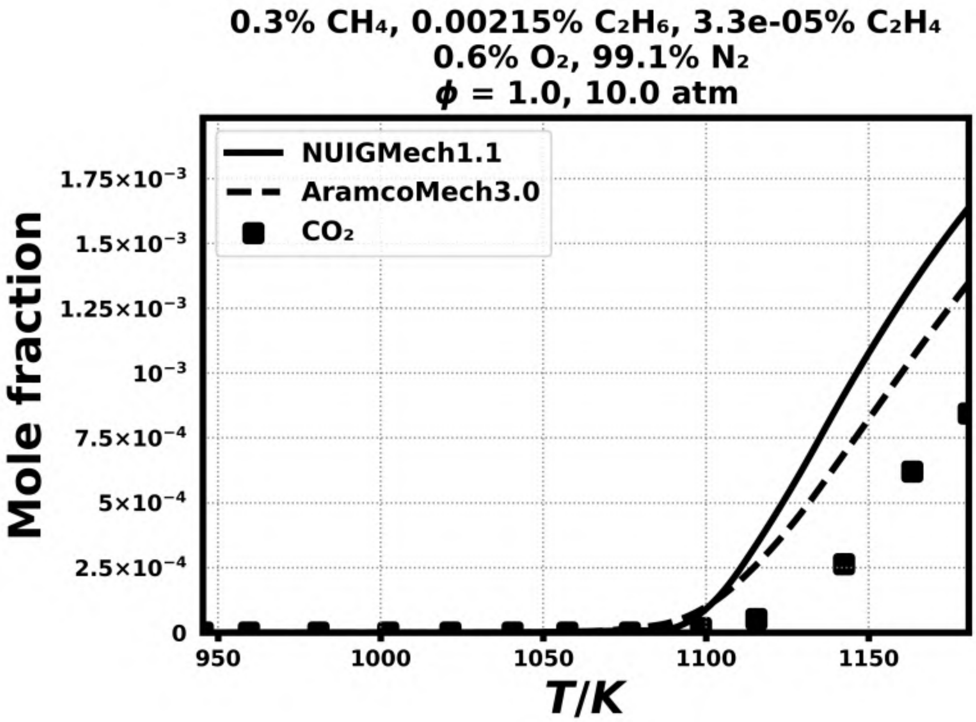
0.3% CH4, 0.00055% C2H6
1.2% O2, 98.5% N2
ϕ = 0.5, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
C2H6

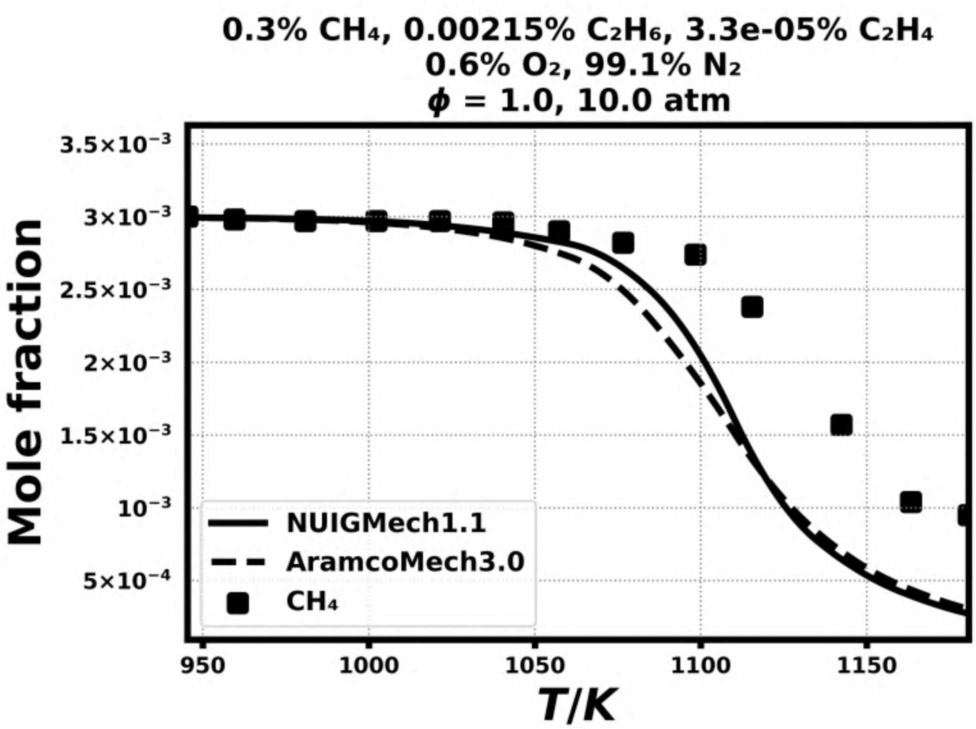

0.3% CH4, 0.00055% C2H6
1.2% O2, 98.5% N2
ϕ = 0.5, 10.0 atm
NUIGMech1.1
AramcoMech3.0
C2H2
Mole fraction
T/K

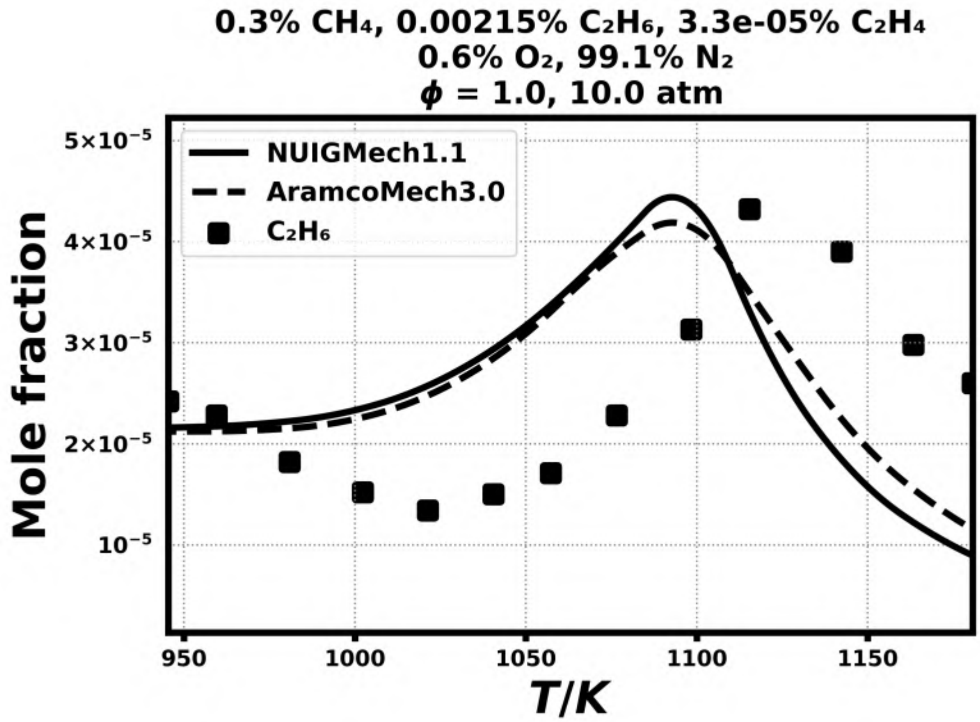

0.3% CH4, 0.00055% C2H6
1.2% O2, 98.5% N2
ϕ = 0.5, 10.0 atm
NUIGMech1.1
AramcoMech3.0
C2H4
Mole fraction
T/K

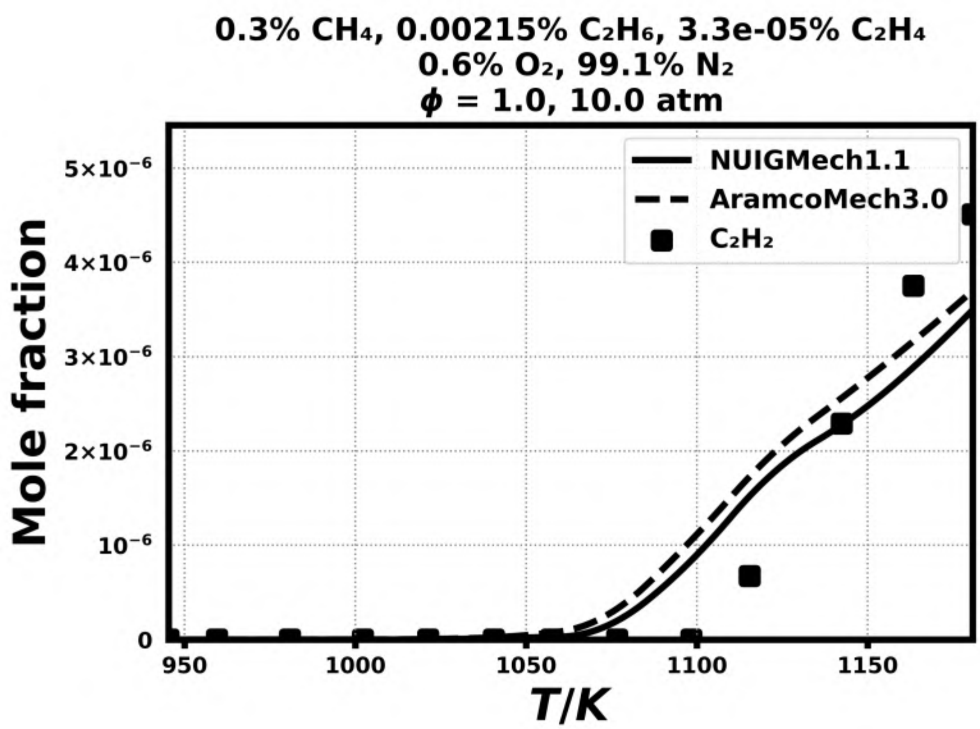

0.3% CH4, 0.00215% C2H6, 3.3e-05% C2H4
0.6% O2, 99.1% N2
ϕ = 1.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
H2
Mole fraction
T/K

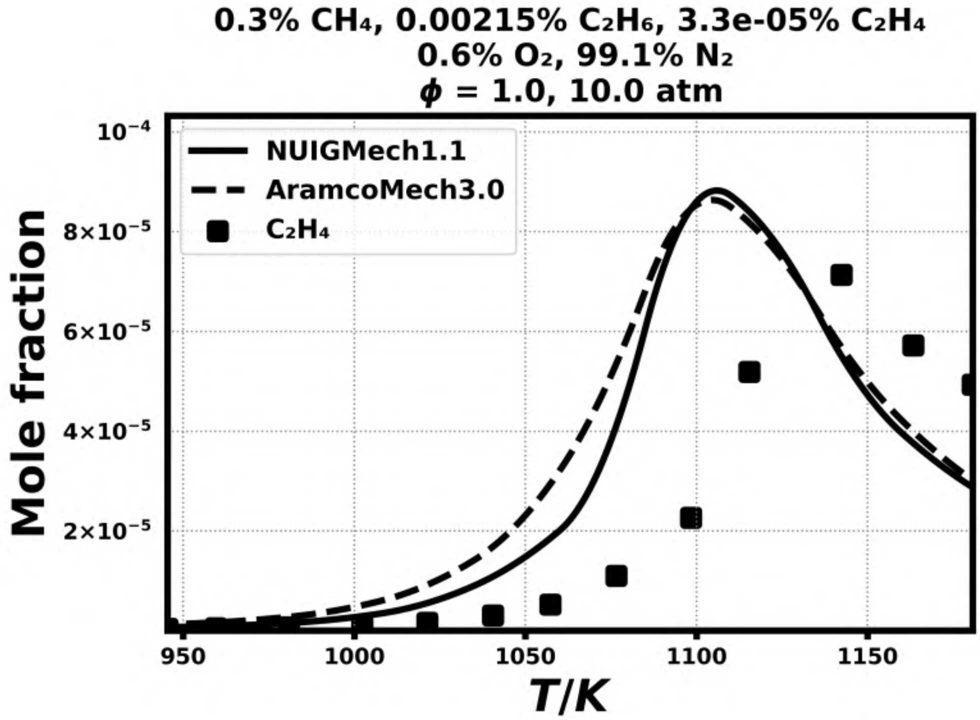

0.3% CH4, 0.00215% C2H6, 3.3e-05% C2H4
0.6% O2, 99.1% N2
ϕ = 1.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
T/K


0.3% CH₄, 0.00215% C₂H₆, 3.3e-05% C₂H₄
0.6% O₂, 99.1% N₂
ϕ = 1.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CO₂
Mole fraction
T/K


0.3% CH₄, 0.00215% C₂H₆, 3.3e-05% C₂H₄
0.6% O₂, 99.1% N₂
ϕ = 1.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CH₄
Mole fraction
T/K

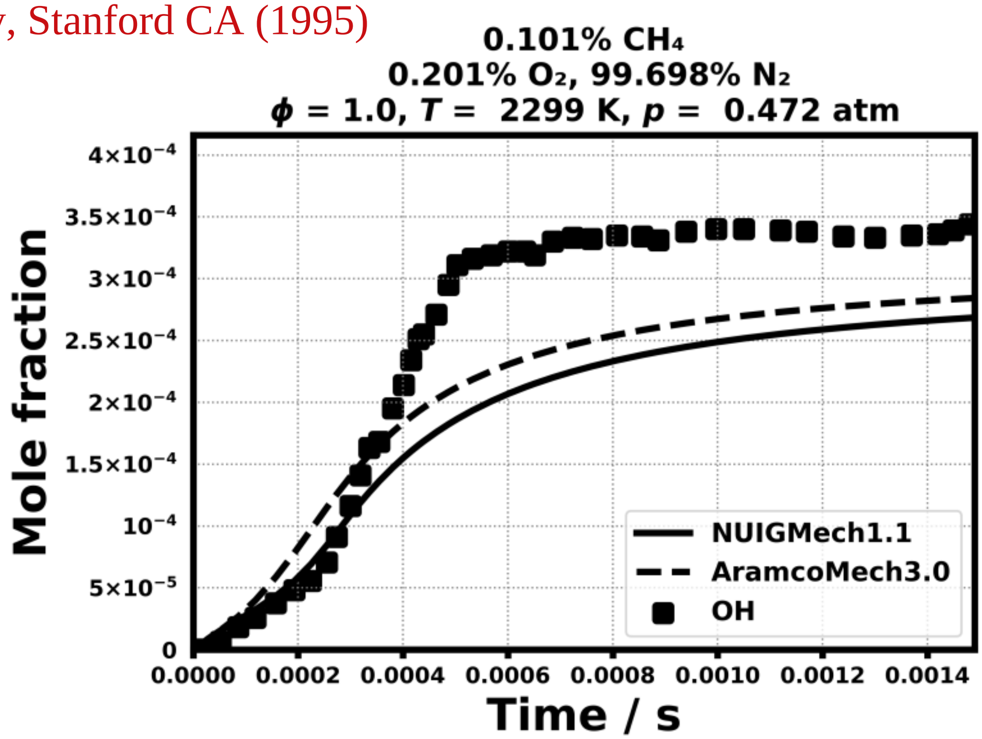

0.3% CH4, 0.00215% C2H6, 3.3e-05% C2H4
0.6% O2, 99.1% N2
ϕ = 1.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
C2H6
Mole fraction
5×10⁻⁵
4×10⁻⁵
3×10⁻⁵
2×10⁻⁵
10⁻⁵
950
1000
1050
1100
1150
T/K

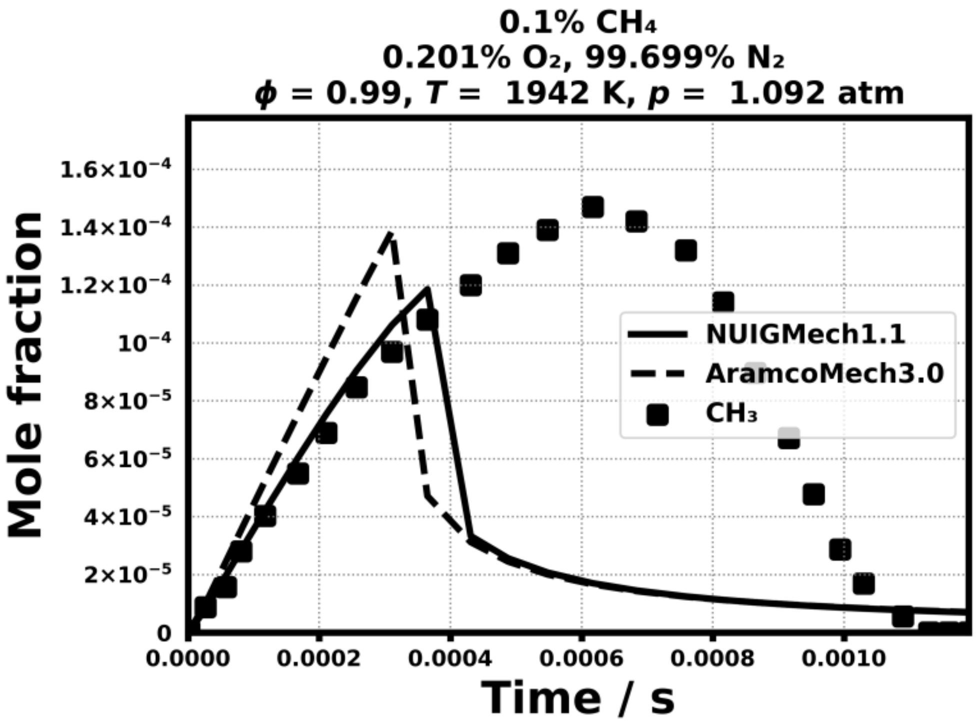

0.3% CH4, 0.00215% C2H6, 3.3e-05% C2H4
0.6% O2, 99.1% N2
ϕ = 1.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
C2H2
Mole fraction
5×10⁻⁶
4×10⁻⁶
3×10⁻⁶
2×10⁻⁶
10⁻⁶
0
950
1000
1050
1100
1150
T/K

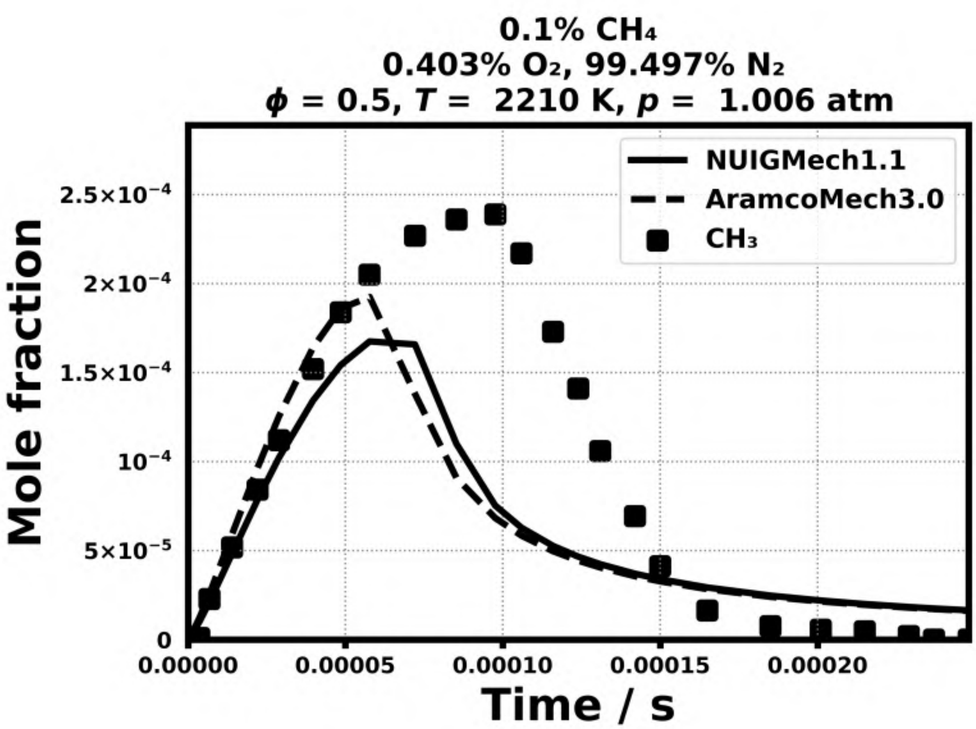


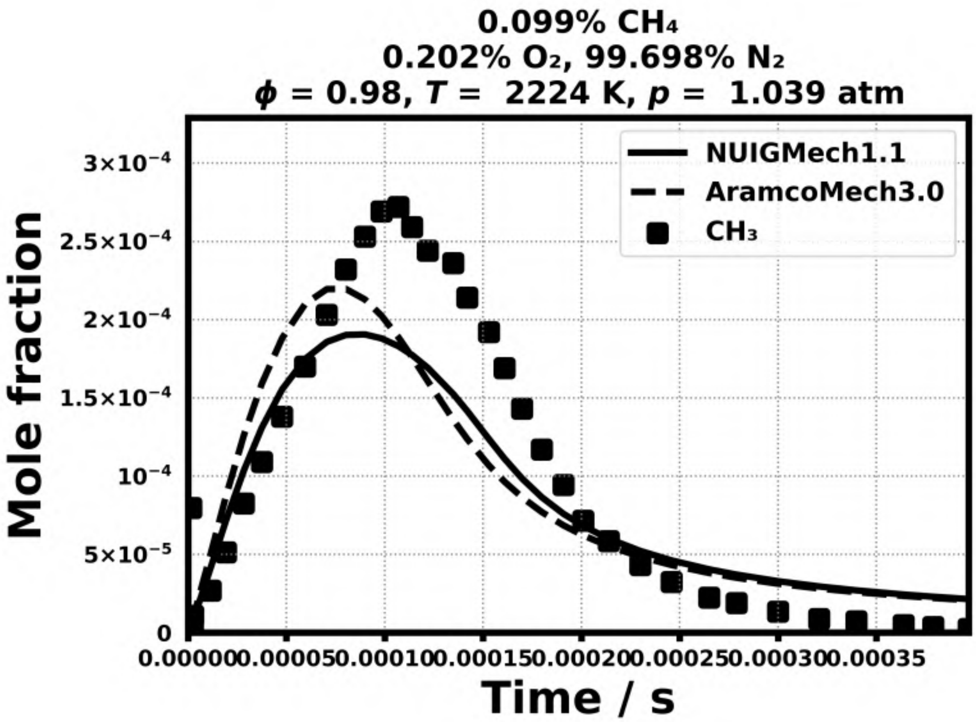
Speciation in Flow reactor

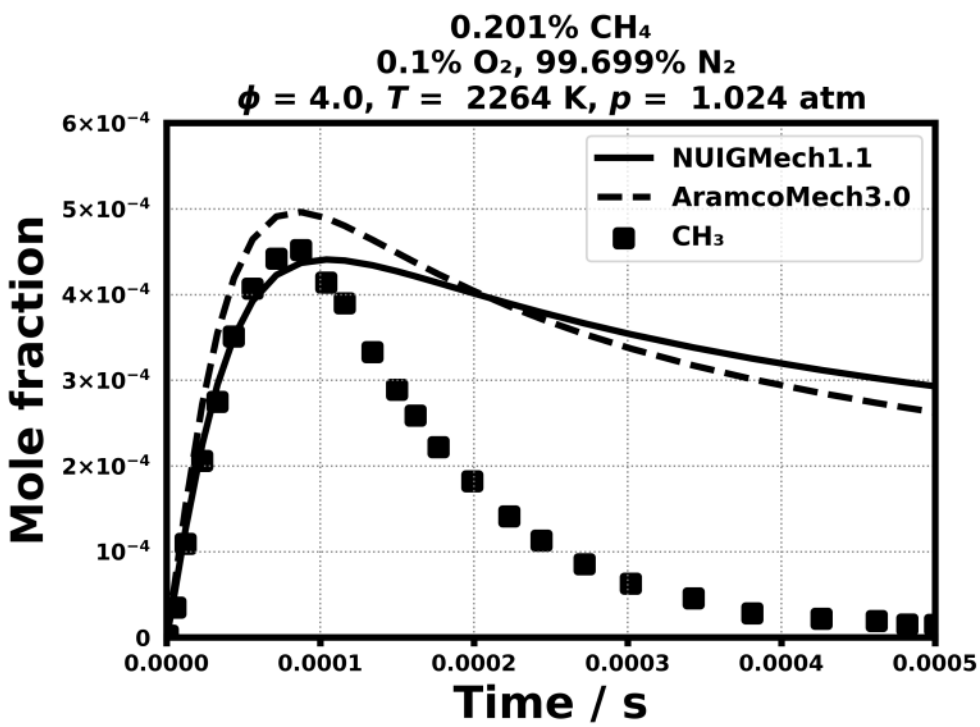
3.12) E.J.Chang, M. ENG. Thesis, Mechanical Engineering Department, Stanford University, Stanford CA (1995)



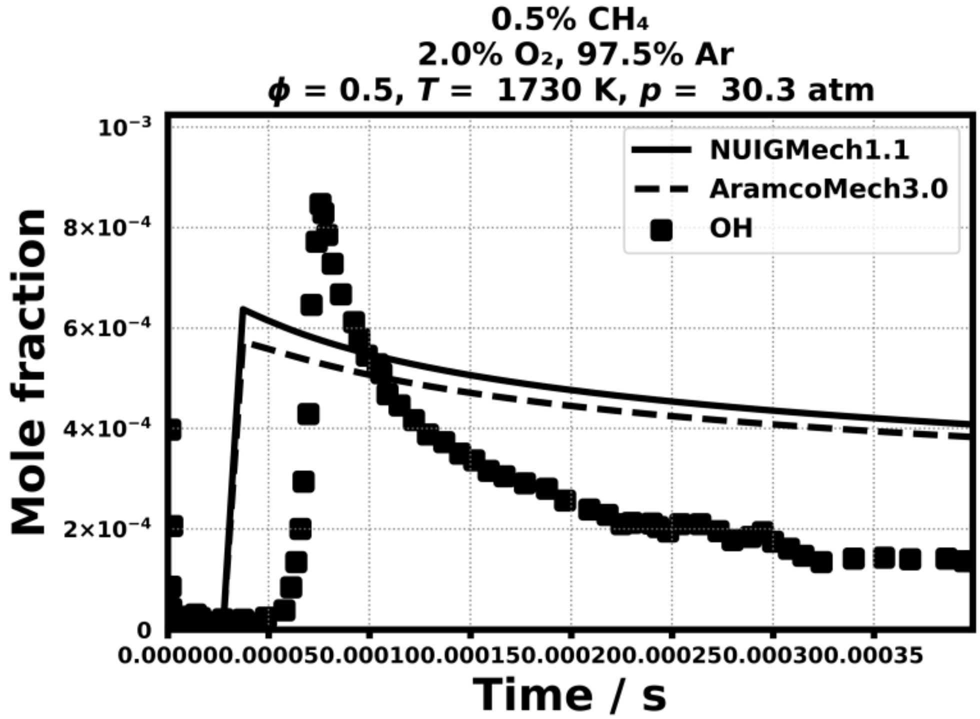

0.1% CH₄
0.201% O₂, 99.699% N₂
ϕ = 0.99, T = 1942 K, p = 1.092 atm
Mole fraction
Time / s
NUIGMech1.1
AramcoMech3.0
CH₃
1.6×10⁻⁴
1.4×10⁻⁴
1.2×10⁻⁴
10⁻⁴
8×10⁻⁵
6×10⁻⁵
4×10⁻⁵
2×10⁻⁵
0
0.0000
0.0002
0.0004
0.0006
0.0008
0.0010

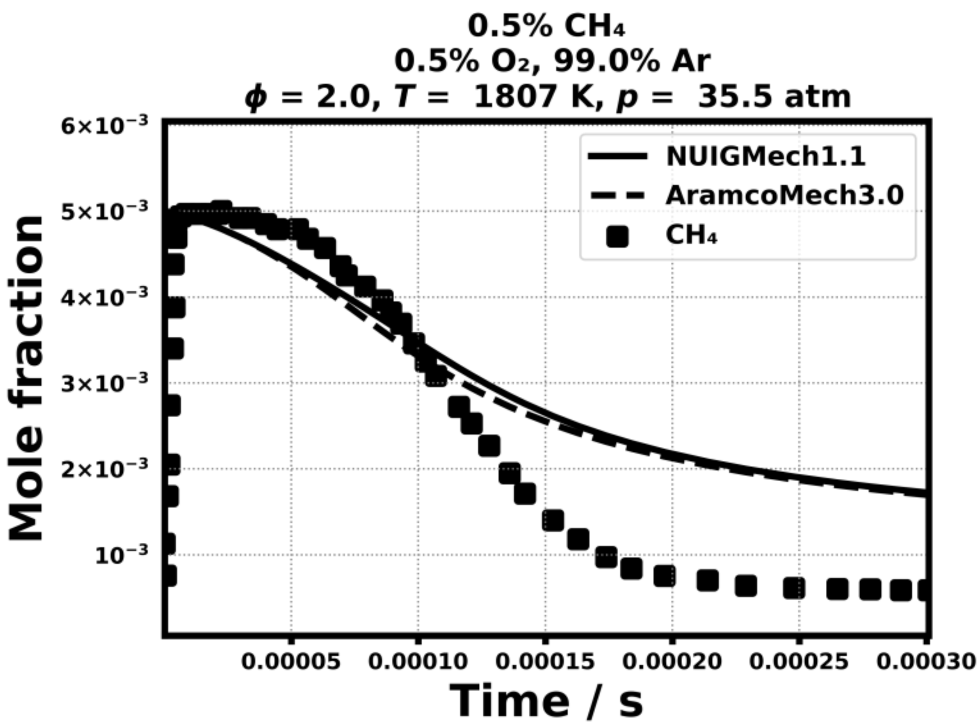

0.1% CH₄
0.403% O₂, 99.497% N₂
ϕ = 0.5, T = 2210 K, p = 1.006 atm
Mole fraction
Time / s
NUIGMech1.1
AramcoMech3.0
CH₃
2.5×10⁻⁴
2×10⁻⁴
1.5×10⁻⁴
10⁻⁴
5×10⁻⁵
0
0.00000
0.00005
0.00010
0.00015
0.00020


0.099% CH4
0.202% O2, 99.698% N2
ϕ = 0.98, T = 2224 K, p = 1.039 atm
NUIGMech1.1
AramcoMech3.0
CH3
Mole fraction
Time / s
3×10⁻⁴
2.5×10⁻⁴
2×10⁻⁴
1.5×10⁻⁴
10⁻⁴
5×10⁻⁵
0
0.00000
0.00005
0.00010
0.00015
0.00020
0.00025
0.00030
0.00035


0.201% CH4
0.1% O2, 99.699% N2
ϕ = 4.0, T = 2264 K, p = 1.024 atm
NUIGMech1.1
AramcoMech3.0
CH3
Mole fraction
Time / s
6×10⁻⁴
5×10⁻⁴
4×10⁻⁴
3×10⁻⁴
2×10⁻⁴
10⁻⁴
0
0.0000
0.0001
0.0002
0.0003
0.0004
0.0005

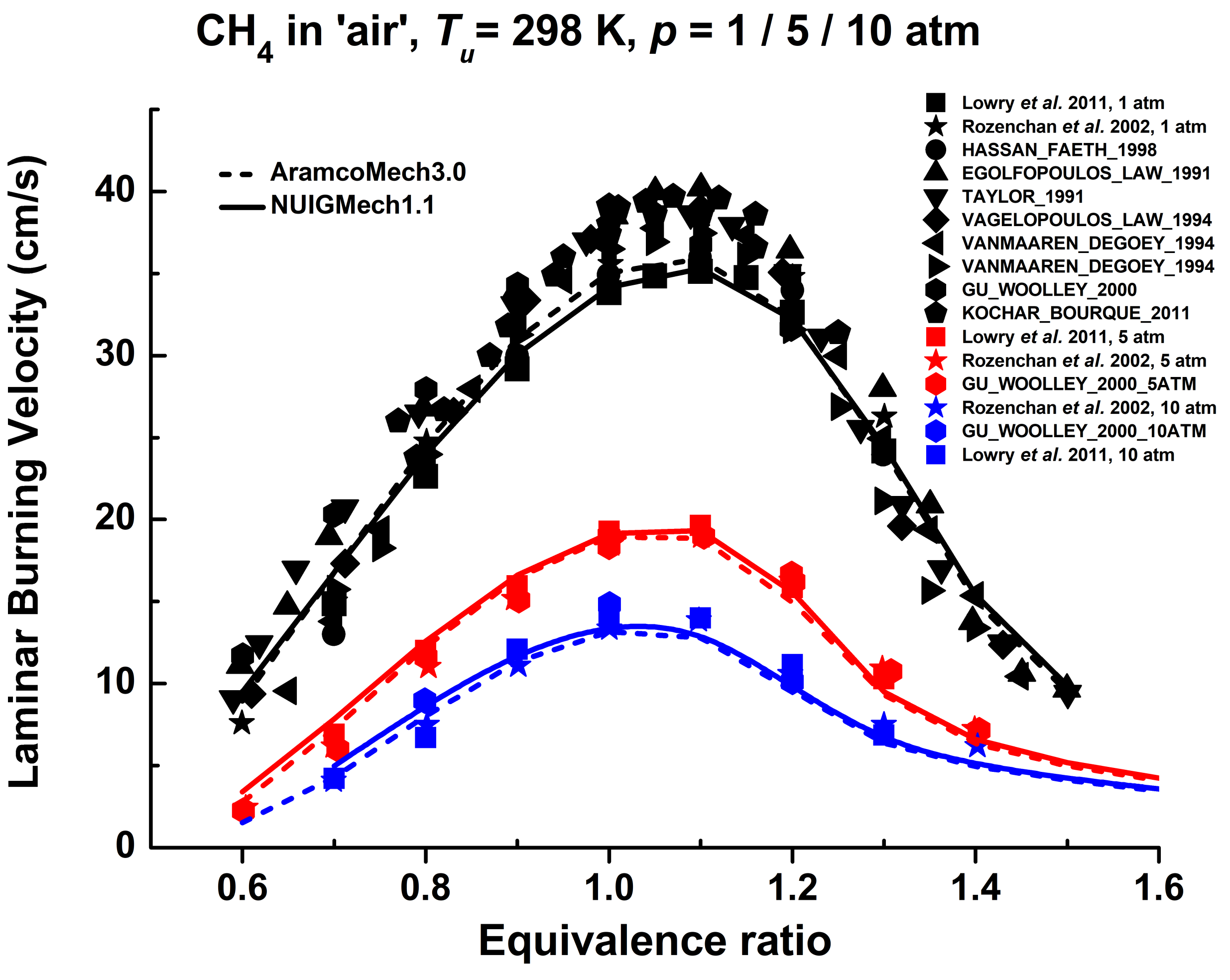
3.13) Petersen, E. L., Röhrig, M., Davidson, D. F., Hanson, R. K., & Bowman, C. T., In Symposium (International) on Combustion, 26 (1996, January) 799-806





Laminar flame speed

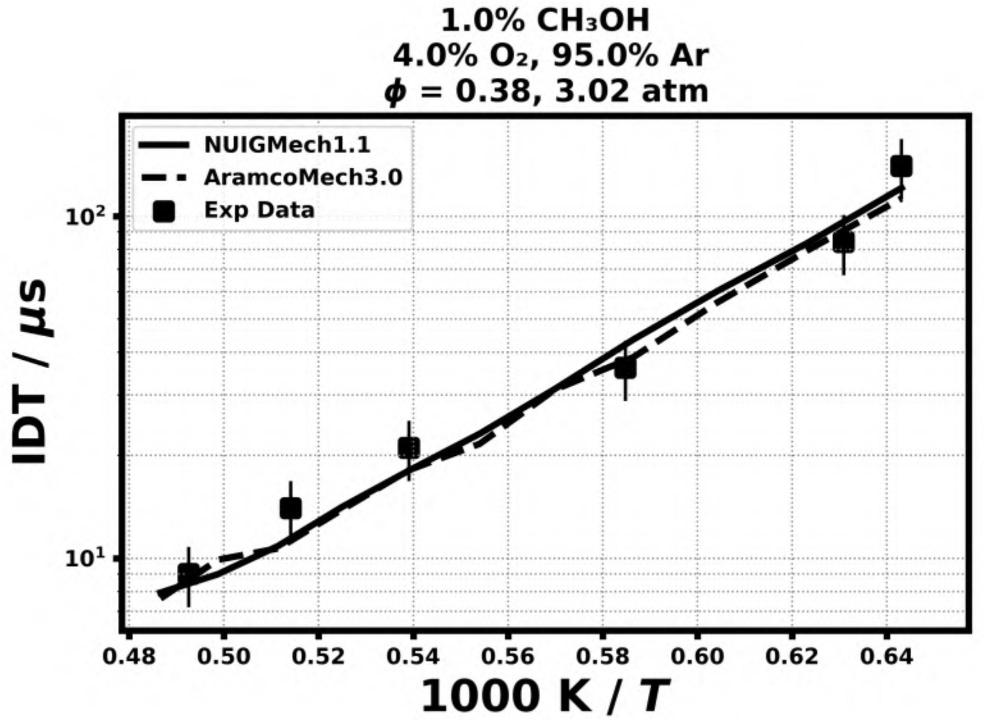
3.14) Gu, X. J., Haq, M. Z., Lawes, M., & Woolley, R., Combustion and flame, 121(1-2) (2000) 41-58.
3.15) Rozenchan, G., Zhu, D. L., Law, C. K., & Tse, S. D., Proceedings of the Combustion Institute, 29(2) (2002) 1461-1470.
3.16) Hassan, M. I., Aung, K. T., & Faeth, G. M., Combustion and flame, 115(4) (1998) 539-550..
3.17) Zhu, D. L., Egolfopoulos, F. N., & Law, C. K., In Symposium (International) on Combustion,22, (1989, January) 1537-1545
3.18) Lowry, W., de Vries, J., Krejci, M., Petersen, E., Serinyel, Z., Metcalfe, W., Bourque, G., Jornal of Engineering for Gas Turbines and Power, 133(9) (2011).
3.19) Egolfopoulos, F. N., Zhu, D. L., & Law, C. K., In Symposium (International) on Combustion, 23 (1991, January) 471-478.
3.20) S. Taylor, PhD diss., University of Leeds, 1991.
3.21) Vagelopoulos, C. M., Egolfopoulos, F. N., & Law, C. K., In Symposium (international) on combustion, 25 (1994, January) 1341-1347
3.22) Van Maaren, A., Thung, D. S., & DE GOEY, L. R. H., Combustion Science and Technology, 96(4-6) (1994) 327-344.
3.23) U. Kochar, Turbo Expo: Power for Land, Sea, and Air (Vol. 54624 (2011) 129-140.

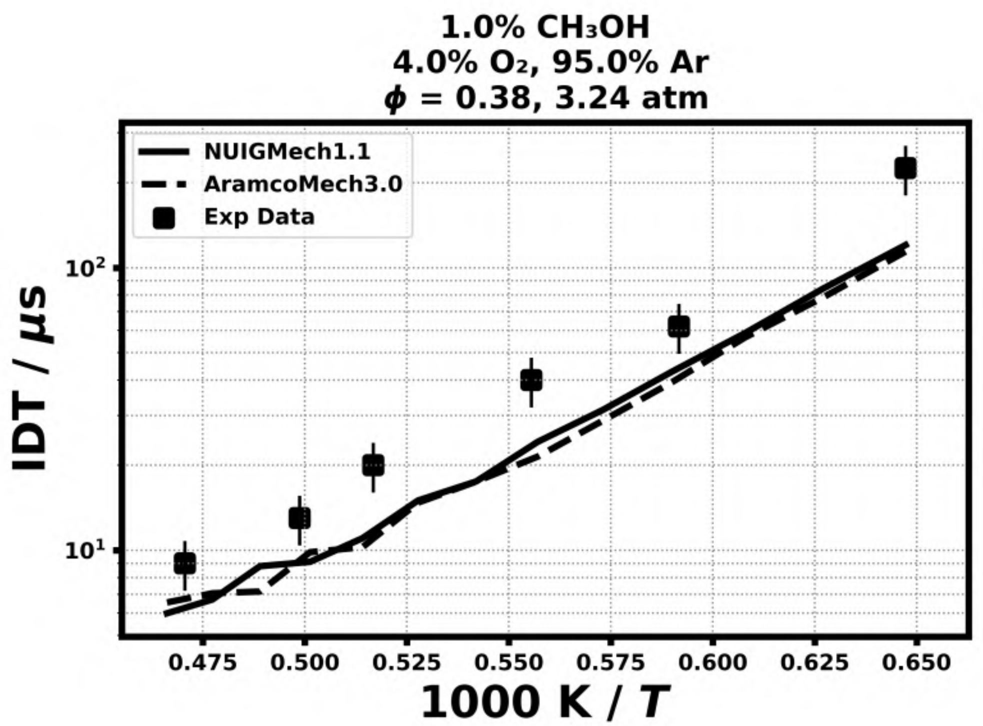


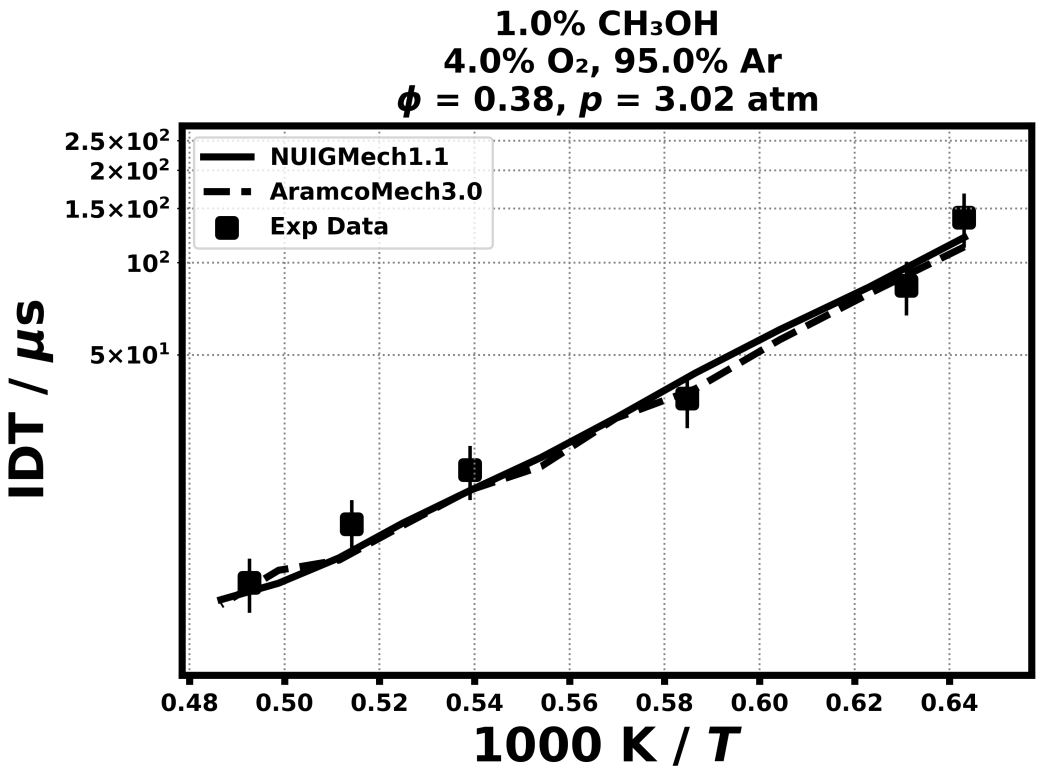
4. Validation for CH_3OH

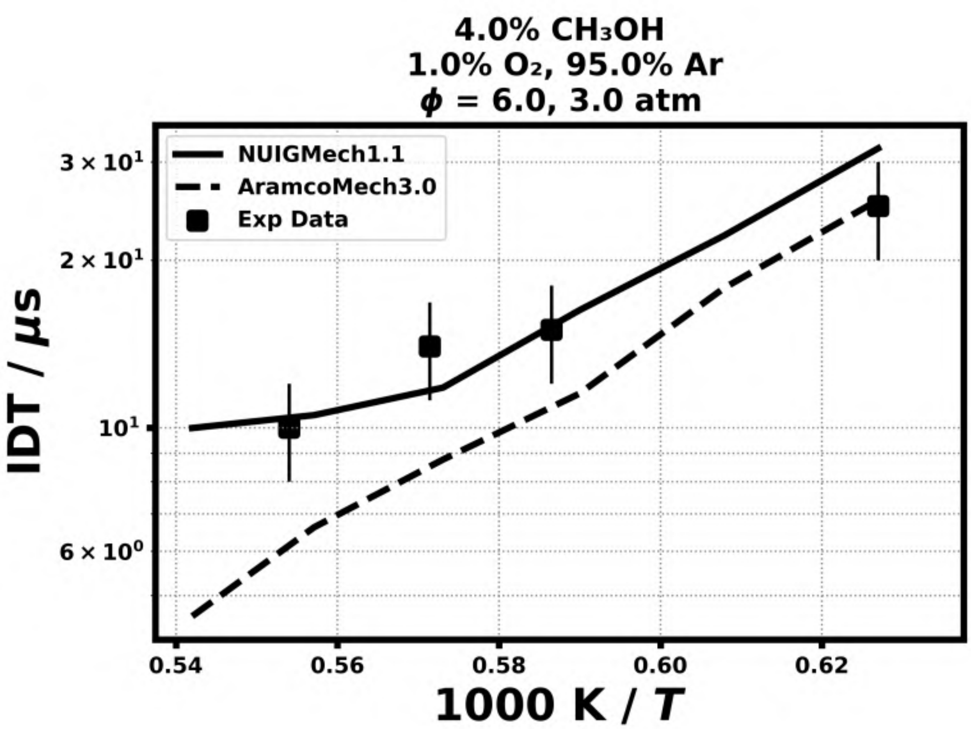
Shock tube ignition delay time

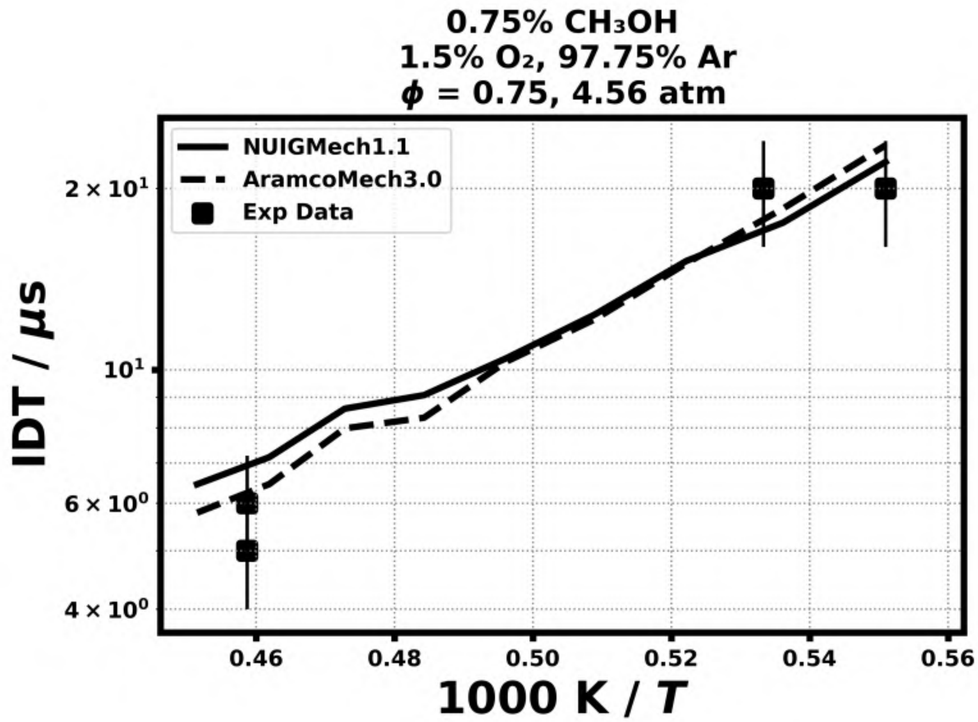
4.1) Bowman, C. T., Combustion and Flame 25 (1975) 343-354.

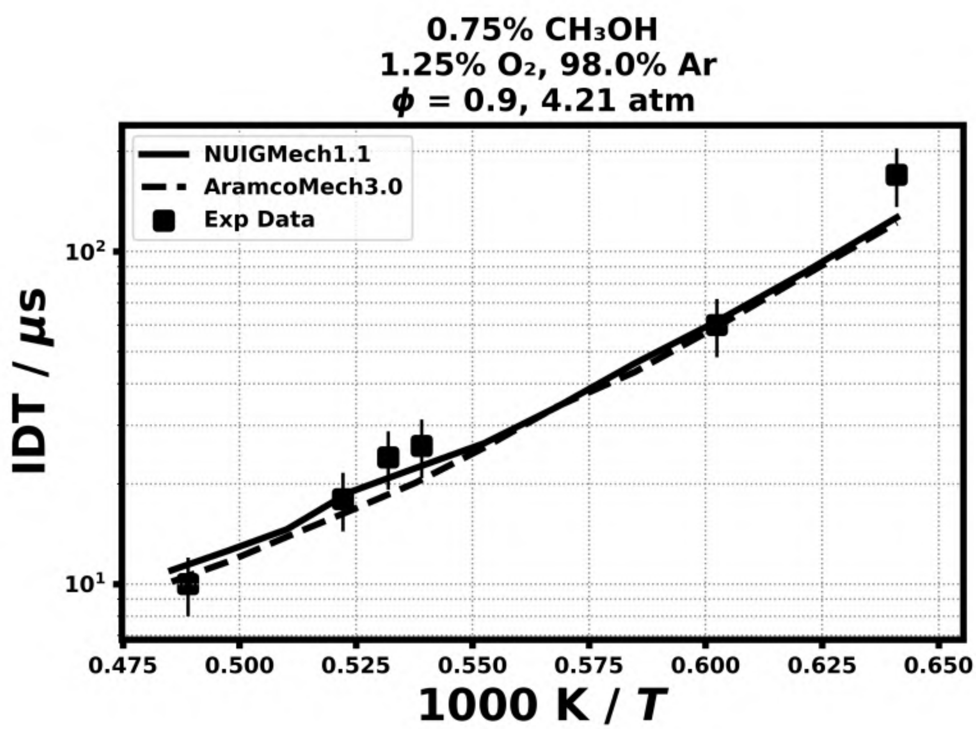




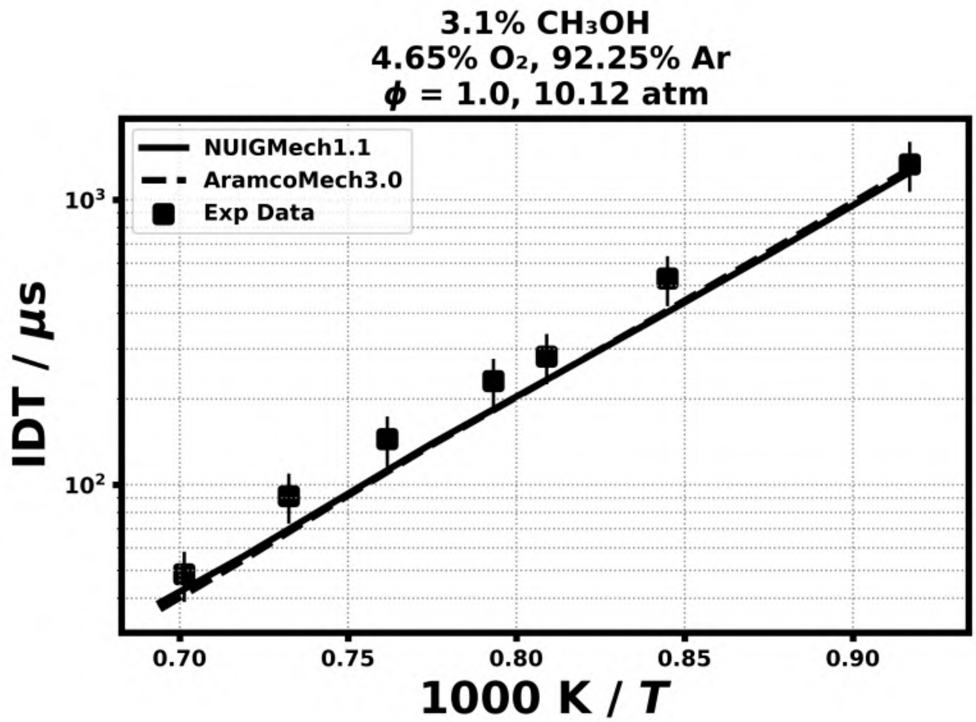

1.0% CH₃OH
4.0% O₂, 95.0% Ar
ϕ = 0.38, p = 3.02 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
2.5×10²
2×10²
1.5×10²
10²
5×10¹
0.48
0.50
0.52
0.54
0.56
0.58
0.60
0.62
0.64

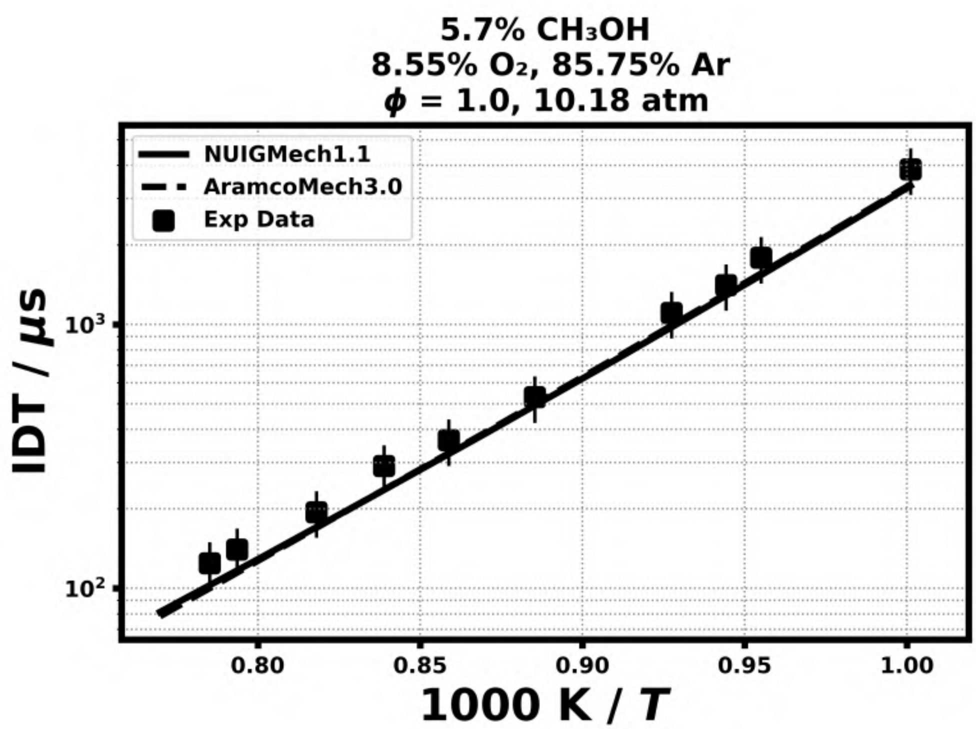

4.0% CH₃OH
1.0% O₂, 95.0% Ar
ϕ = 6.0, 3.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
3 × 10¹
2 × 10¹
10¹
6 × 10⁰
0.54
0.56
0.58
0.60
0.62

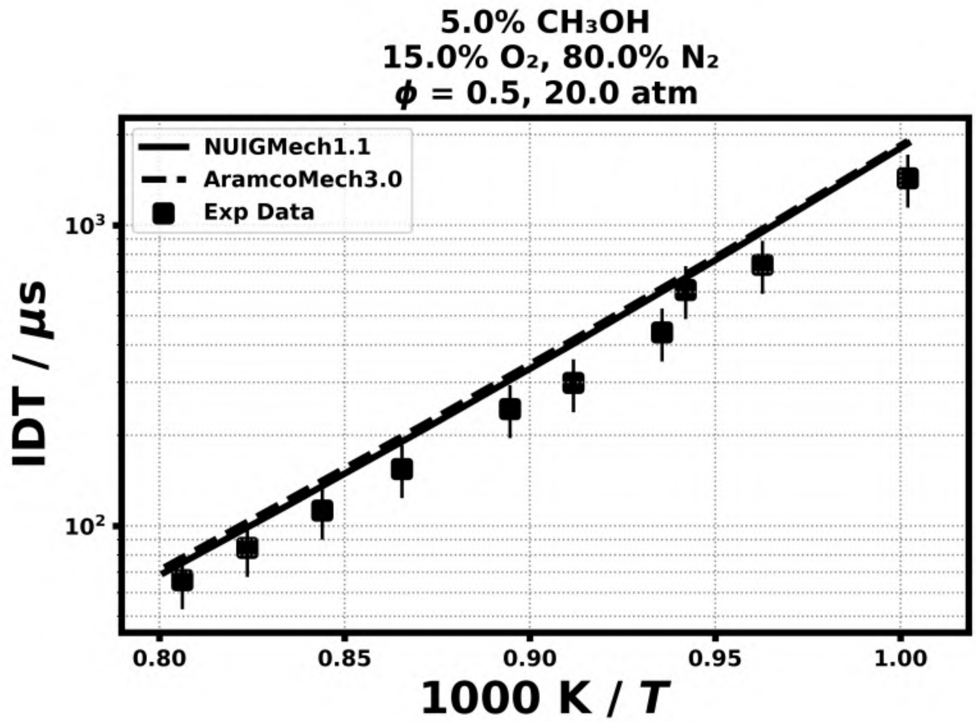

0.75% CH₃OH
1.5% O₂, 97.75% Ar
ϕ = 0.75, 4.56 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
2 × 10¹
10¹
6 × 10⁰
4 × 10⁰
0.46
0.48
0.50
0.52
0.54
0.56
1000 K / T

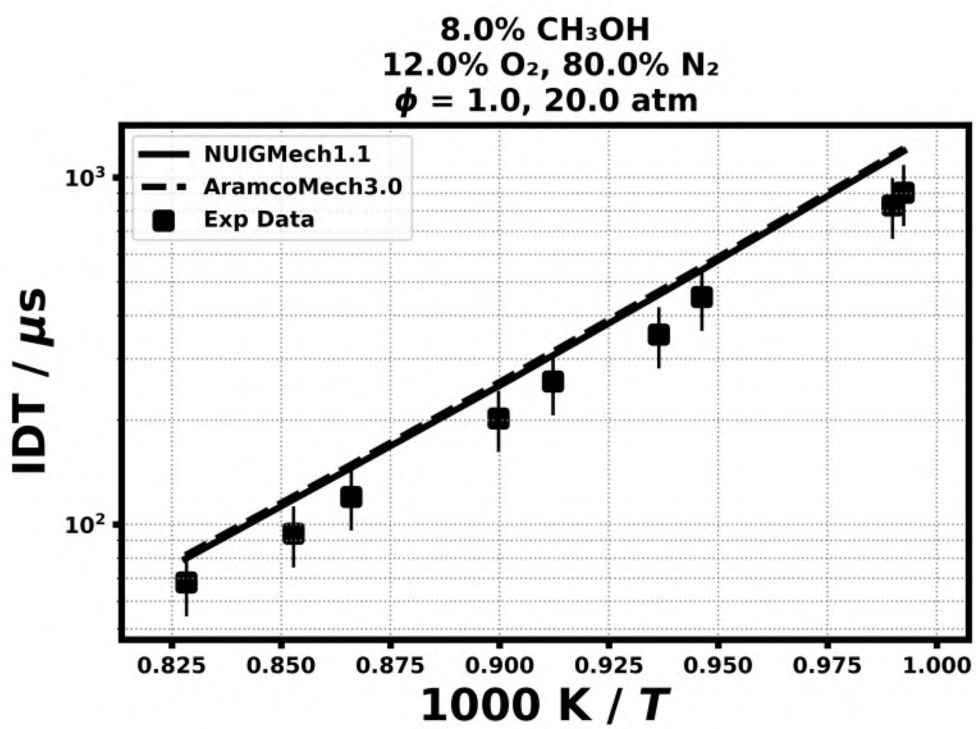

0.75% CH₃OH
1.25% O₂, 98.0% Ar
ϕ = 0.9, 4.21 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10²
10¹
0.475
0.500
0.525
0.550
0.575
0.600
0.625
0.650
1000 K / T

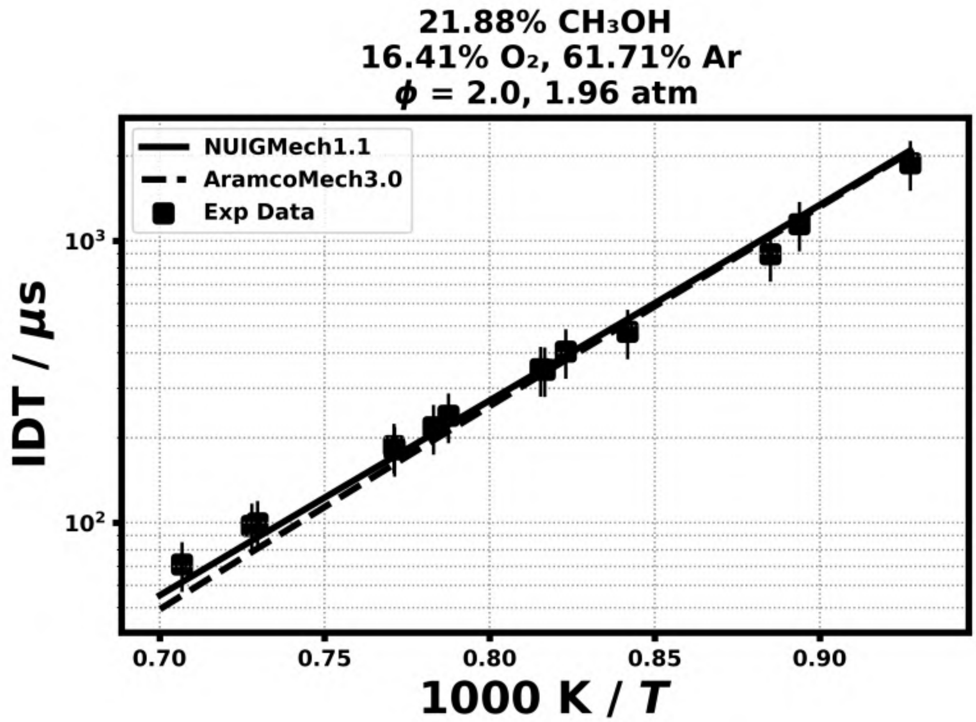
4.2) Burke, U., Metcalfe, W. K., Burke, S. M., Heufer, K. A., Dagaut, P., & Curran, H. J. Combustion and Flame, 165 (2016) 125-136.

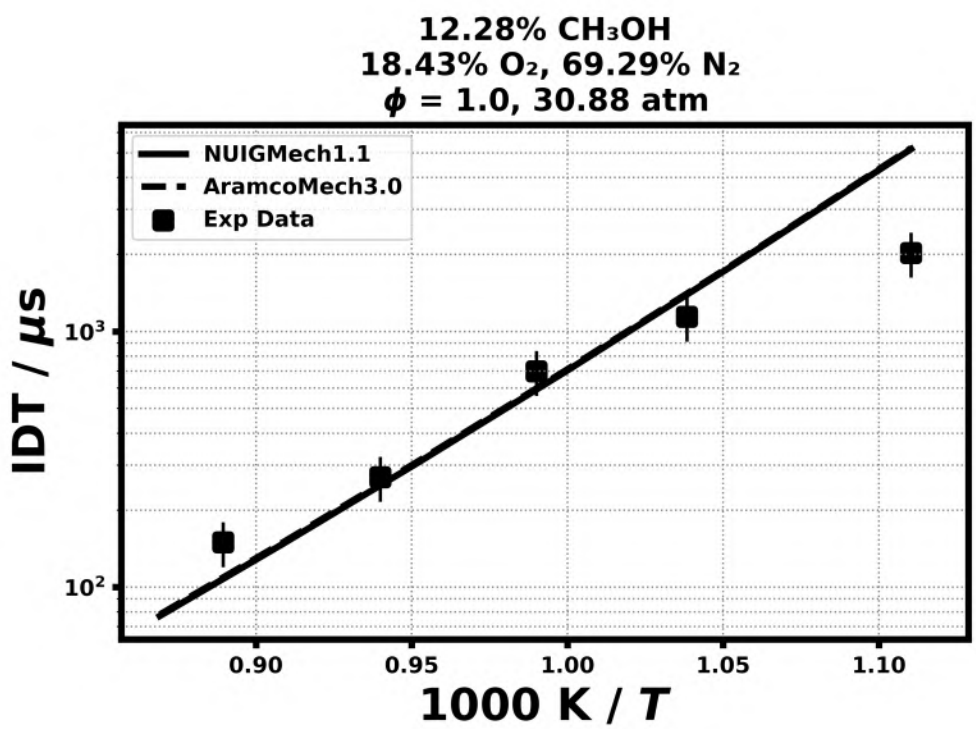


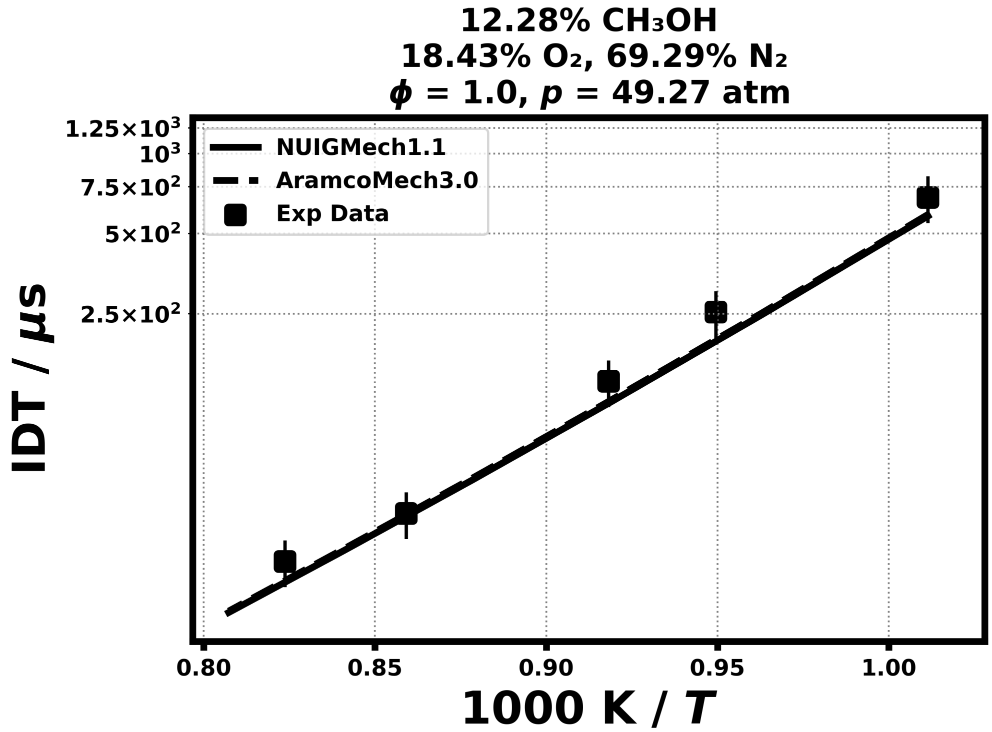


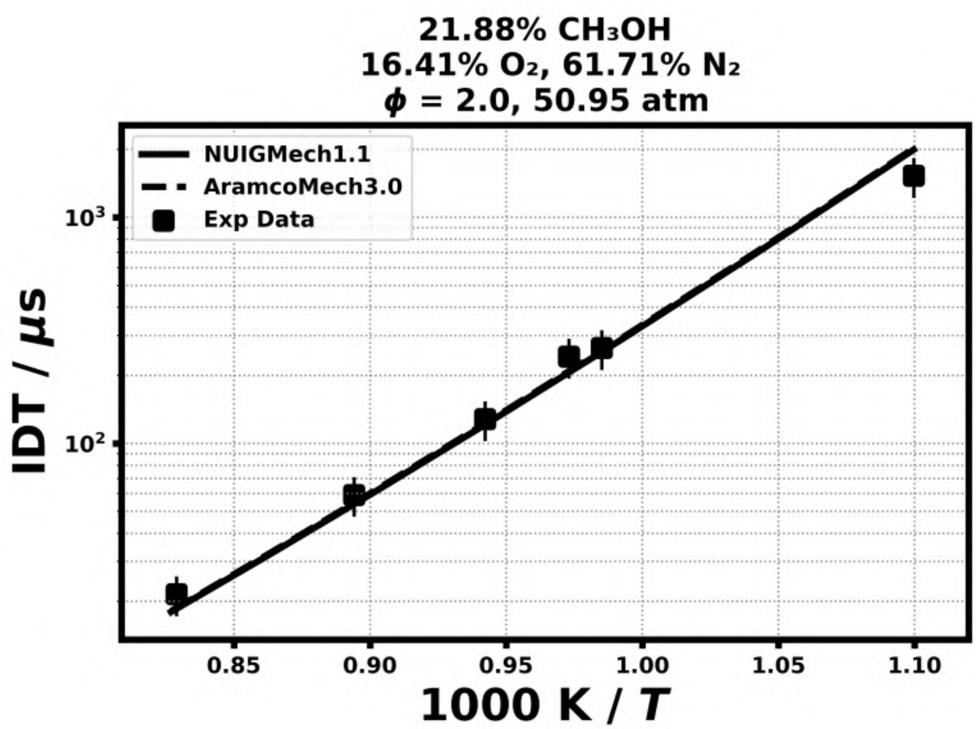

5.0% CH₃OH
15.0% O₂, 80.0% N₂
ϕ = 0.5, 20.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.80
0.85
0.90
0.95
1.00
1000 K / T

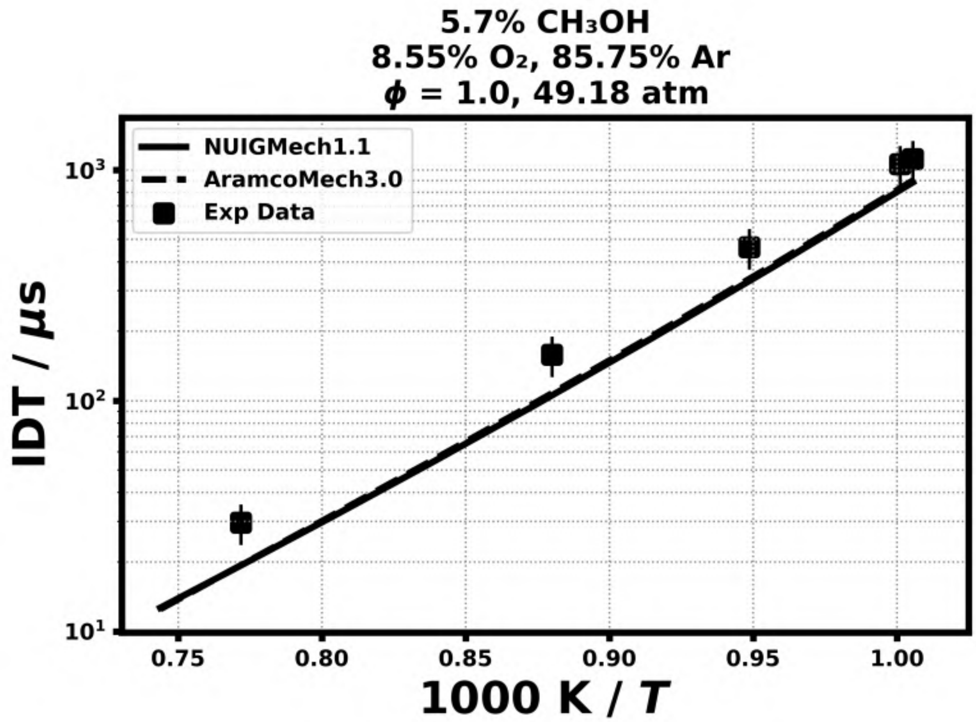

8.0% CH₃OH
12.0% O₂, 80.0% N₂
ϕ = 1.0, 20.0 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.825
0.850
0.875
0.900
0.925
0.950
0.975
1.000
1000 K / T

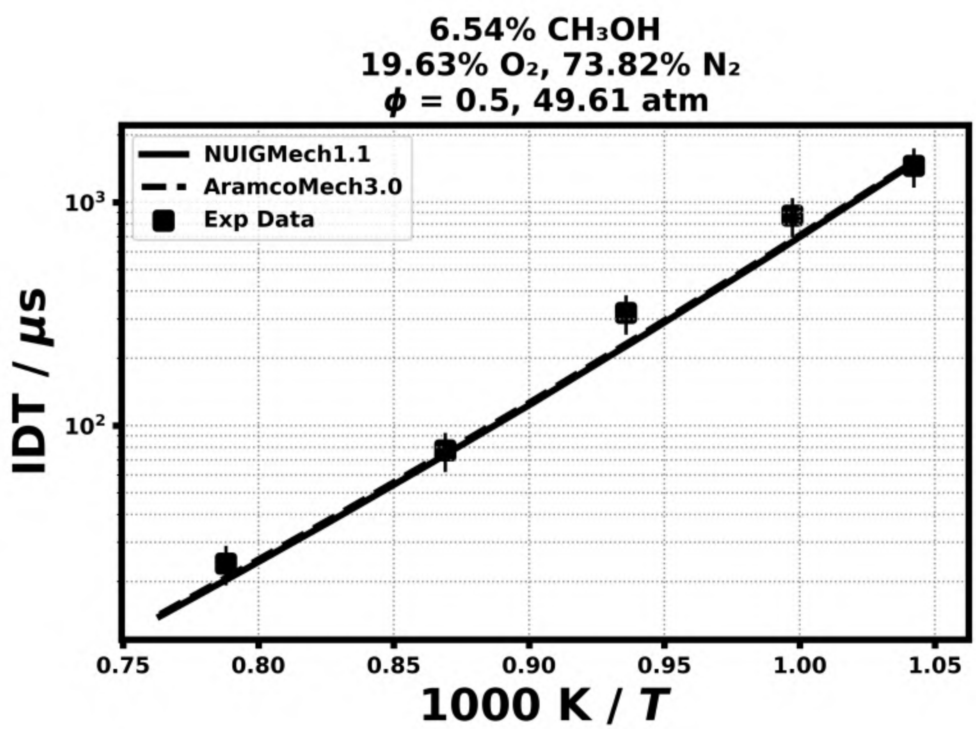

21.88% CH3OH
16.41% O2, 61.71% Ar
ϕ = 2.0, 1.96 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.70
0.75
0.80
0.85
0.90
1000 K / T


12.28% CH3OH
18.43% O2, 69.29% N2
ϕ = 1.0, 30.88 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.90
0.95
1.00
1.05
1.10
1000 K / T

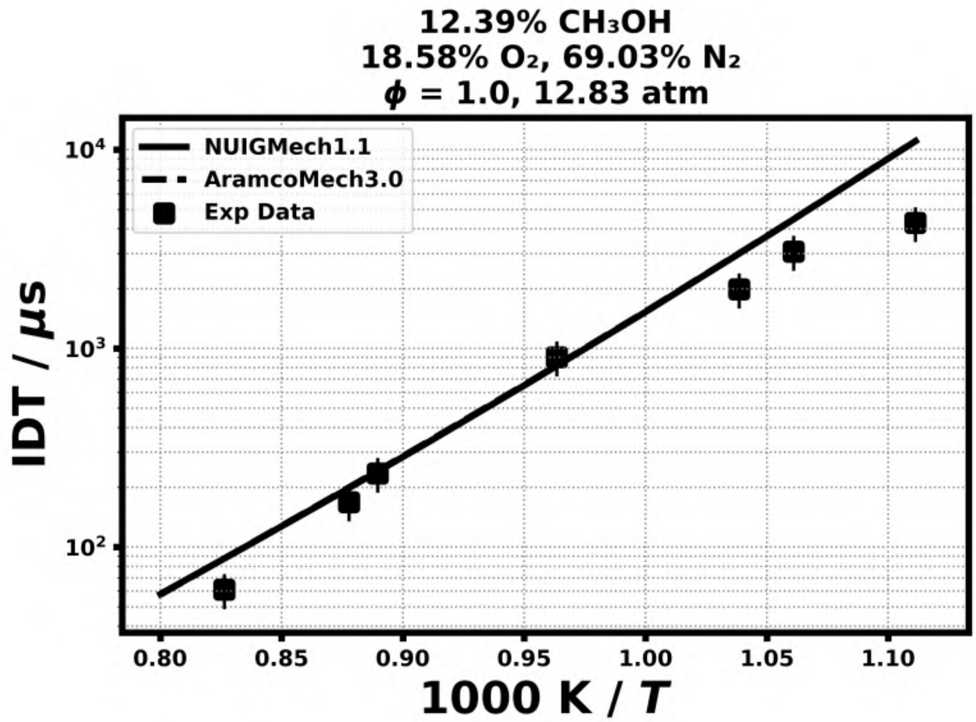

12.28% CH₃OH
18.43% O₂, 69.29% N₂
ϕ = 1.0, p = 49.27 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1.25×10³
10³
7.5×10²
5×10²
2.5×10²
0.80
0.85
0.90
0.95
1.00
1000 K / T

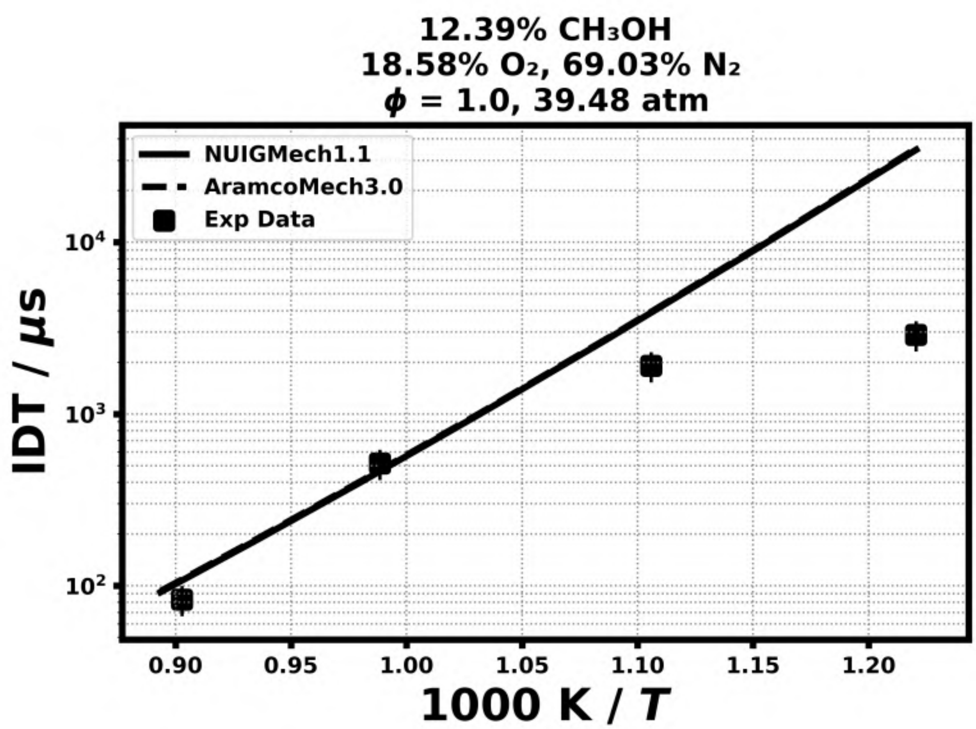

21.88% CH₃OH
16.41% O₂, 61.71% N₂
ϕ = 2.0, 50.95 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.85
0.90
0.95
1.00
1.05
1.10
1000 K / T


5.7% CH₃OH
8.55% O₂, 85.75% Ar
ϕ = 1.0, 49.18 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
10¹
0.75
0.80
0.85
0.90
0.95
1.00
1000 K / T

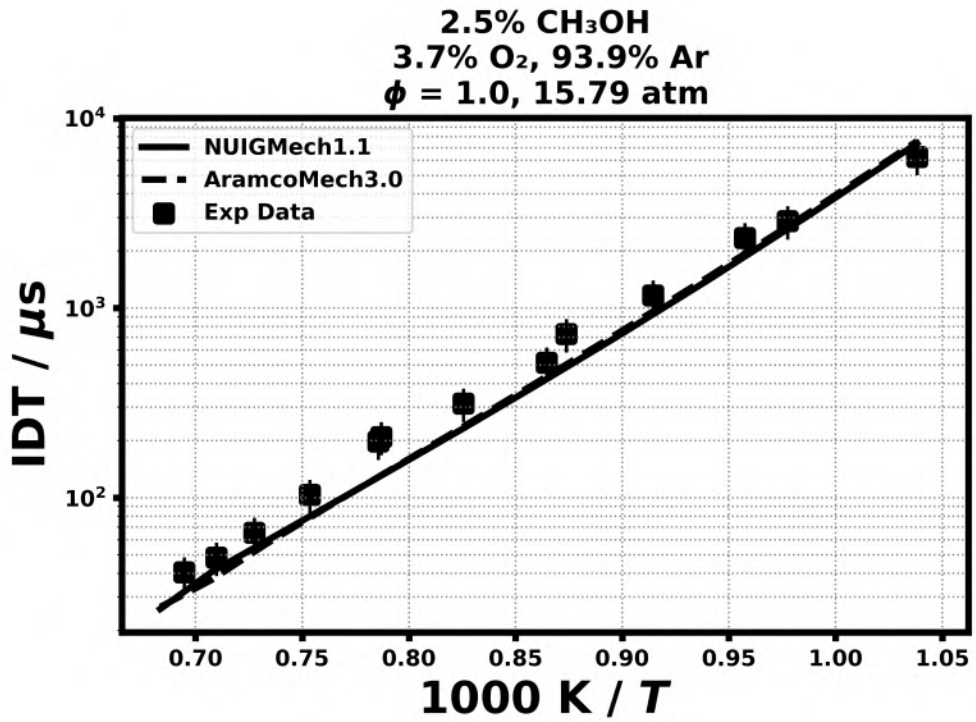

6.54% CH₃OH
19.63% O₂, 73.82% N₂
ϕ = 0.5, 49.61 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.75
0.80
0.85
0.90
0.95
1.00
1.05
1000 K / T

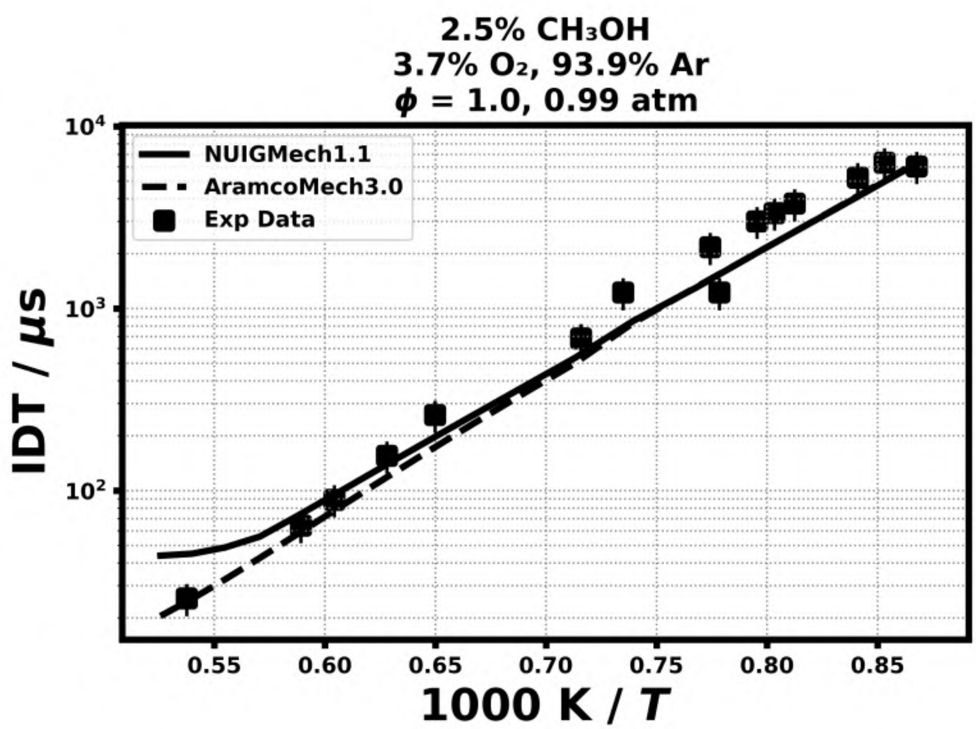
4.3) Fieweger, K., Blumenthal, R., & Adomeit, G., Combustion and Flame, 109(4) (1997) 599-619.

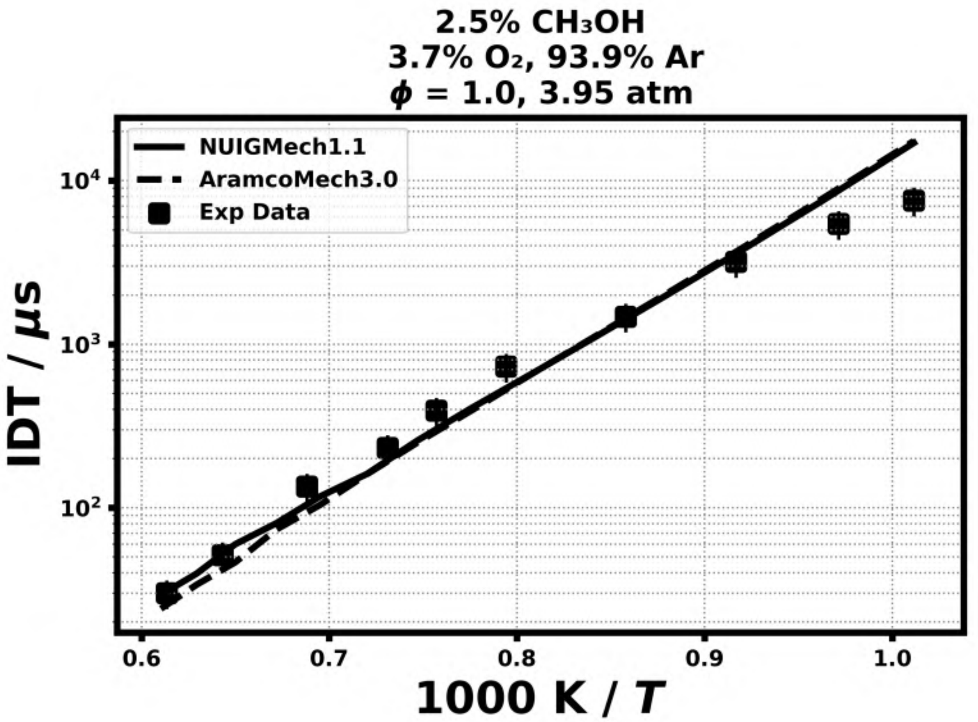




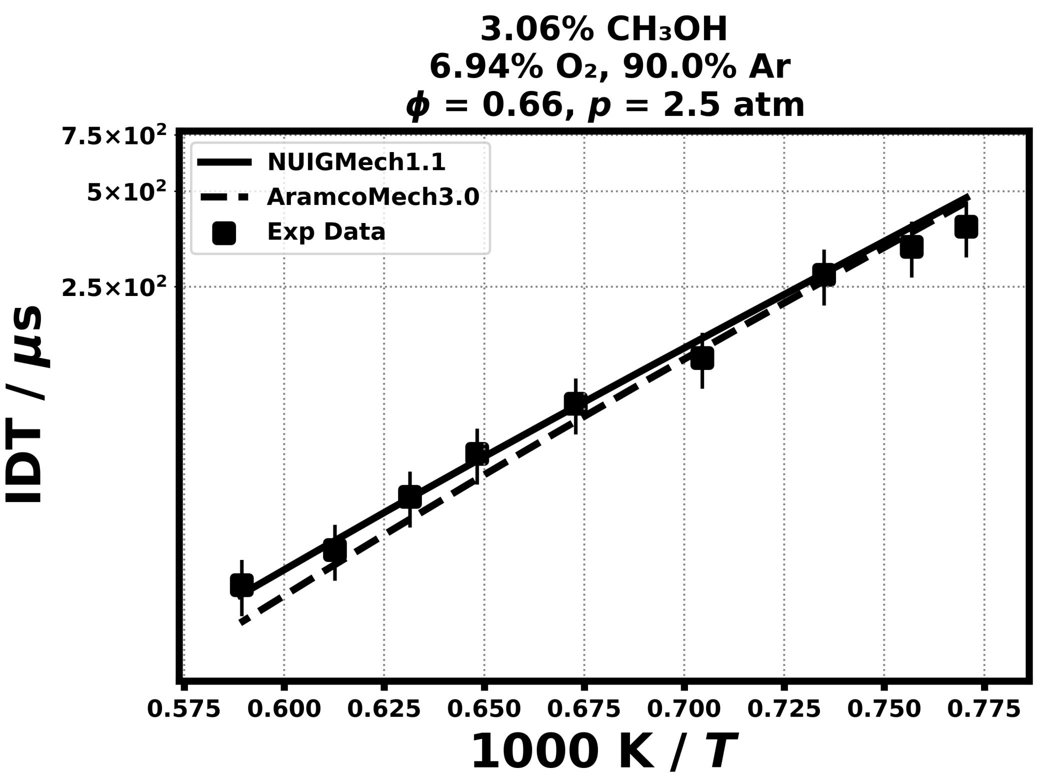
4.4) J. Herzler, European Combust. Meeting, Lund Sweden, 2013

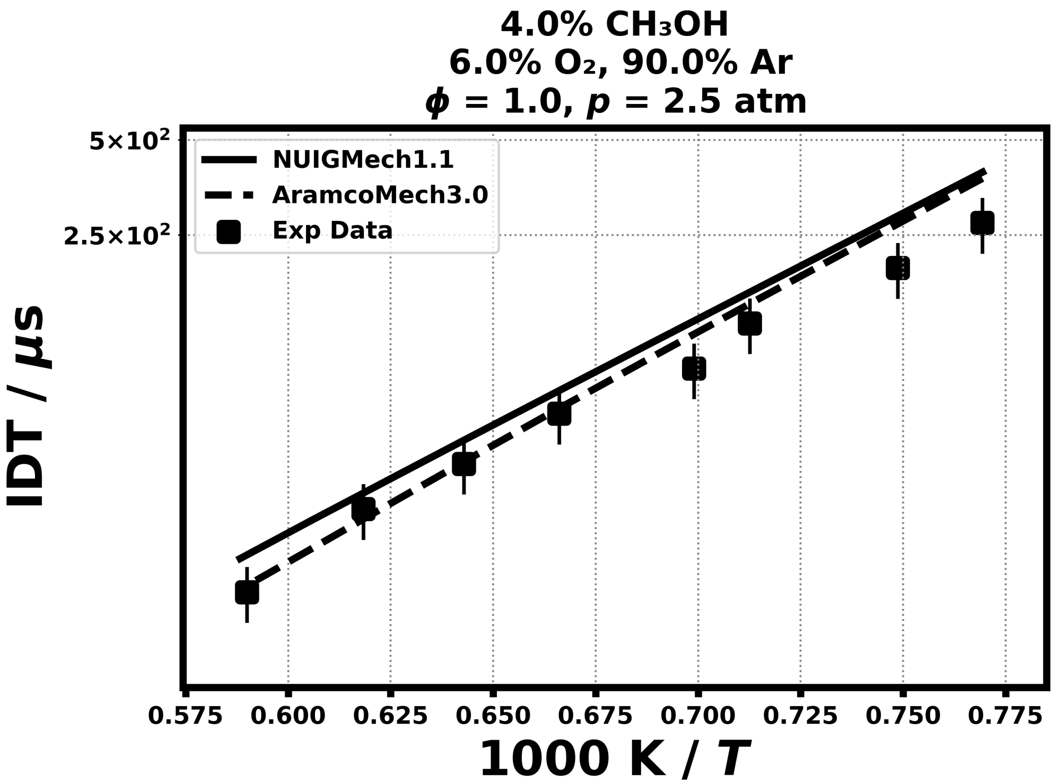


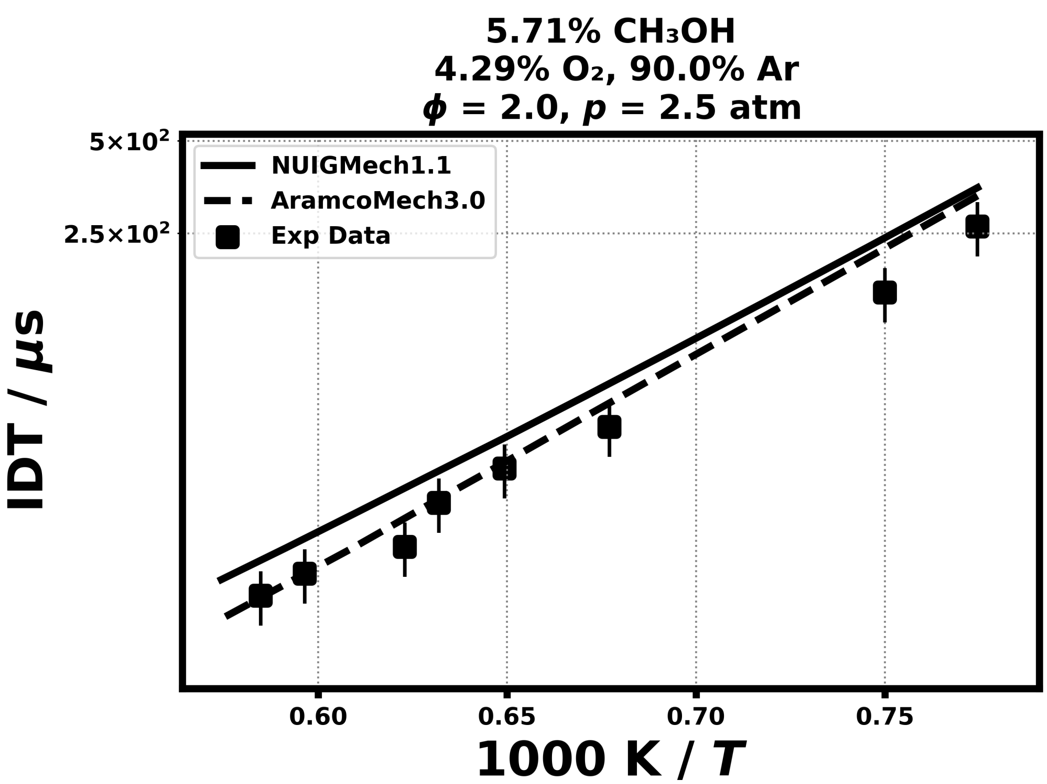




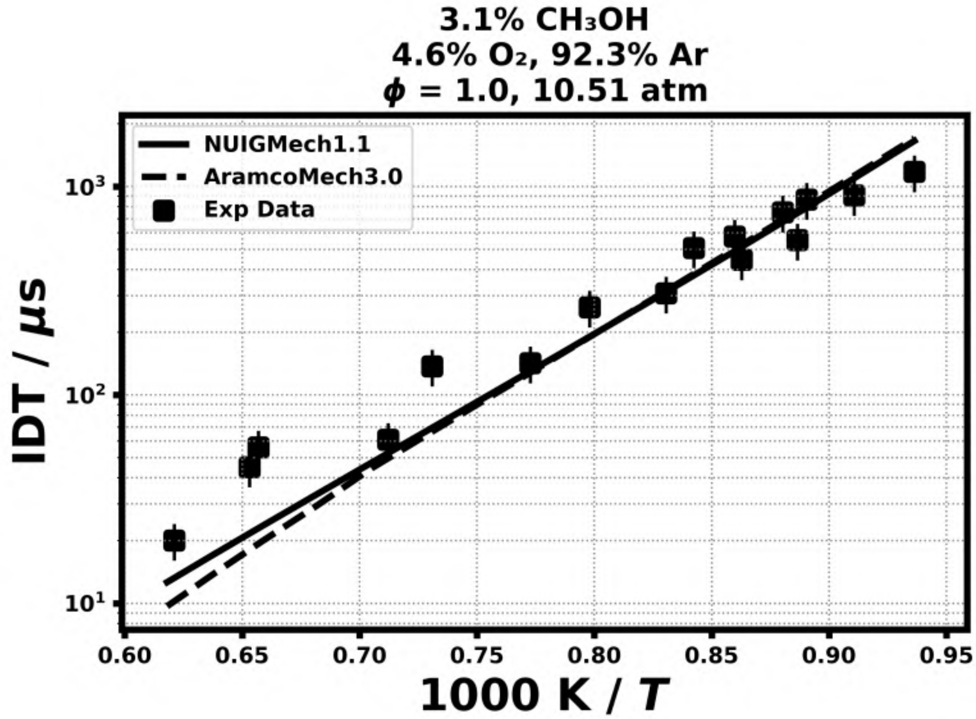
4.5) Natarajan, K., & Bhaskaran, K. A., Combustion and Flame, 43 (1981) 35-49.

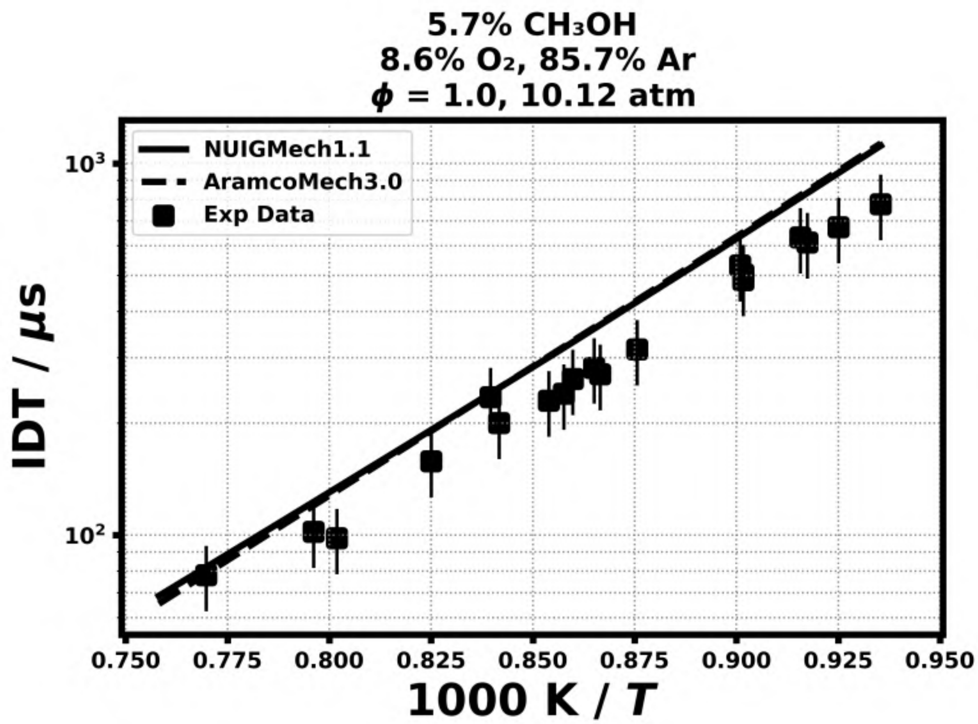


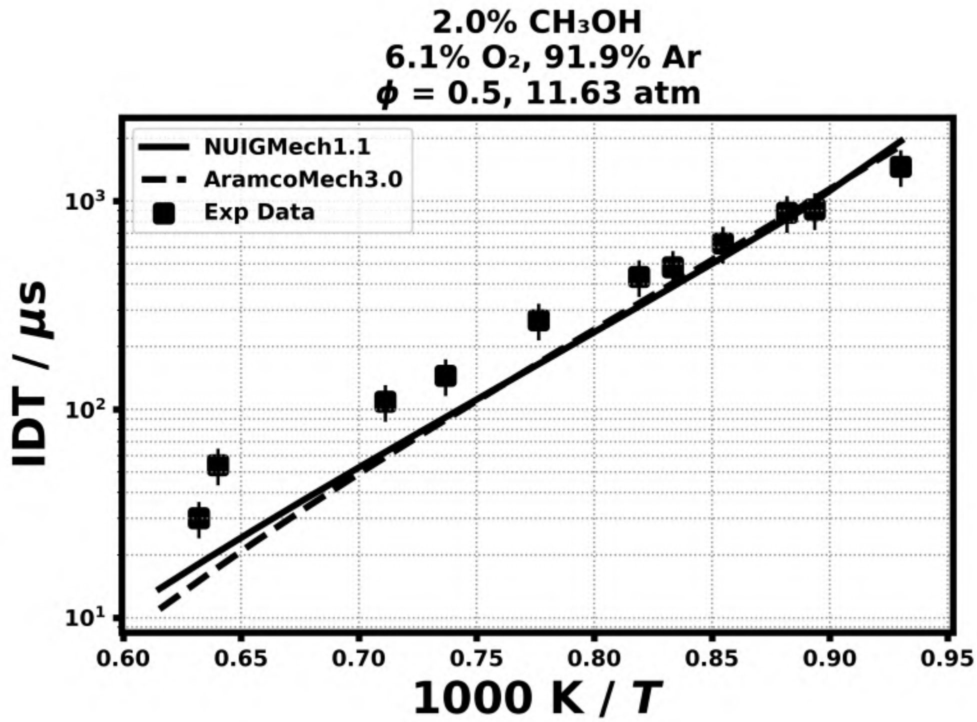

4.0% CH₃OH
6.0% O₂, 90.0% Ar
ϕ = 1.0, p = 2.5 atm
5×10²
2.5×10²
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
0.575
0.600
0.625
0.650
0.675
0.700
0.725
0.750
0.775
1000 K / T

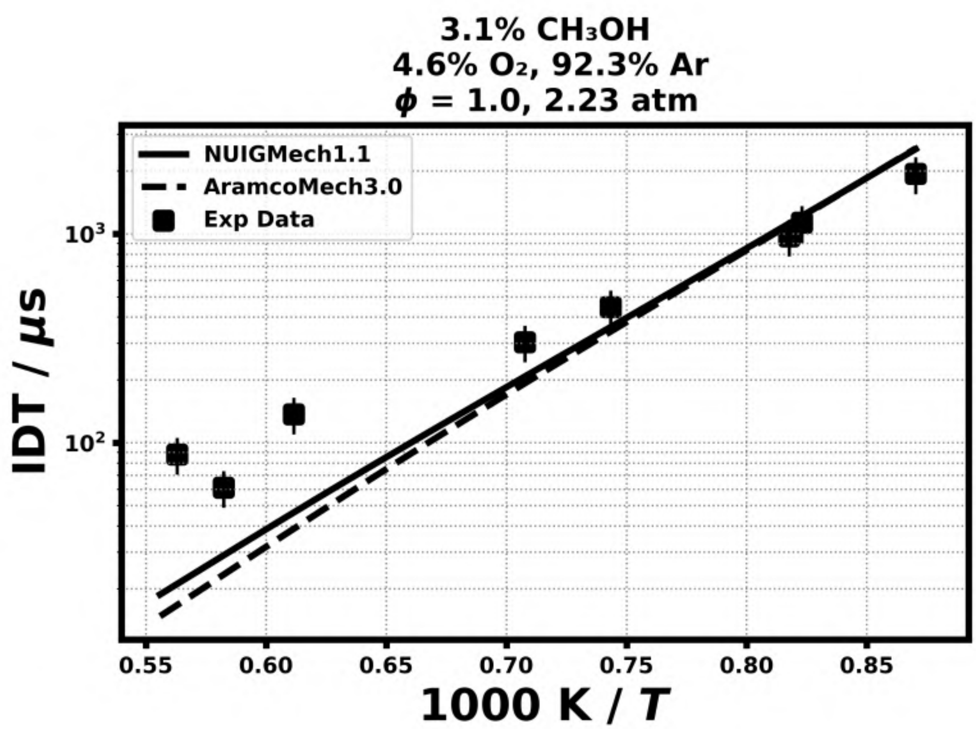

5.71% CH₃OH
4.29% O₂, 90.0% Ar
ϕ = 2.0, p = 2.5 atm
5×10²
2.5×10²
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
0.60
0.65
0.70
0.75
1000 K / T

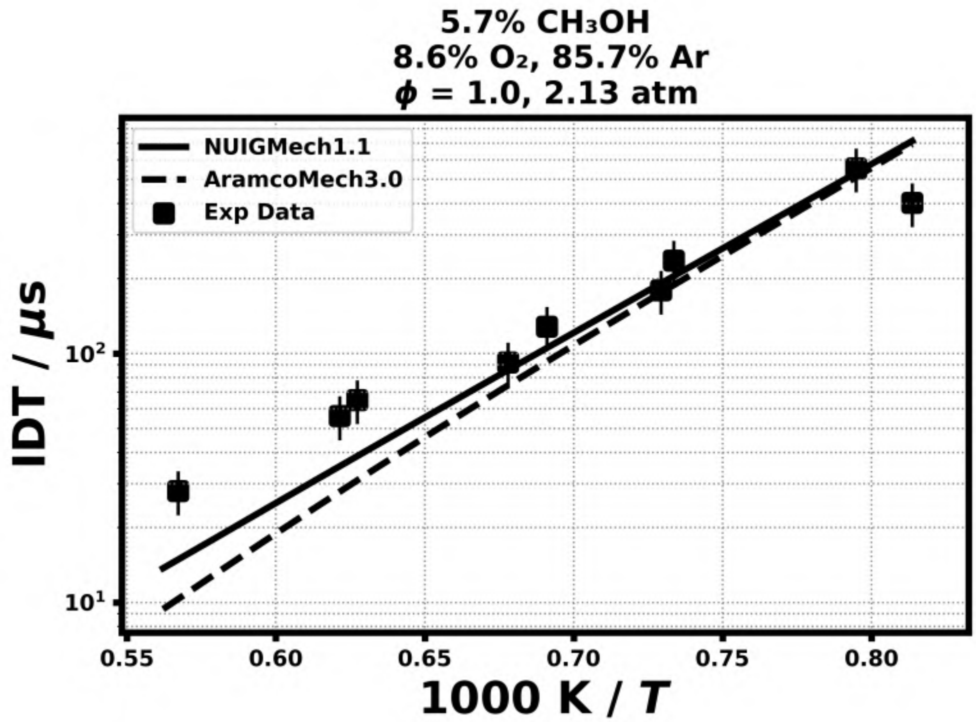
4.6) Noorani, K. E., Akih-Kumgeh, B., & Bergthorson, J. M., Energy & fuels, 24(11) (2010) 5834-5843.

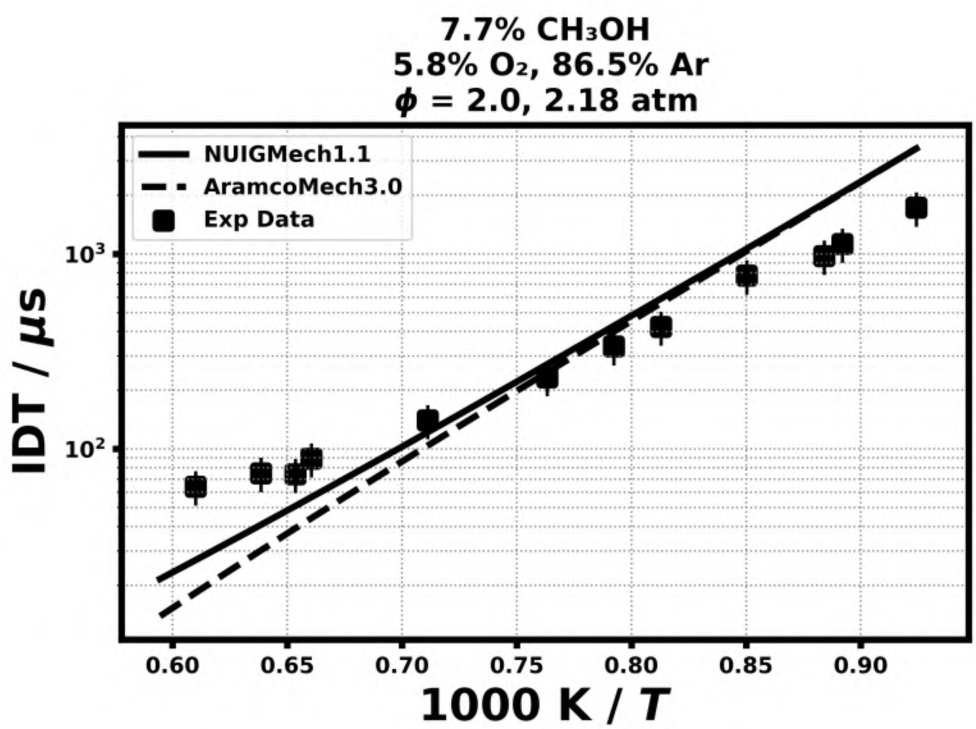





2.0% CH₃OH
6.1% O₂, 91.9% Ar
ϕ = 0.5, 11.63 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
0.60
0.65
0.70
0.75
0.80
0.85
0.90
0.95

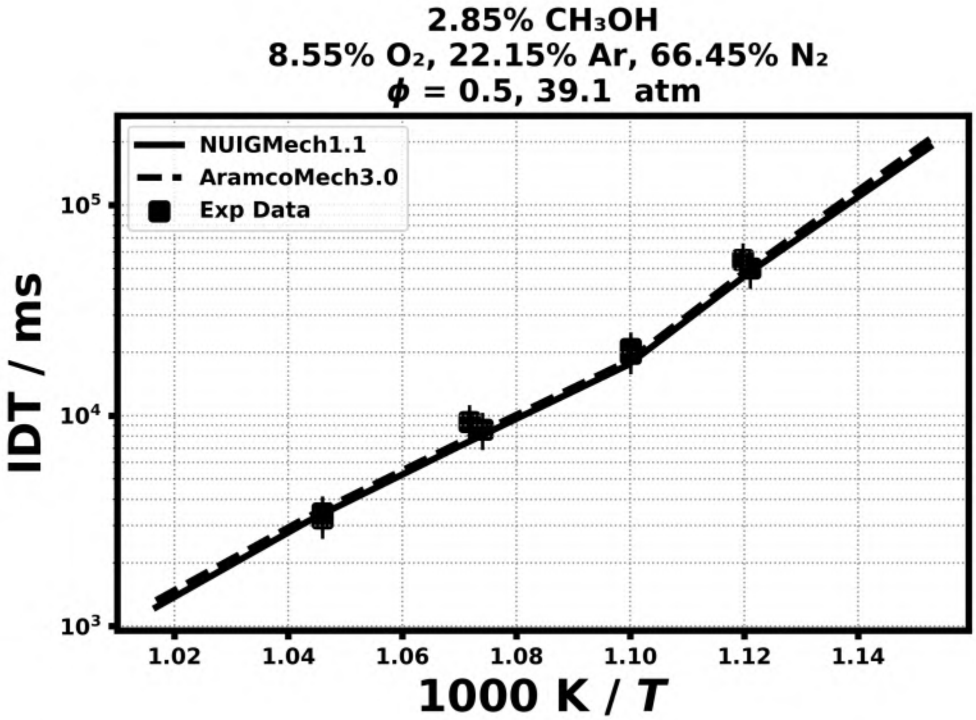

3.1% CH₃OH
4.6% O₂, 92.3% Ar
ϕ = 1.0, 2.23 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
1000 K / T
0.55
0.60
0.65
0.70
0.75
0.80
0.85

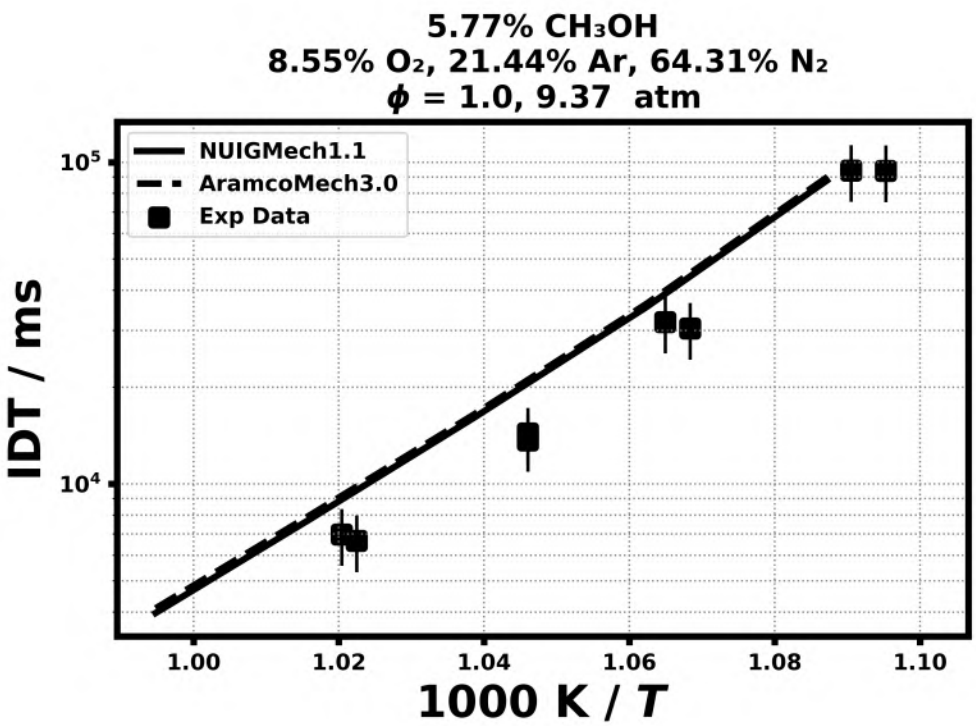

5.7% CH₃OH
8.6% O₂, 85.7% Ar
ϕ = 1.0, 2.13 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10²
10¹
0.55
0.60
0.65
0.70
0.75
0.80
1000 K / T

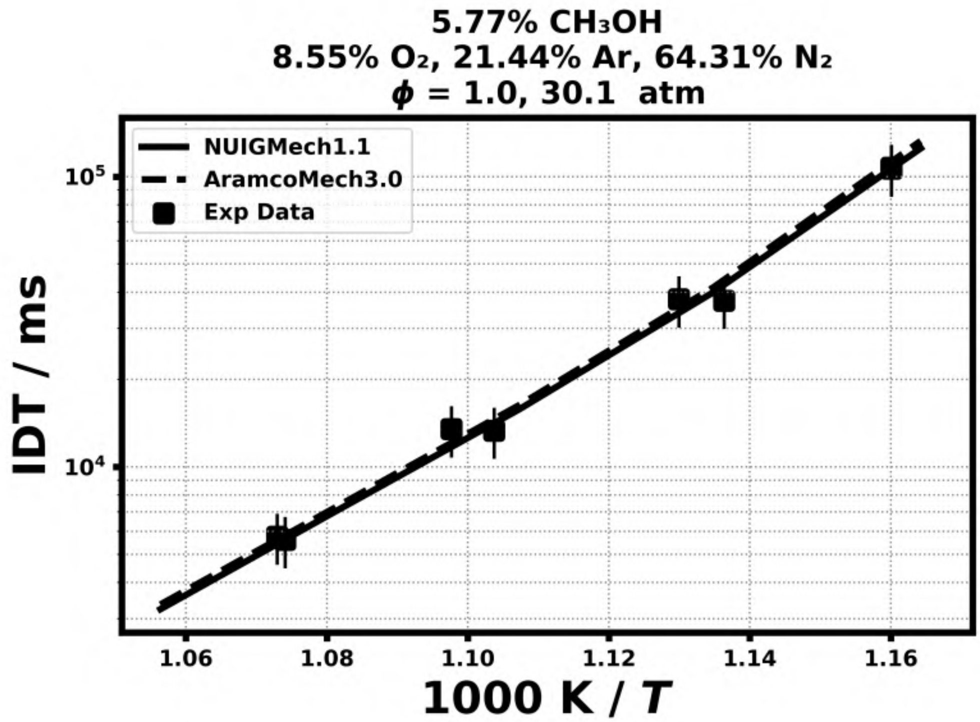

7.7% CH₃OH
5.8% O₂, 86.5% Ar
ϕ = 2.0, 2.18 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / μs
10³
10²
0.60
0.65
0.70
0.75
0.80
0.85
0.90
1000 K / T

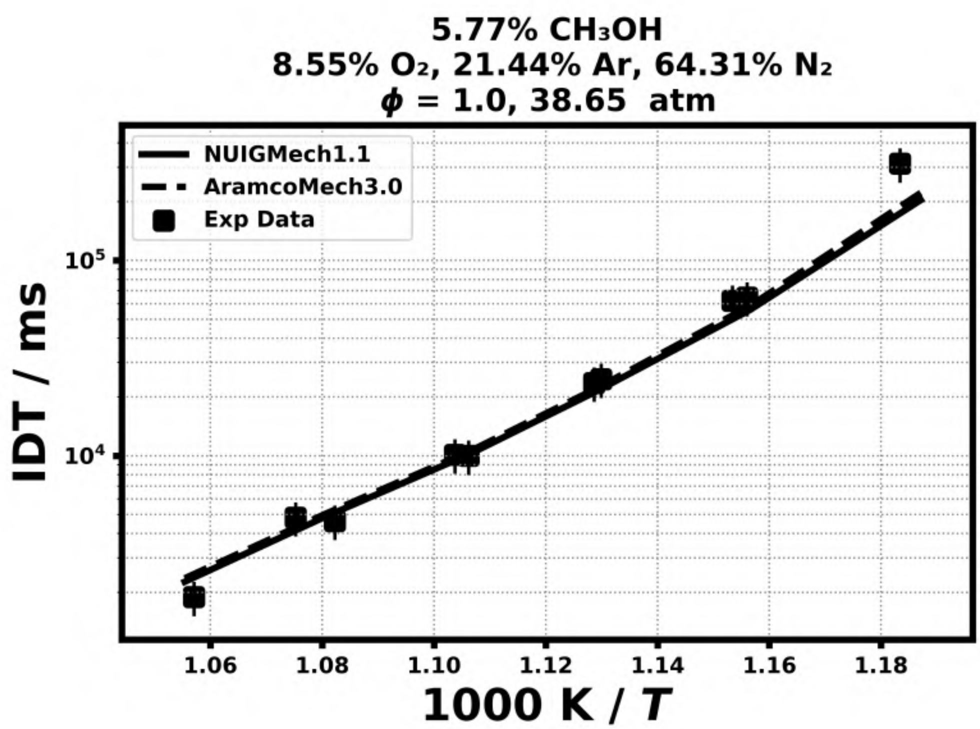
RCM Ignition delay time

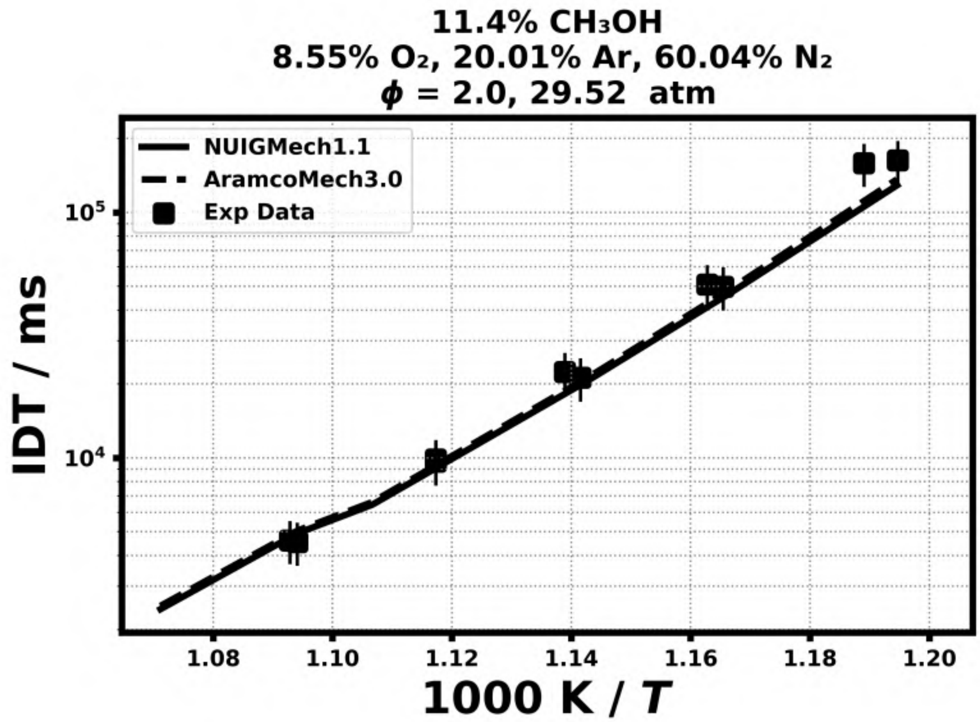
4.7) Burke, U., Metcalfe, W. K., Burke, S. M., Heufer, K. A., Dagaut, P., & Curran, H. J., Combustion and Flame, 165 (2016) 125-136.

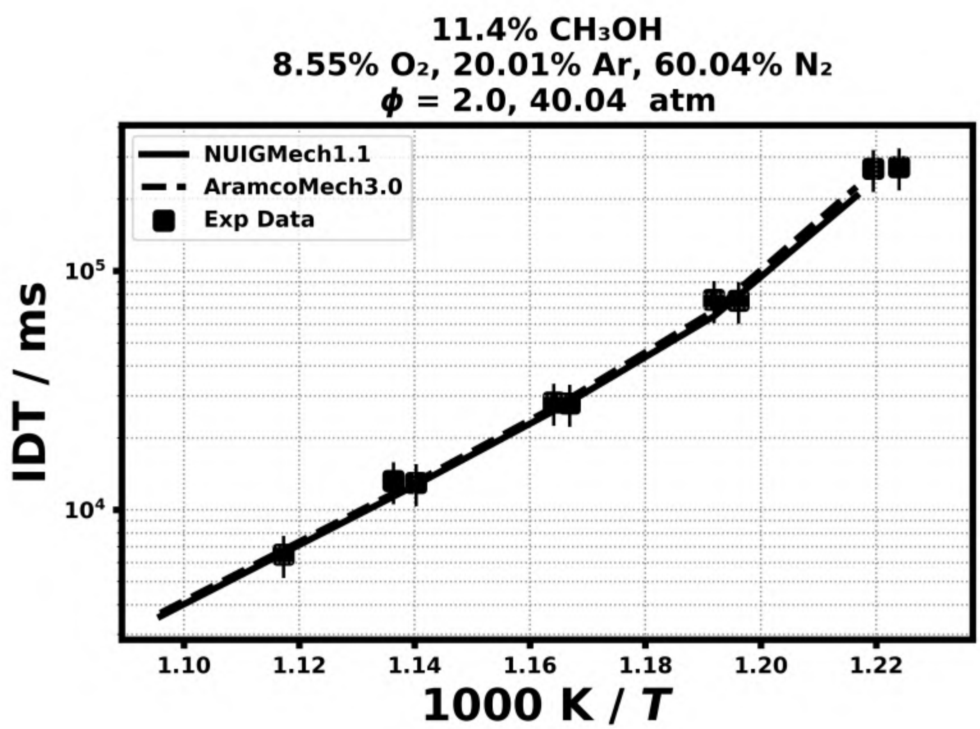





5.77% CH3OH
8.55% O2, 21.44% Ar, 64.31% N2
ϕ = 1.0, 30.1 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / ms
10^5
10^4
1.06
1.08
1.10
1.12
1.14
1.16
1000 K / T

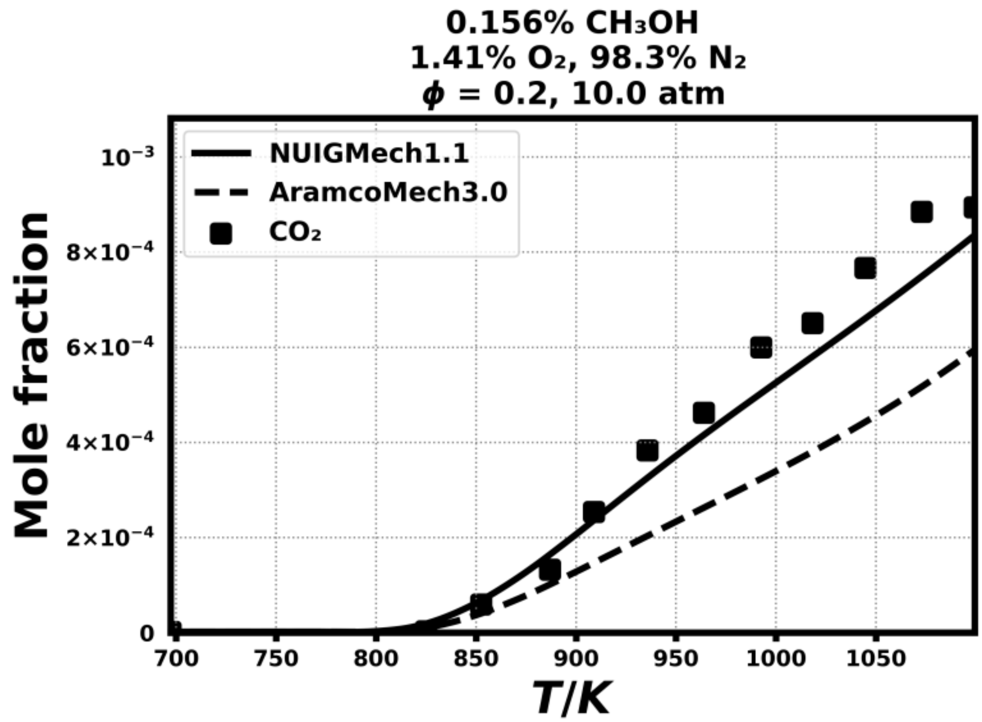

5.77% CH3OH
8.55% O2, 21.44% Ar, 64.31% N2
ϕ = 1.0, 38.65 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / ms
10^5
10^4
1.06
1.08
1.10
1.12
1.14
1.16
1.18
1000 K / T

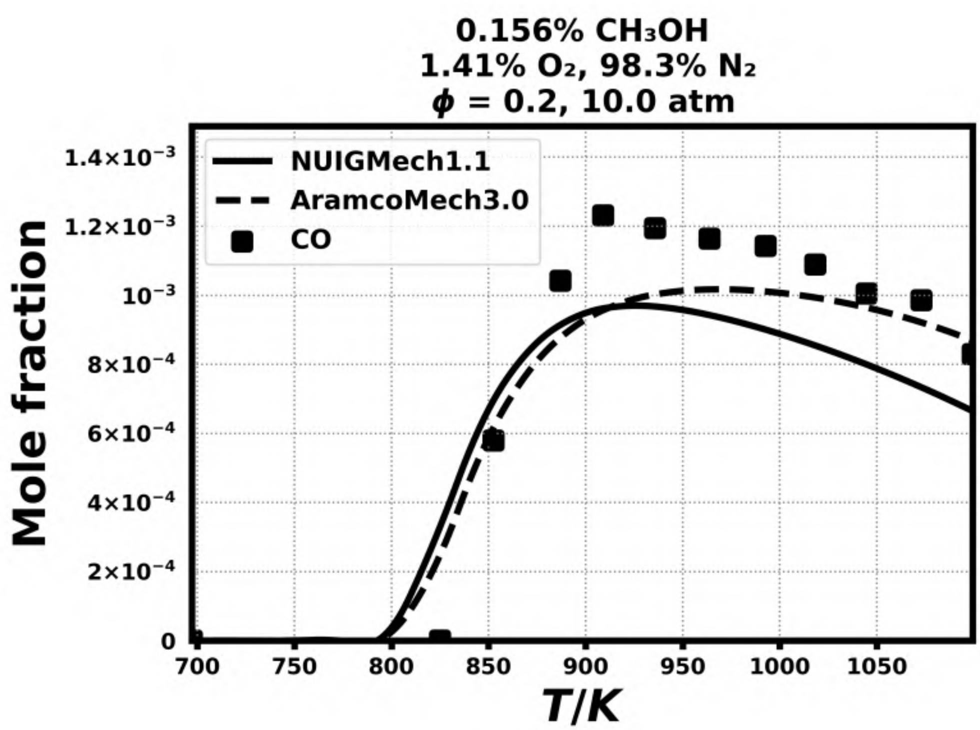

11.4% CH3OH
8.55% O2, 20.01% Ar, 60.04% N2
ϕ = 2.0, 29.52 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / ms
10^5
10^4
1.08
1.10
1.12
1.14
1.16
1.18
1.20
1000 K / T

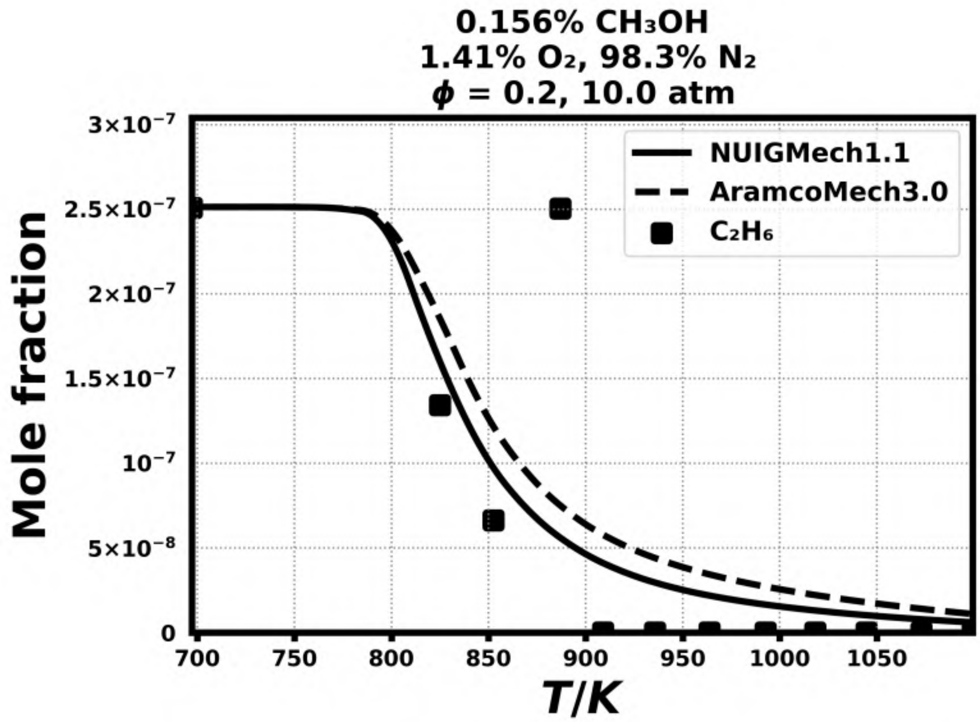

11.4% CH3OH
8.55% O2, 20.01% Ar, 60.04% N2
ϕ = 2.0, 40.04 atm
NUIGMech1.1
AramcoMech3.0
Exp Data
IDT / ms
10^5
10^4
1.10
1.12
1.14
1.16
1.18
1.20
1.22
1000 K / T

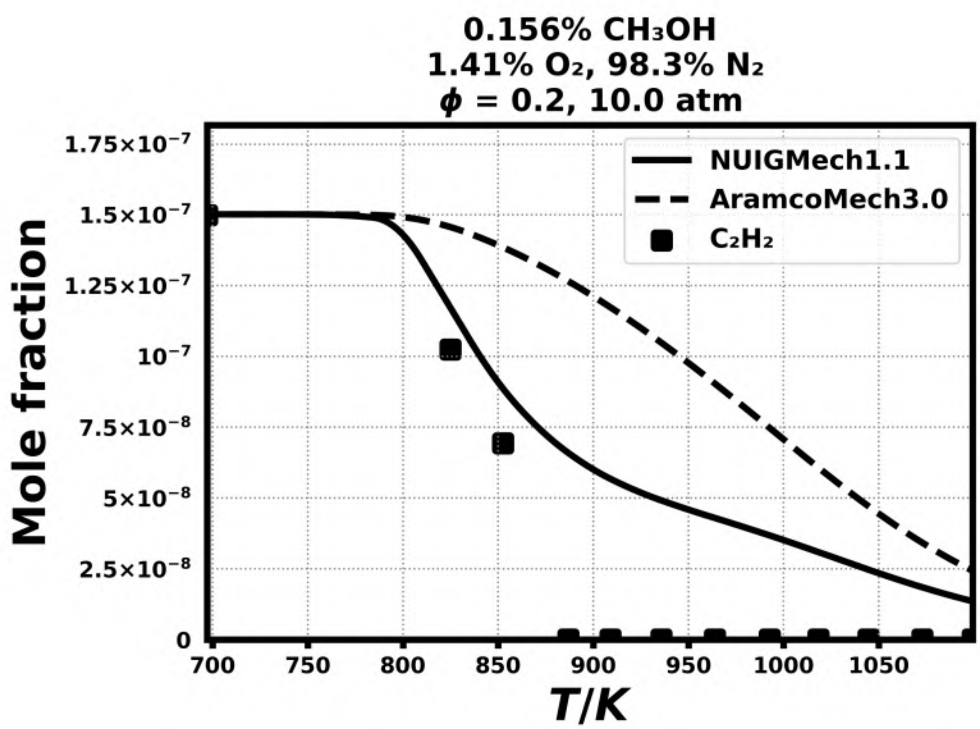
Speciation in Jet-stirred reactor

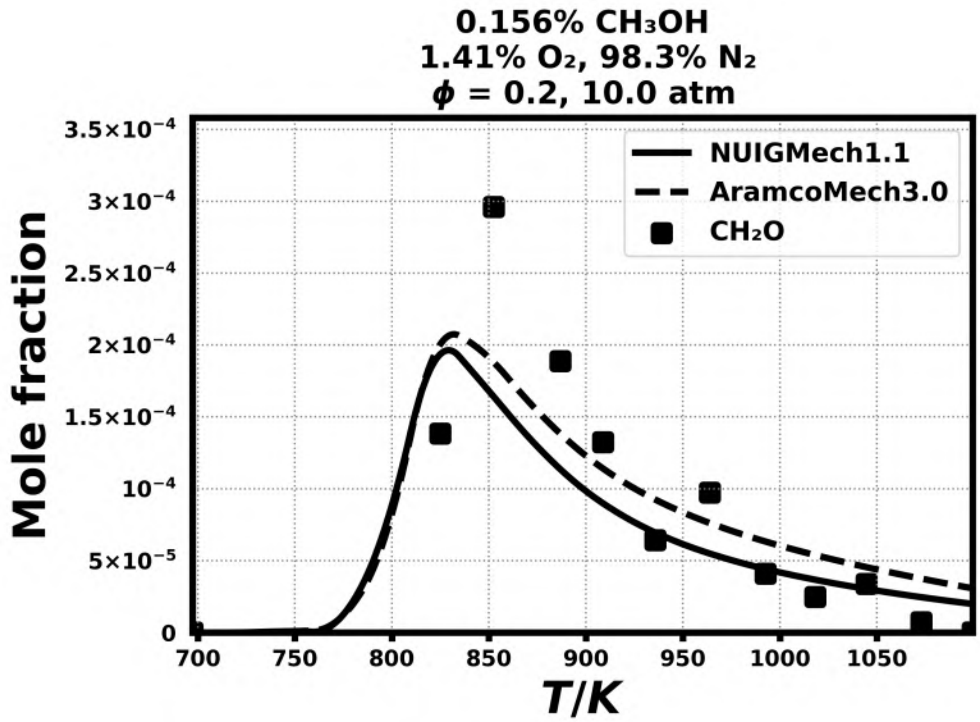
4.8) Burke, U., Metcalfe, W. K., Burke, S. M., Heufer, K. A., Dagaut, P., & Curran, H. J., Combustion and Flame, 165 (2016) 125-136.

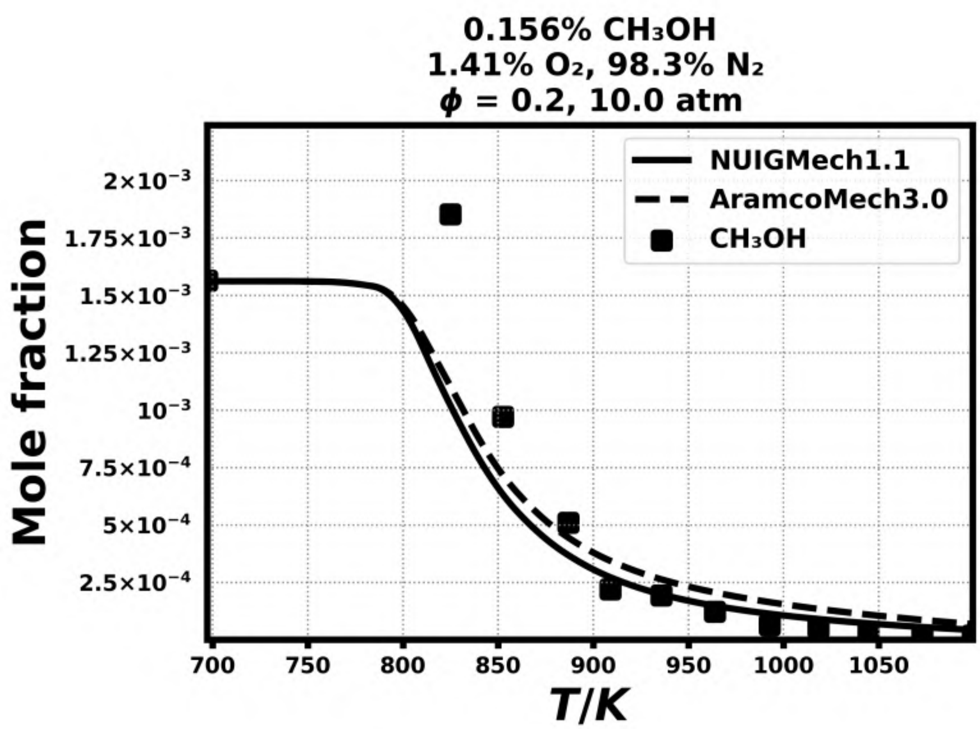


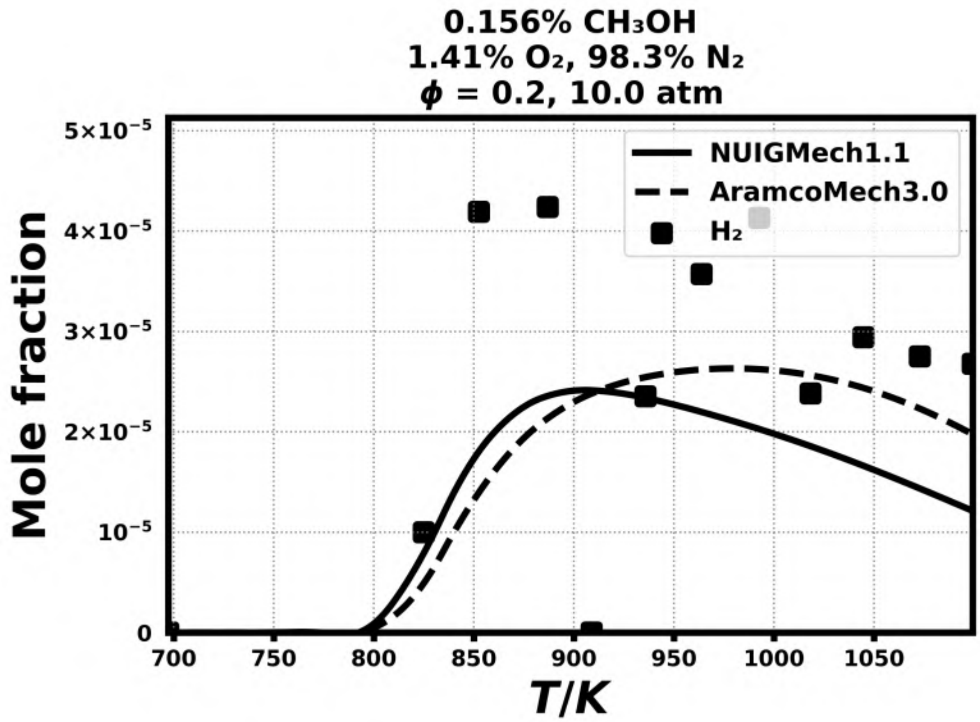


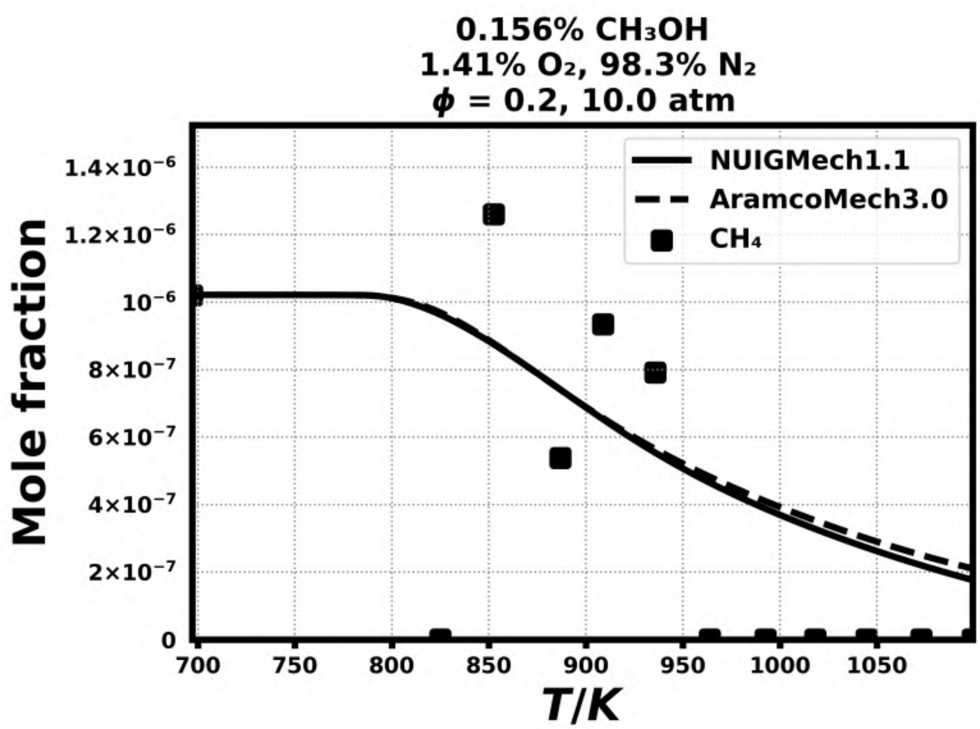

0.156% CH3OH
1.41% O2, 98.3% N2
ϕ = 0.2, 10.0 atm
NUIGMech1.1
AramcoMech3.0
C2H6
Mole fraction
T/K
3×10⁻⁷
2.5×10⁻⁷
2×10⁻⁷
1.5×10⁻⁷
10⁻⁷
5×10⁻⁸
0
700
750
800
850
900
950
1000
1050

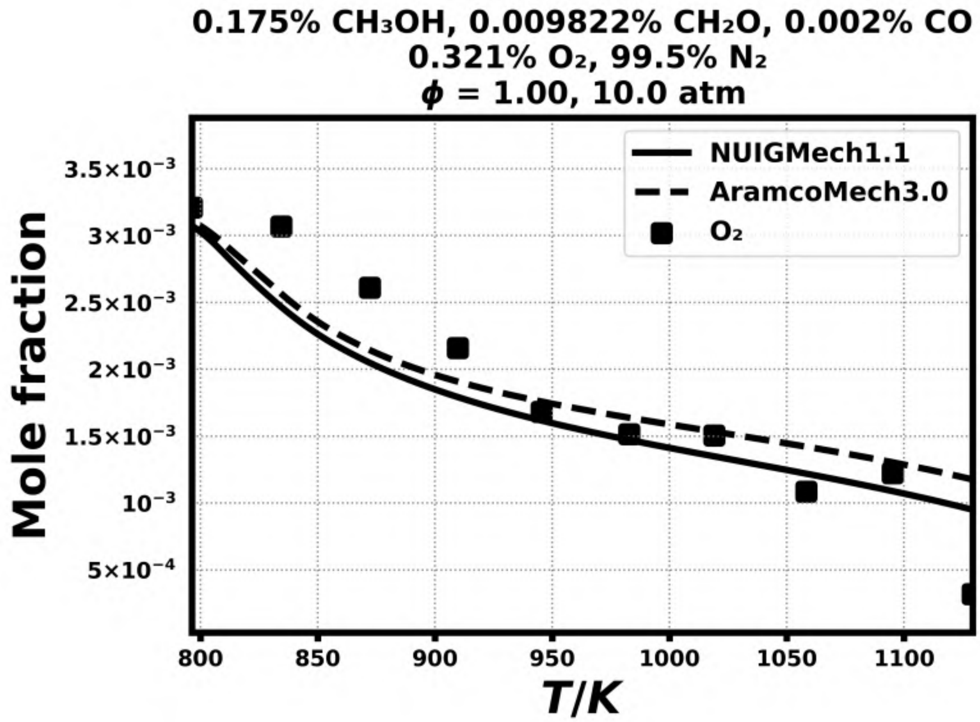

0.156% CH3OH
1.41% O2, 98.3% N2
ϕ = 0.2, 10.0 atm
NUIGMech1.1
AramcoMech3.0
C2H2
Mole fraction
T/K
1.75×10⁻⁷
1.5×10⁻⁷
1.25×10⁻⁷
10⁻⁷
7.5×10⁻⁸
5×10⁻⁸
2.5×10⁻⁸
0
700
750
800
850
900
950
1000
1050

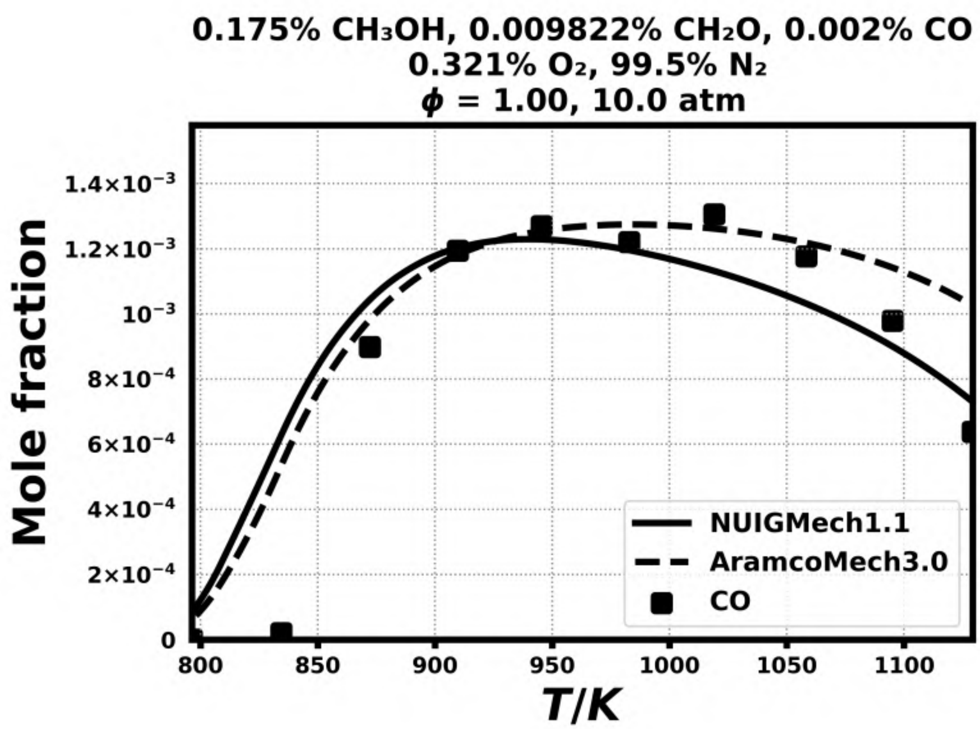

0.156% CH₃OH
1.41% O₂, 98.3% N₂
ϕ = 0.2, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
T/K

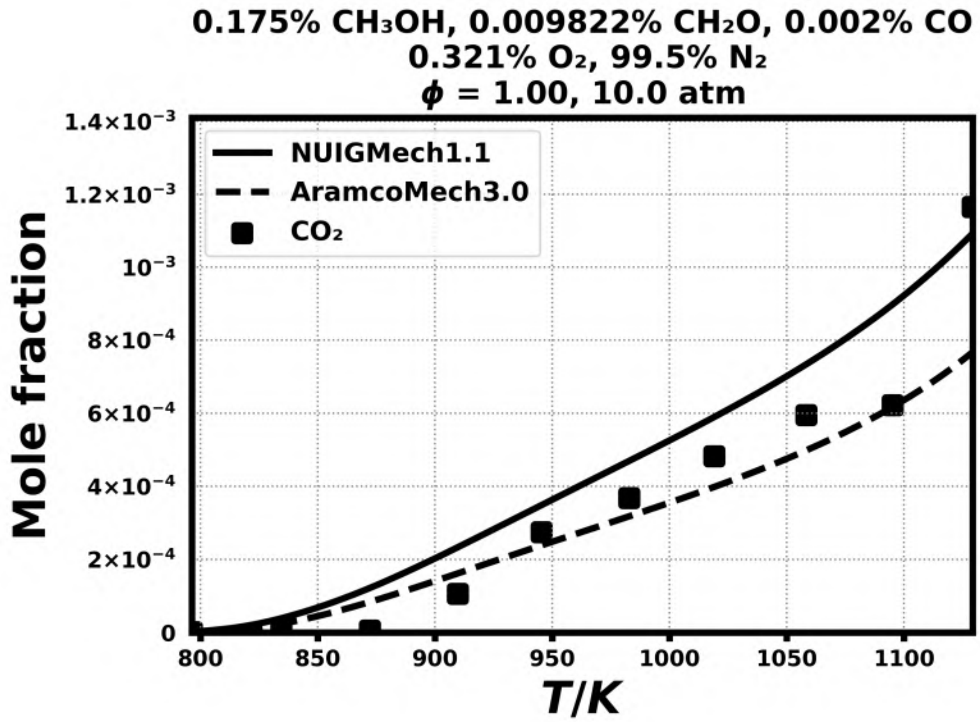

0.156% CH₃OH
1.41% O₂, 98.3% N₂
ϕ = 0.2, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CH₃OH
Mole fraction
T/K

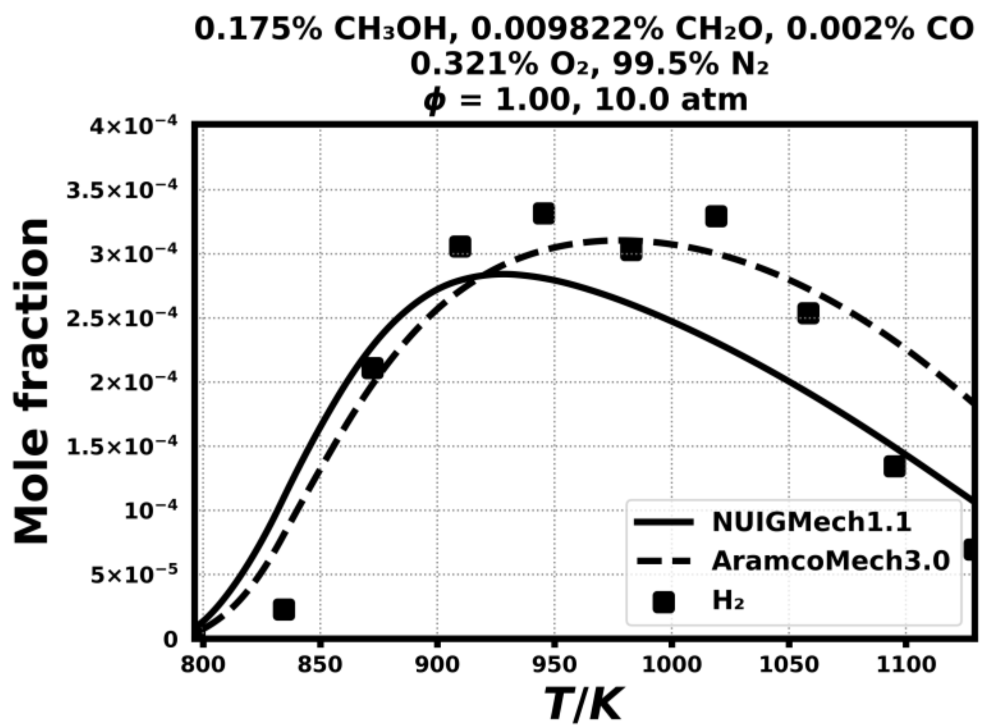

0.156% CH₃OH
1.41% O₂, 98.3% N₂
ϕ = 0.2, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
H₂
5×10⁻⁵
4×10⁻⁵
3×10⁻⁵
2×10⁻⁵
10⁻⁵
0
700
750
800
850
900
950
1000
1050

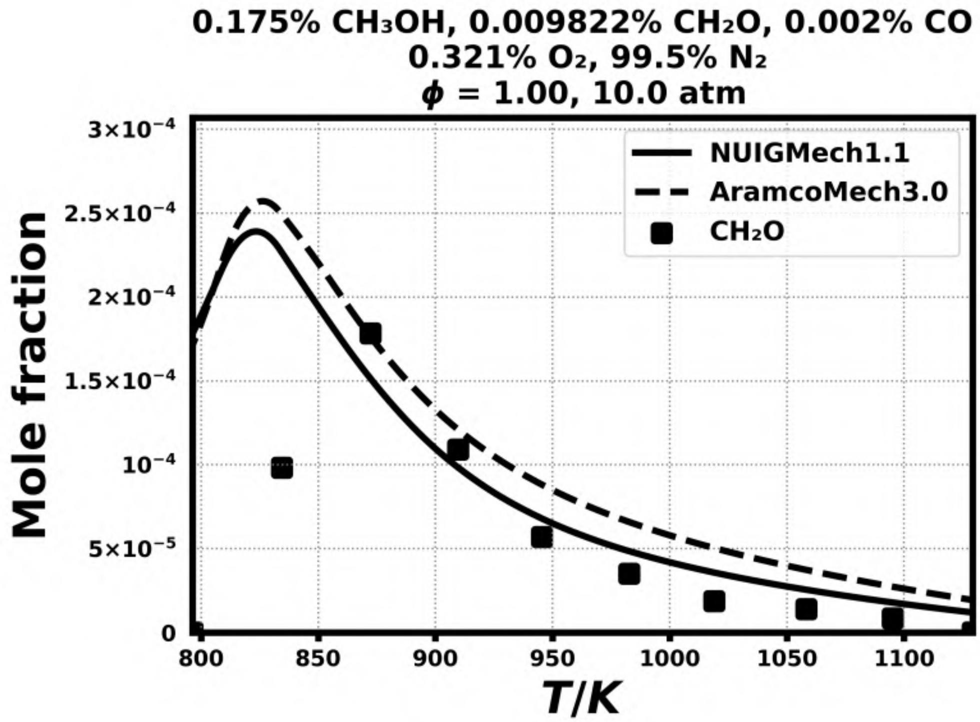

0.156% CH₃OH
1.41% O₂, 98.3% N₂
ϕ = 0.2, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH₄
1.4×10⁻⁶
1.2×10⁻⁶
10⁻⁶
8×10⁻⁷
6×10⁻⁷
4×10⁻⁷
2×10⁻⁷
0
700
750
800
850
900
950
1000
1050


0.175% CH₃OH, 0.009822% CH₂O, 0.002% CO
0.321% O₂, 99.5% N₂
ϕ = 1.00, 10.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
T/K
3.5×10⁻³
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
800
850
900
950
1000
1050
1100

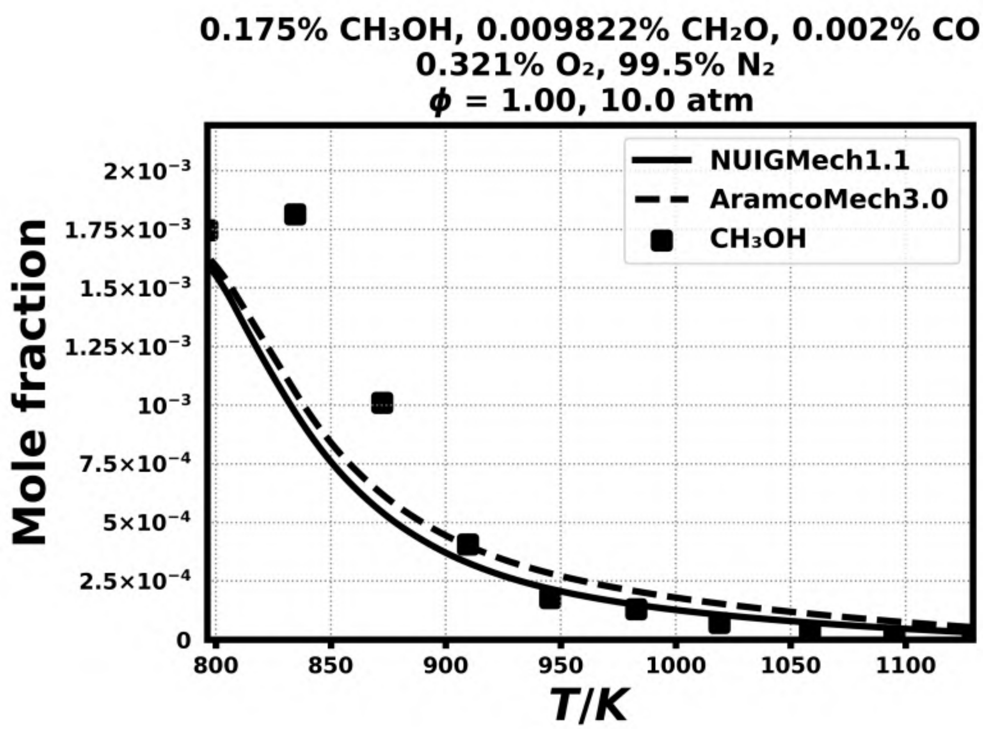

0.175% CH₃OH, 0.009822% CH₂O, 0.002% CO
0.321% O₂, 99.5% N₂
ϕ = 1.00, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
T/K
1.4×10⁻³
1.2×10⁻³
10⁻³
8×10⁻⁴
6×10⁻⁴
4×10⁻⁴
2×10⁻⁴
0
800
850
900
950
1000
1050
1100


0.175% CH₃OH, 0.009822% CH₂O, 0.002% CO
0.321% O₂, 99.5% N₂
ϕ = 1.00, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CO₂
0
2×10⁻⁴
4×10⁻⁴
6×10⁻⁴
8×10⁻⁴
10⁻³
1.2×10⁻³
1.4×10⁻³
800
850
900
950
1000
1050
1100

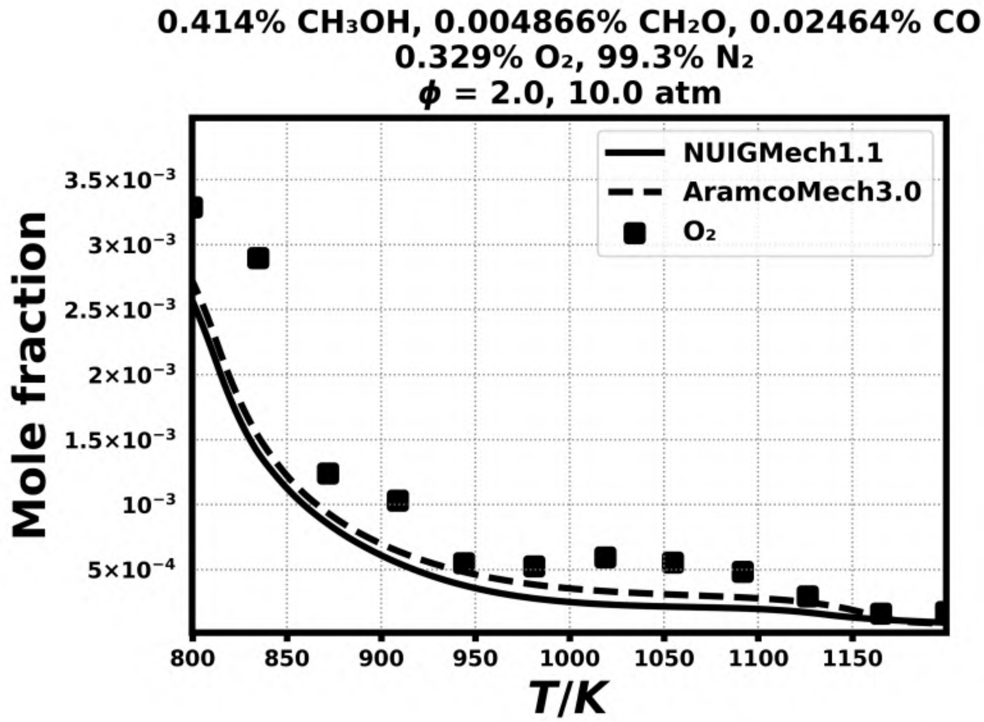

0.175% CH₃OH, 0.009822% CH₂O, 0.002% CO
0.321% O₂, 99.5% N₂
ϕ = 1.00, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
H₂
0
5×10⁻⁵
10⁻⁴
1.5×10⁻⁴
2×10⁻⁴
2.5×10⁻⁴
3×10⁻⁴
3.5×10⁻⁴
4×10⁻⁴
800
850
900
950
1000
1050
1100

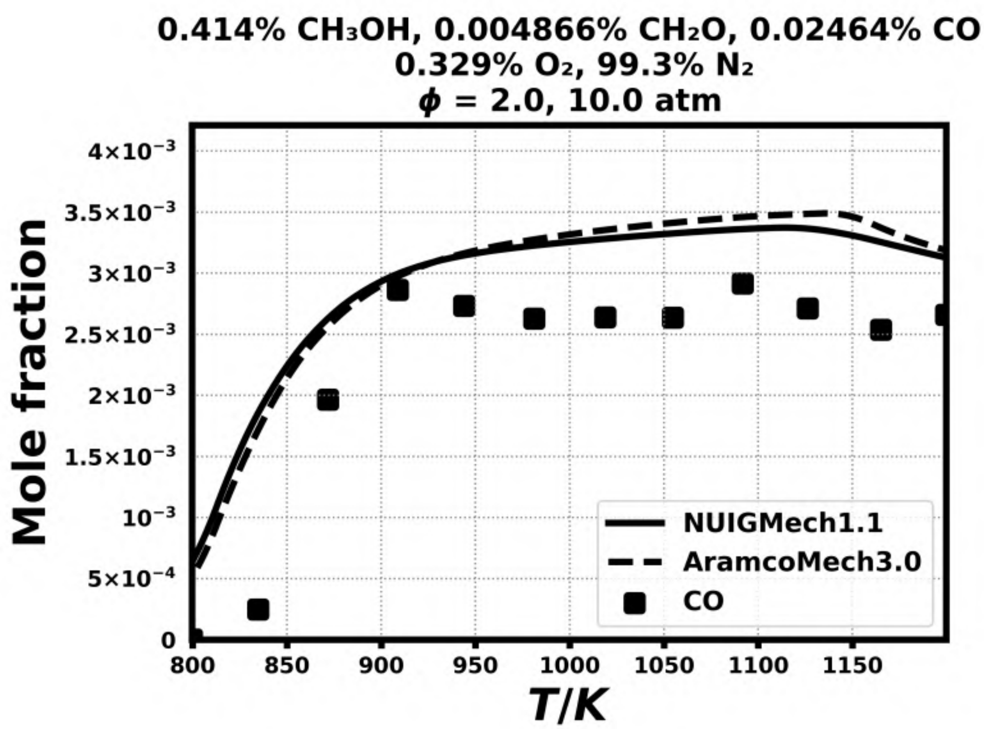


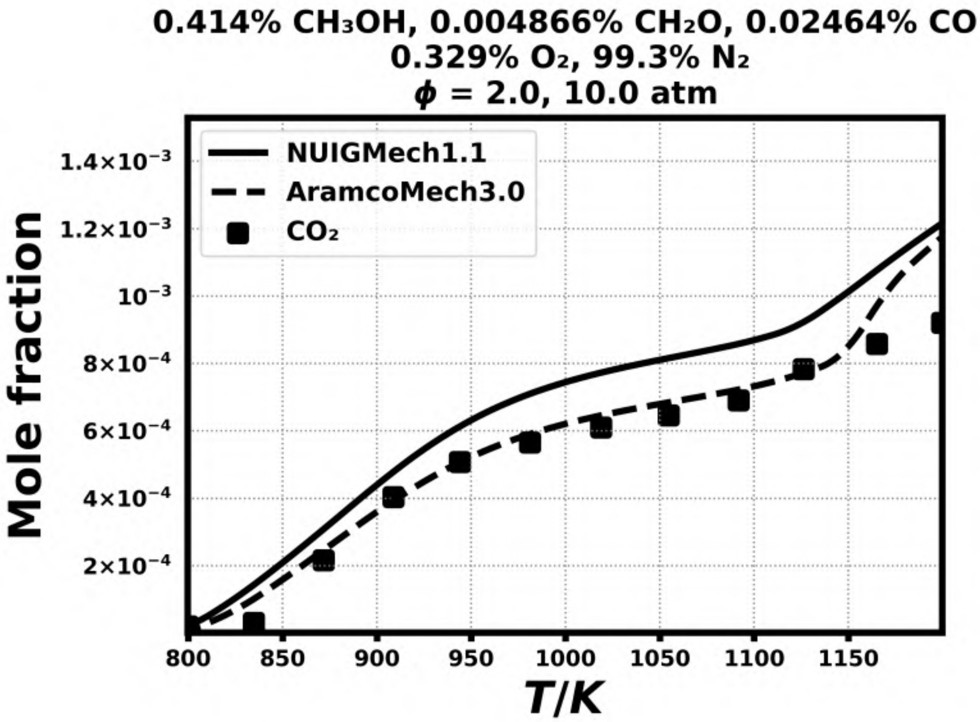
0.175% CH₃OH, 0.009822% CH₂O, 0.002% CO
0.321% O₂, 99.5% N₂
ϕ = 1.00, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
T/K

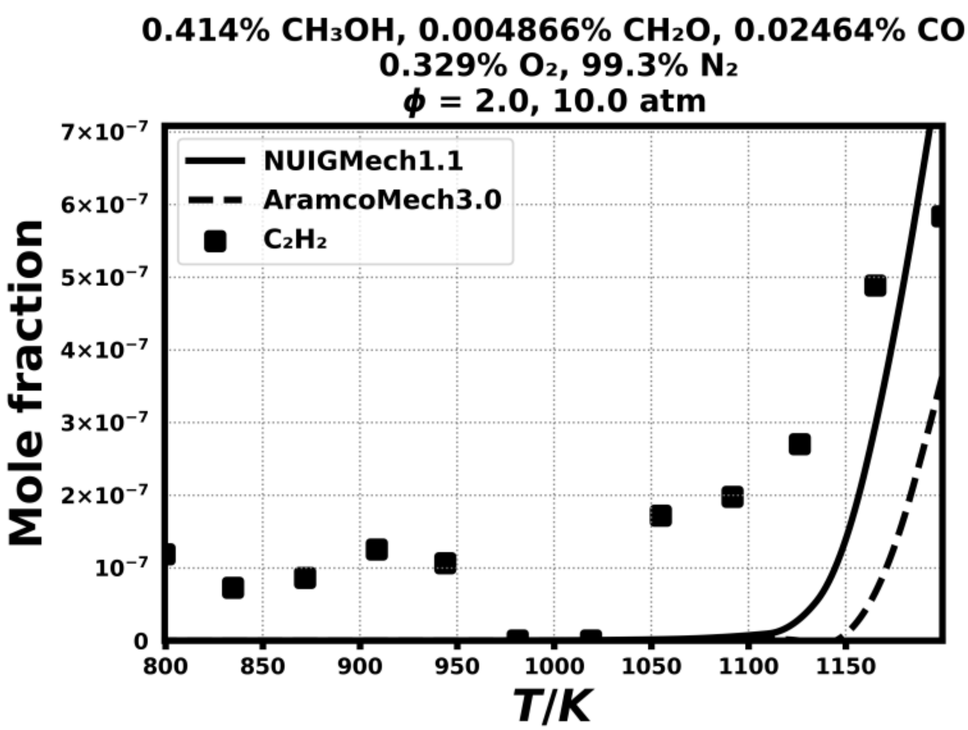


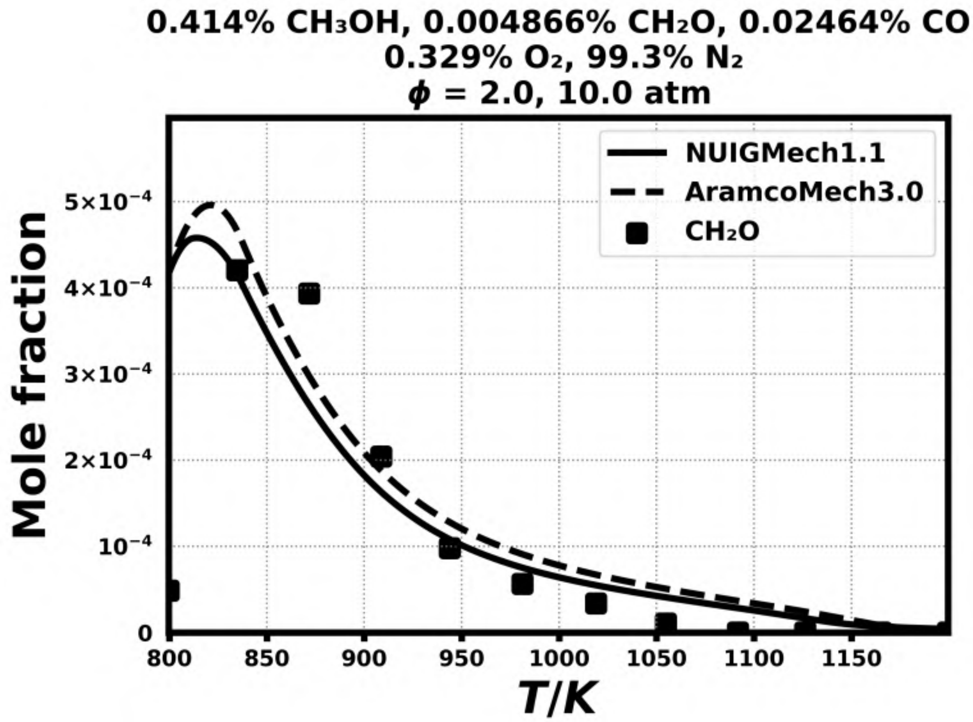
0.175% CH₃OH, 0.009822% CH₂O, 0.002% CO
0.321% O₂, 99.5% N₂
ϕ = 1.00, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CH₃OH
Mole fraction
T/K

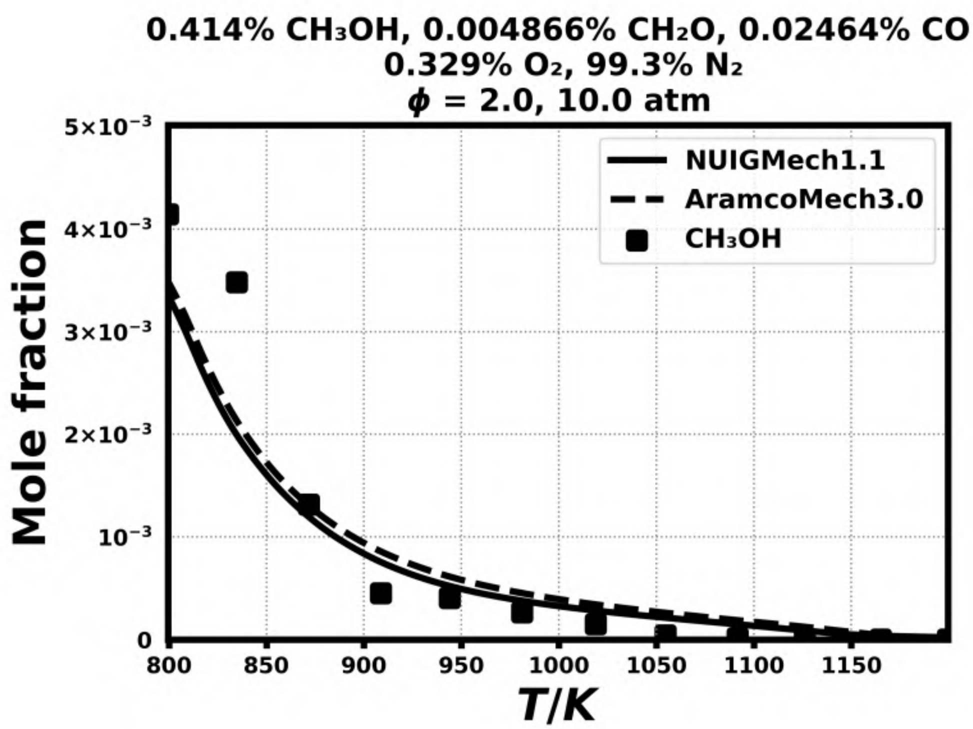

0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
T/K

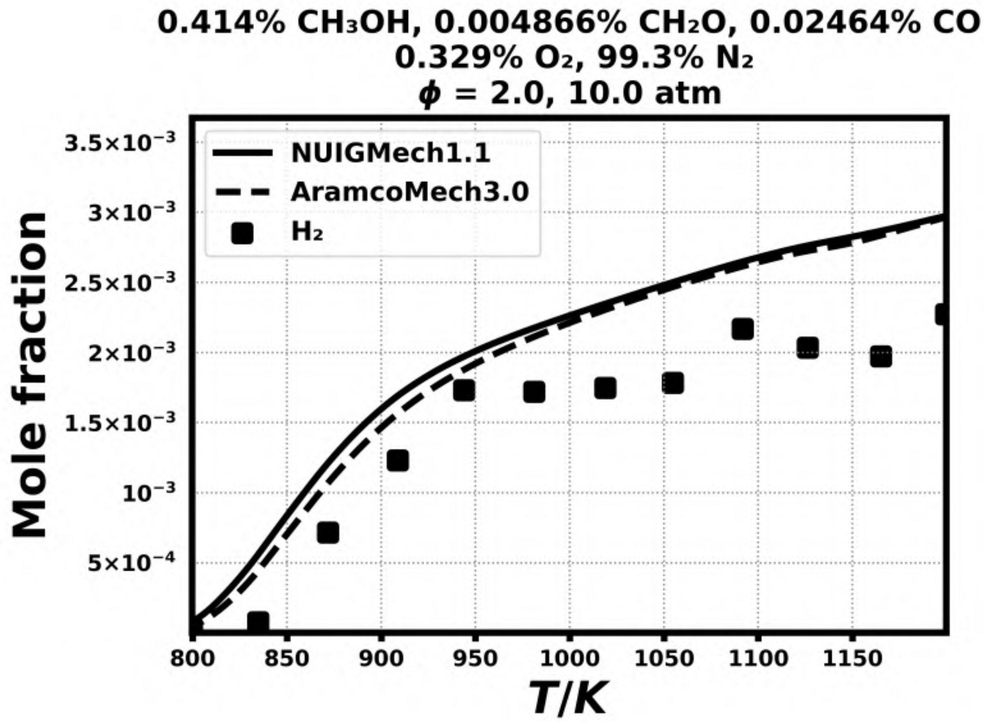

0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
T/K

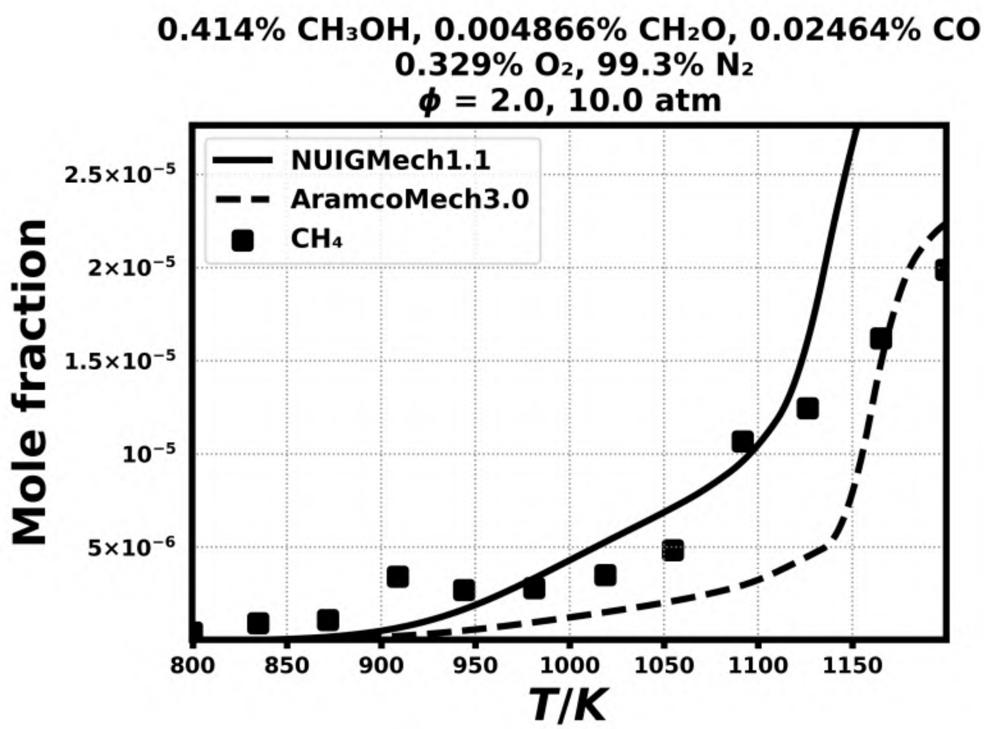

0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CO₂
Mole fraction
T/K

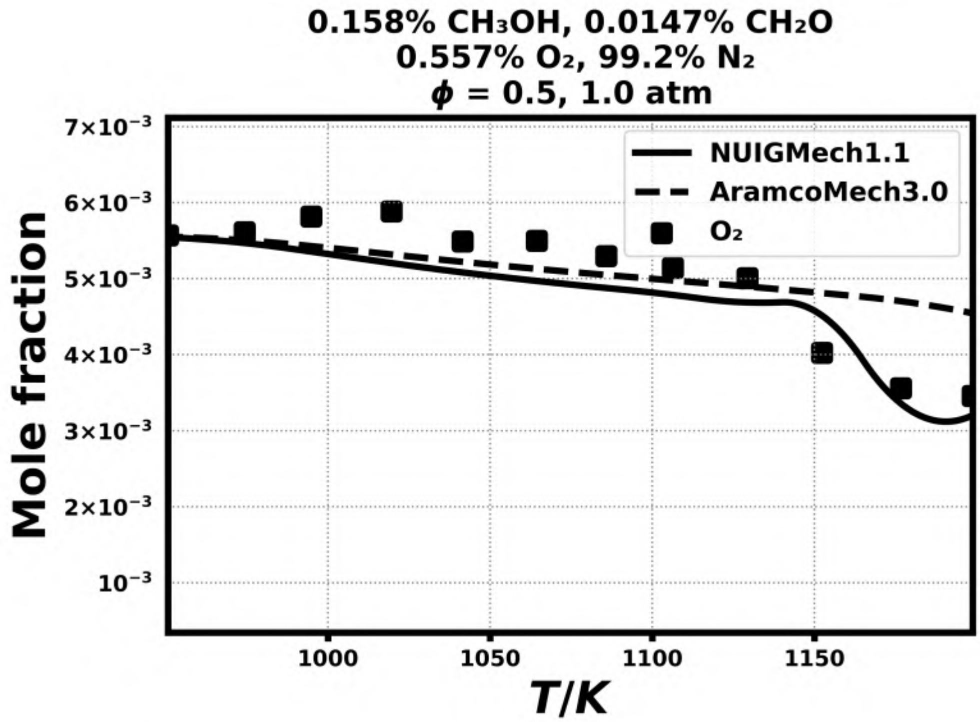

0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
C₂H₂
Mole fraction
T/K


0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH₂O
5×10⁻⁴
4×10⁻⁴
3×10⁻⁴
2×10⁻⁴
10⁻⁴
0
800
850
900
950
1000
1050
1100
1150

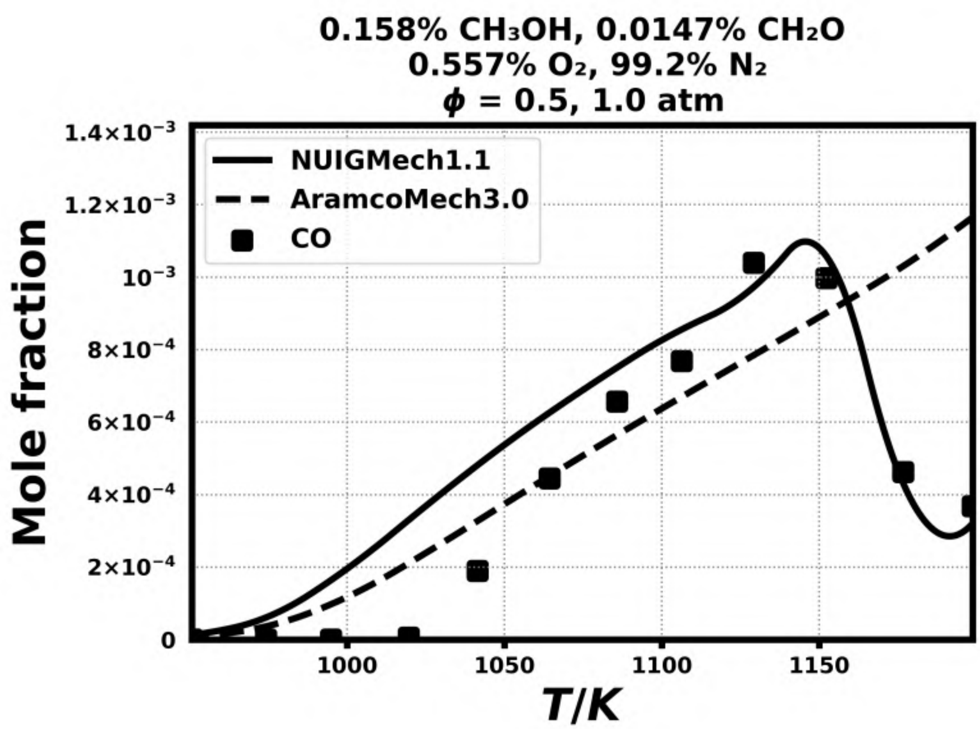

0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH₃OH
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
0
800
850
900
950
1000
1050
1100
1150


0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K

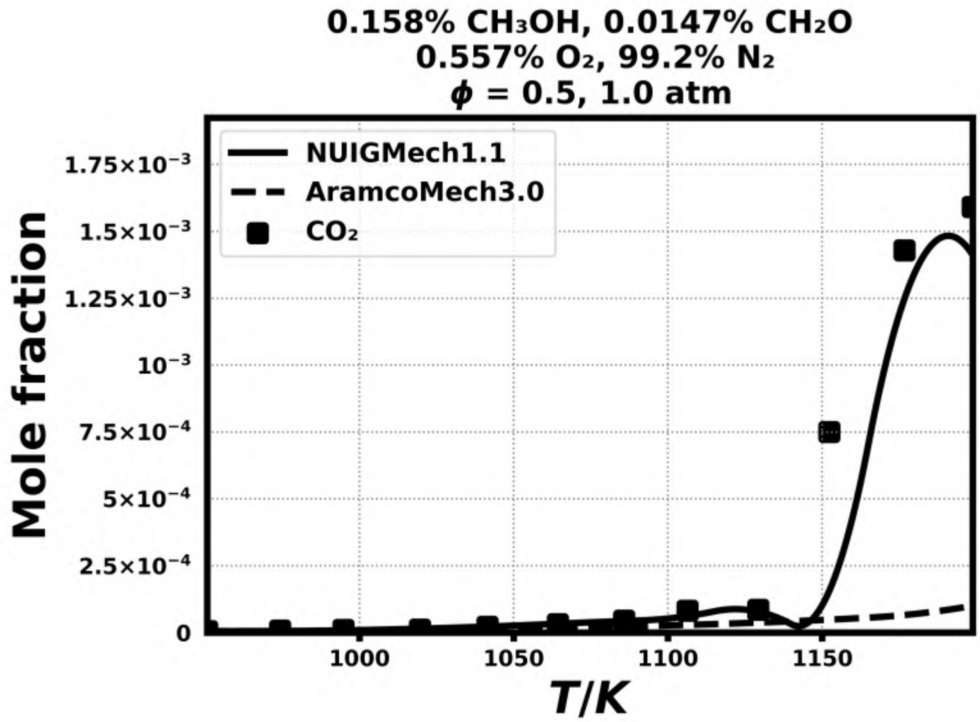

0.414% CH₃OH, 0.004866% CH₂O, 0.02464% CO
0.329% O₂, 99.3% N₂
ϕ = 2.0, 10.0 atm
NUIGMech1.1
AramcoMech3.0
CH₄
Mole fraction
T/K

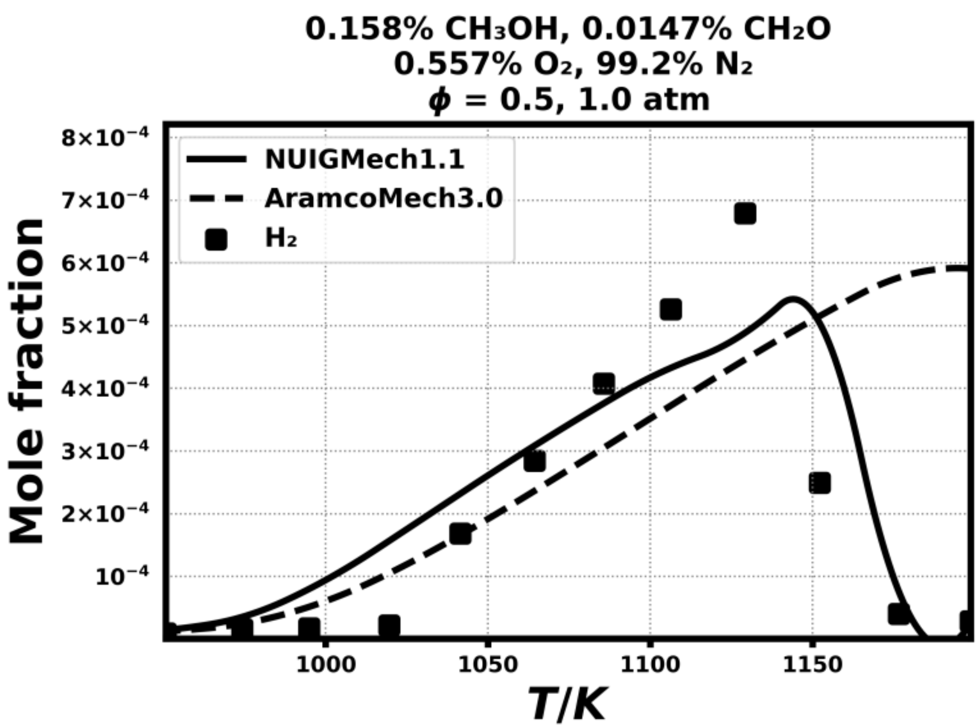


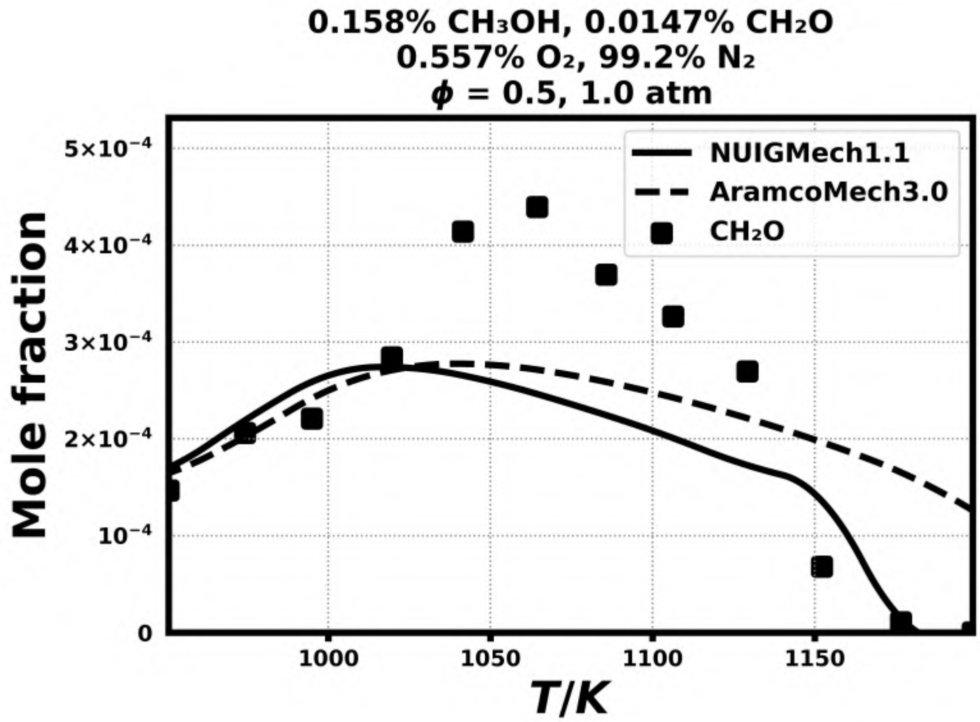
0.158% CH3OH, 0.0147% CH2O
0.557% O2, 99.2% N2
ϕ = 0.5, 1.0 atm
Mole fraction
7×10⁻³
6×10⁻³
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
1000
1050
1100
1150
T/K
NUIGMech1.1
AramcoMech3.0
O2

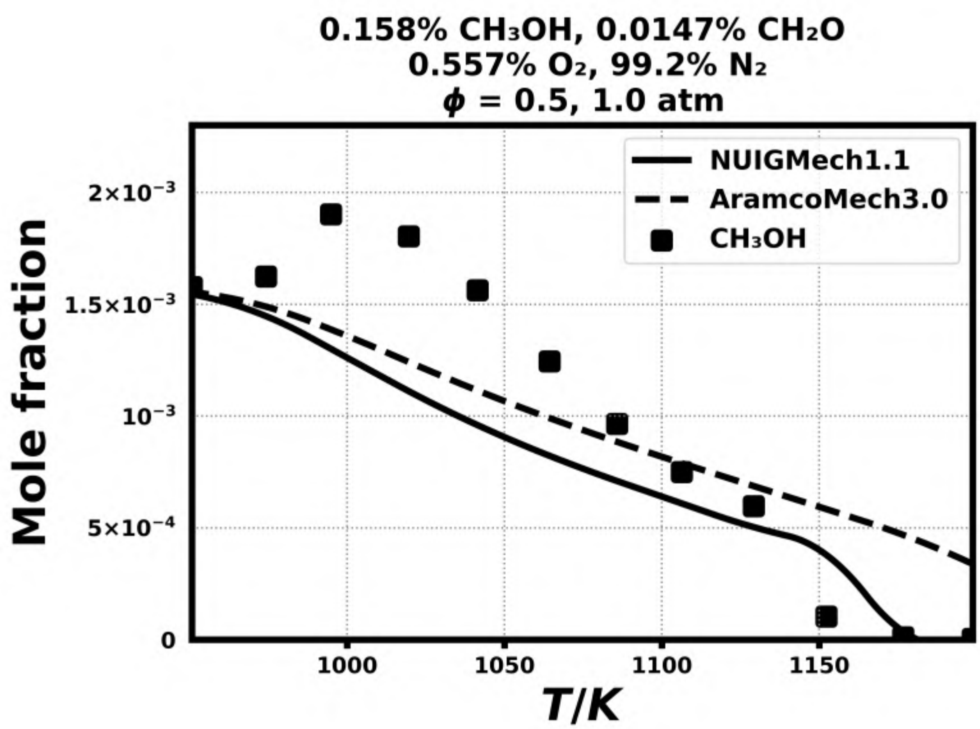


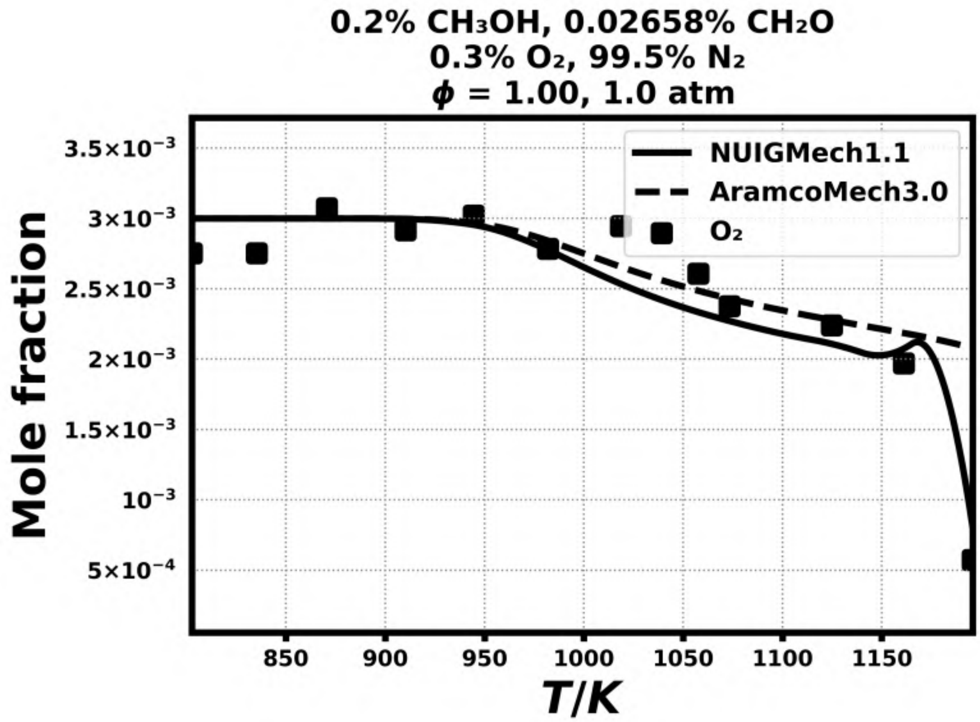
0.158% CH3OH, 0.0147% CH2O
0.557% O2, 99.2% N2
ϕ = 0.5, 1.0 atm
Mole fraction
1.4×10⁻³
1.2×10⁻³
10⁻³
8×10⁻⁴
6×10⁻⁴
4×10⁻⁴
2×10⁻⁴
0
1000
1050
1100
1150
T/K
NUIGMech1.1
AramcoMech3.0
CO

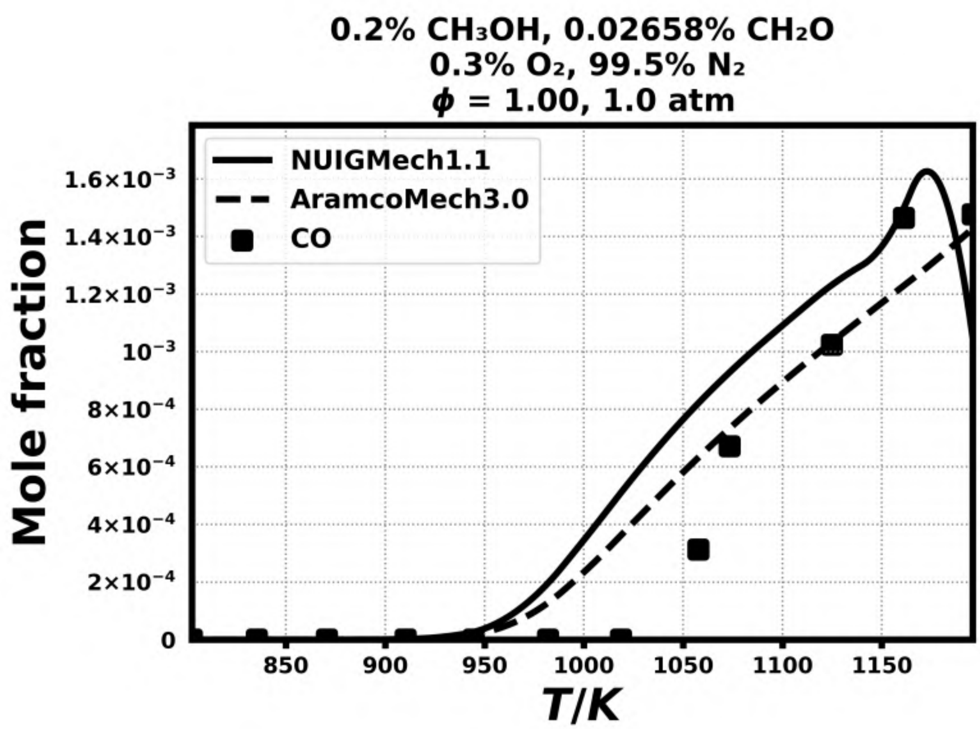

0.158% CH₃OH, 0.0147% CH₂O
0.557% O₂, 99.2% N₂
ϕ = 0.5, 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO₂
Mole fraction
T/K
1.75×10⁻³
1.5×10⁻³
1.25×10⁻³
10⁻³
7.5×10⁻⁴
5×10⁻⁴
2.5×10⁻⁴
0
1000
1050
1100
1150

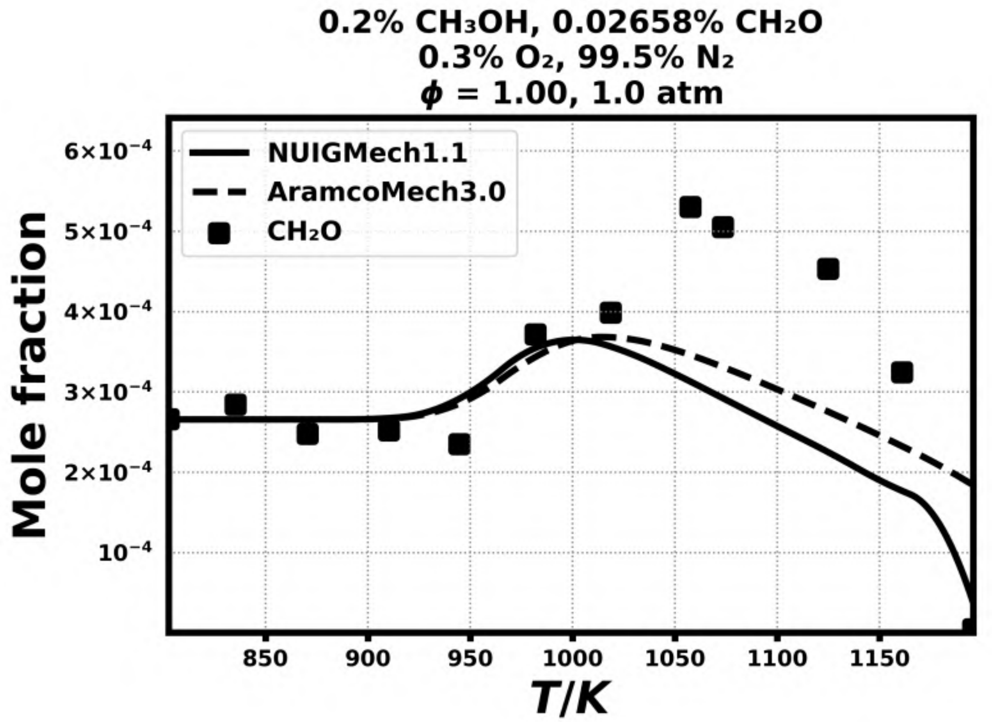

0.158% CH₃OH, 0.0147% CH₂O
0.557% O₂, 99.2% N₂
ϕ = 0.5, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K
8×10⁻⁴
7×10⁻⁴
6×10⁻⁴
5×10⁻⁴
4×10⁻⁴
3×10⁻⁴
2×10⁻⁴
10⁻⁴
1000
1050
1100
1150

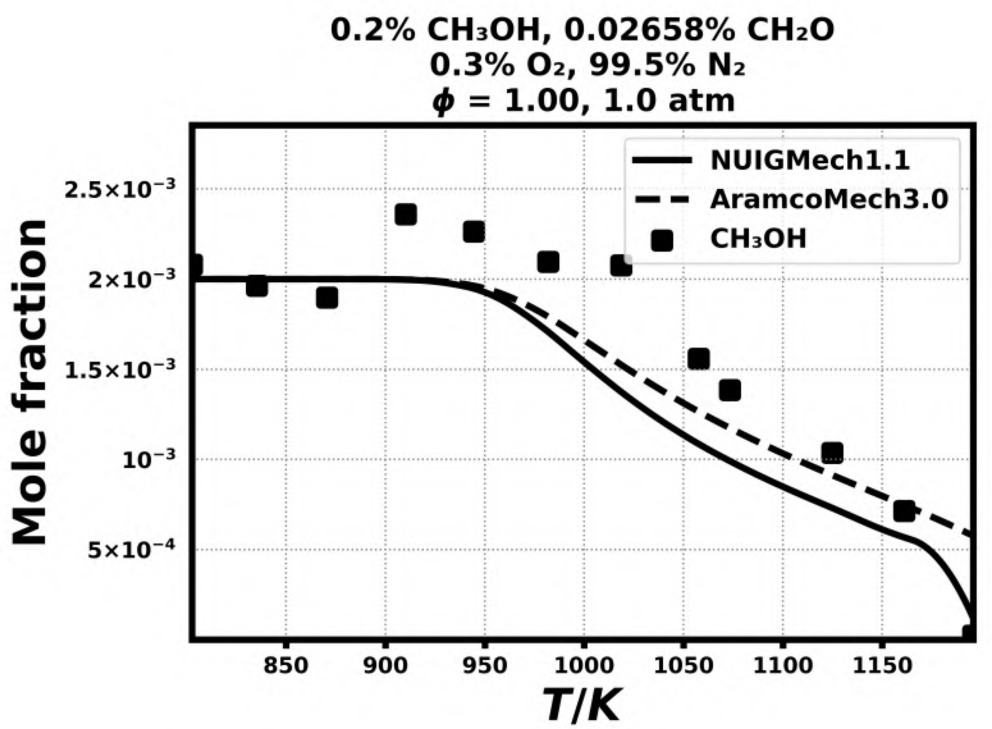

0.158% CH₃OH, 0.0147% CH₂O
0.557% O₂, 99.2% N₂
ϕ = 0.5, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH₂O
5×10⁻⁴
4×10⁻⁴
3×10⁻⁴
2×10⁻⁴
10⁻⁴
0
1000
1050
1100
1150

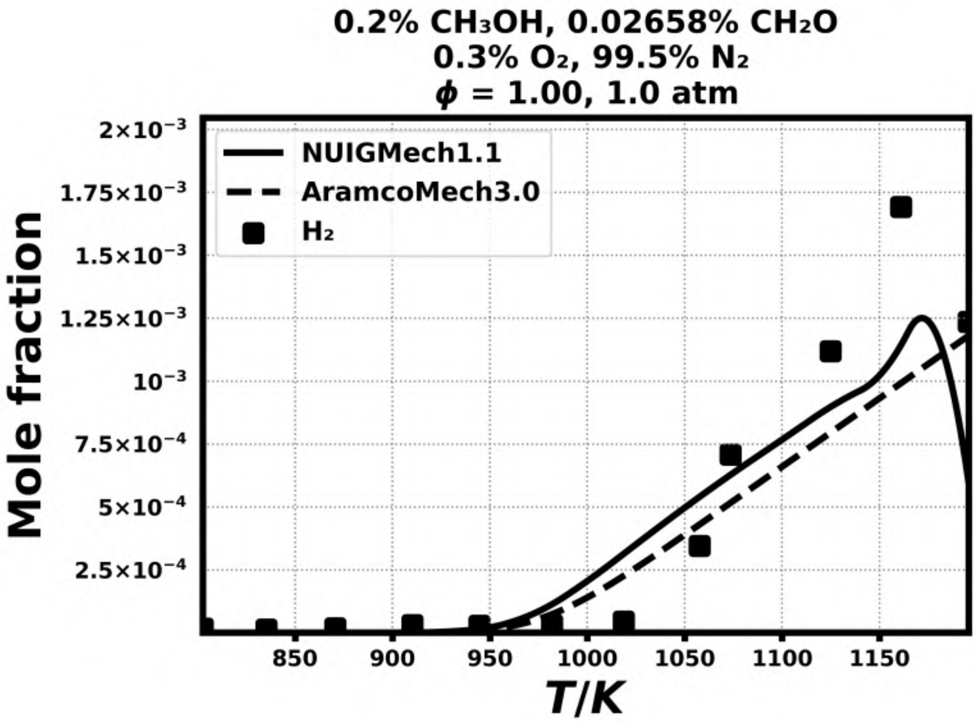

0.158% CH₃OH, 0.0147% CH₂O
0.557% O₂, 99.2% N₂
ϕ = 0.5, 1.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH₃OH
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
0
1000
1050
1100
1150

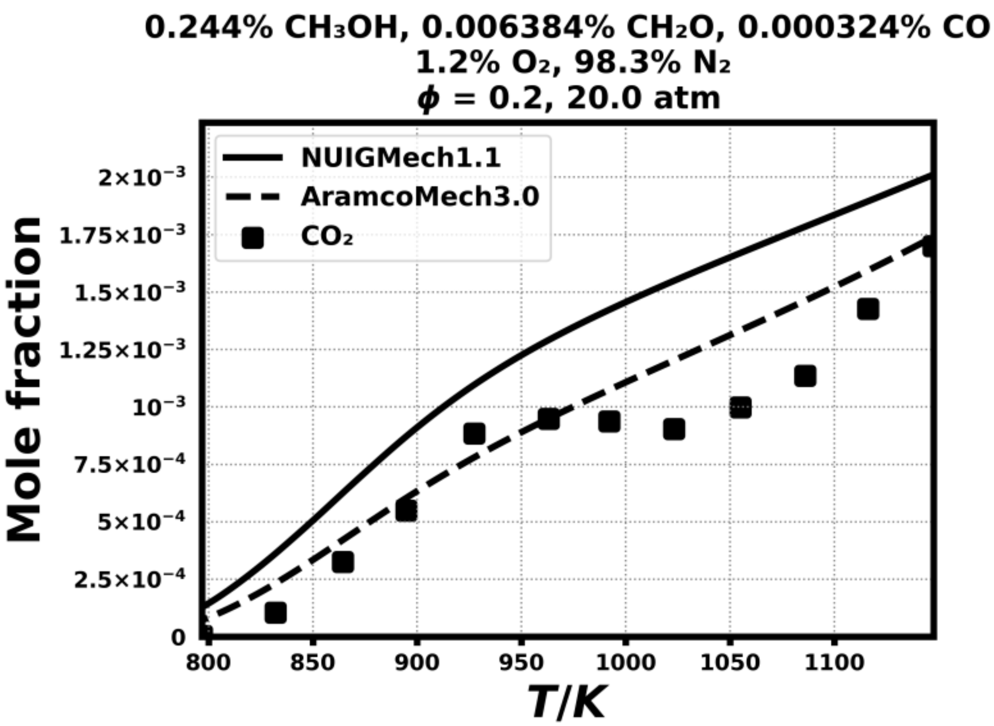

0.2% CH₃OH, 0.02658% CH₂O
0.3% O₂, 99.5% N₂
ϕ = 1.00, 1.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
T/K
3.5×10⁻³
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
850
900
950
1000
1050
1100
1150

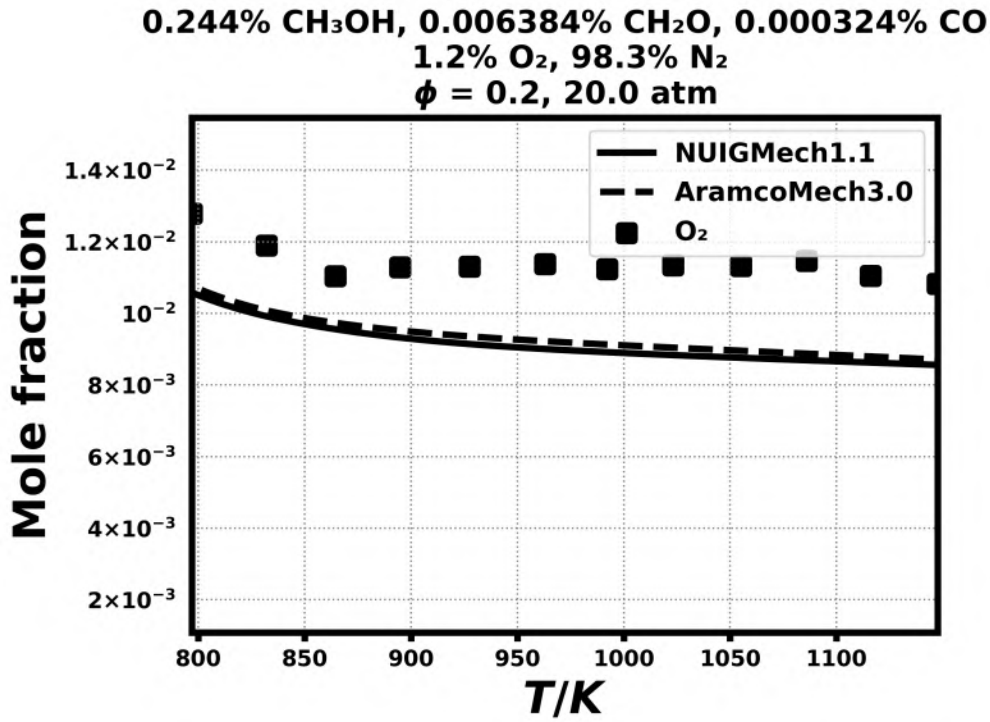

0.2% CH₃OH, 0.02658% CH₂O
0.3% O₂, 99.5% N₂
ϕ = 1.00, 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
T/K
1.6×10⁻³
1.4×10⁻³
1.2×10⁻³
10⁻³
8×10⁻⁴
6×10⁻⁴
4×10⁻⁴
2×10⁻⁴
0
850
900
950
1000
1050
1100
1150


0.2% CH₃OH, 0.02658% CH₂O
0.3% O₂, 99.5% N₂
ϕ = 1.00, 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
T/K

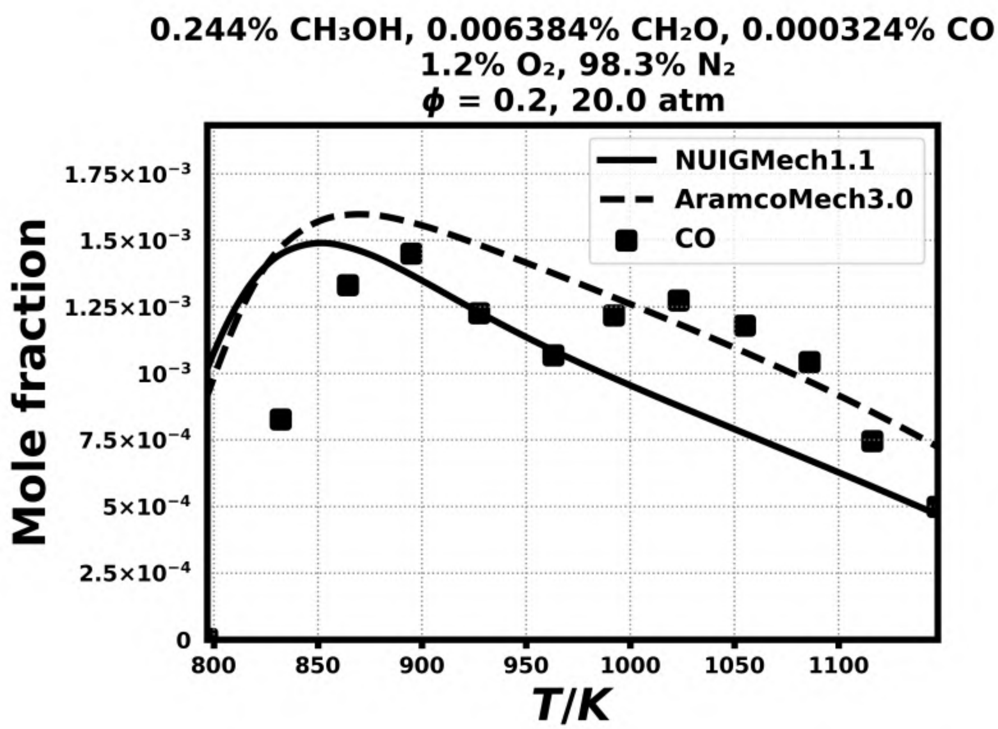

0.2% CH₃OH, 0.02658% CH₂O
0.3% O₂, 99.5% N₂
ϕ = 1.00, 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₃OH
Mole fraction
T/K


0.2% CH₃OH, 0.02658% CH₂O
0.3% O₂, 99.5% N₂
ϕ = 1.00, 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
2×10⁻³
1.75×10⁻³
1.5×10⁻³
1.25×10⁻³
10⁻³
7.5×10⁻⁴
5×10⁻⁴
2.5×10⁻⁴
850
900
950
1000
1050
1100
1150
T/K

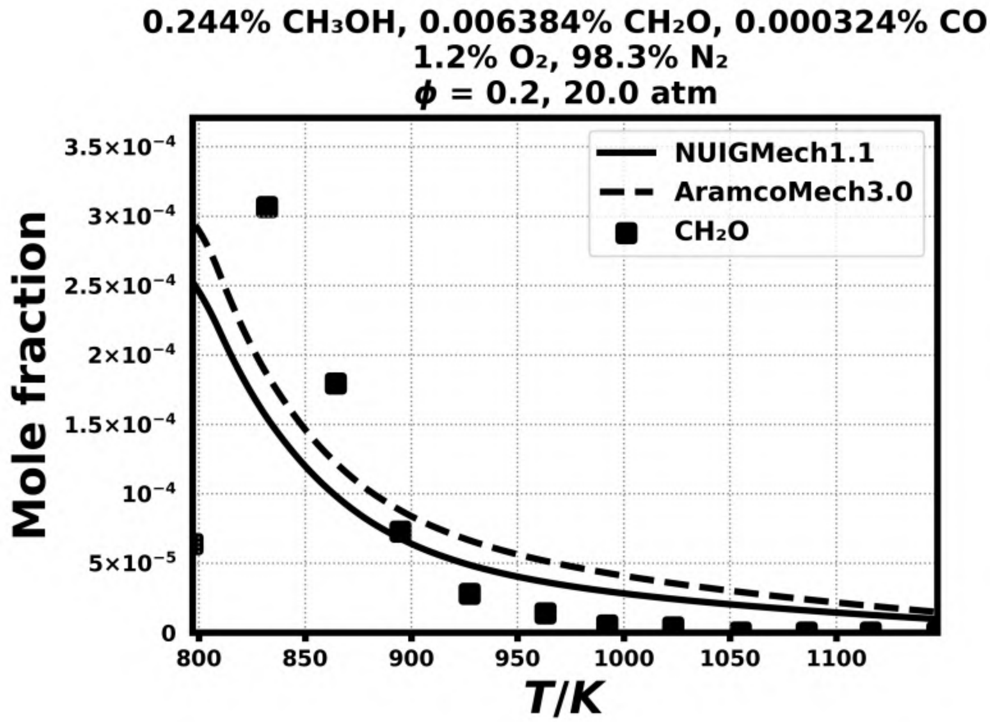

0.244% CH₃OH, 0.006384% CH₂O, 0.000324% CO
1.2% O₂, 98.3% N₂
ϕ = 0.2, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CO₂
Mole fraction
2×10⁻³
1.75×10⁻³
1.5×10⁻³
1.25×10⁻³
10⁻³
7.5×10⁻⁴
5×10⁻⁴
2.5×10⁻⁴
0
800
850
900
950
1000
1050
1100
T/K

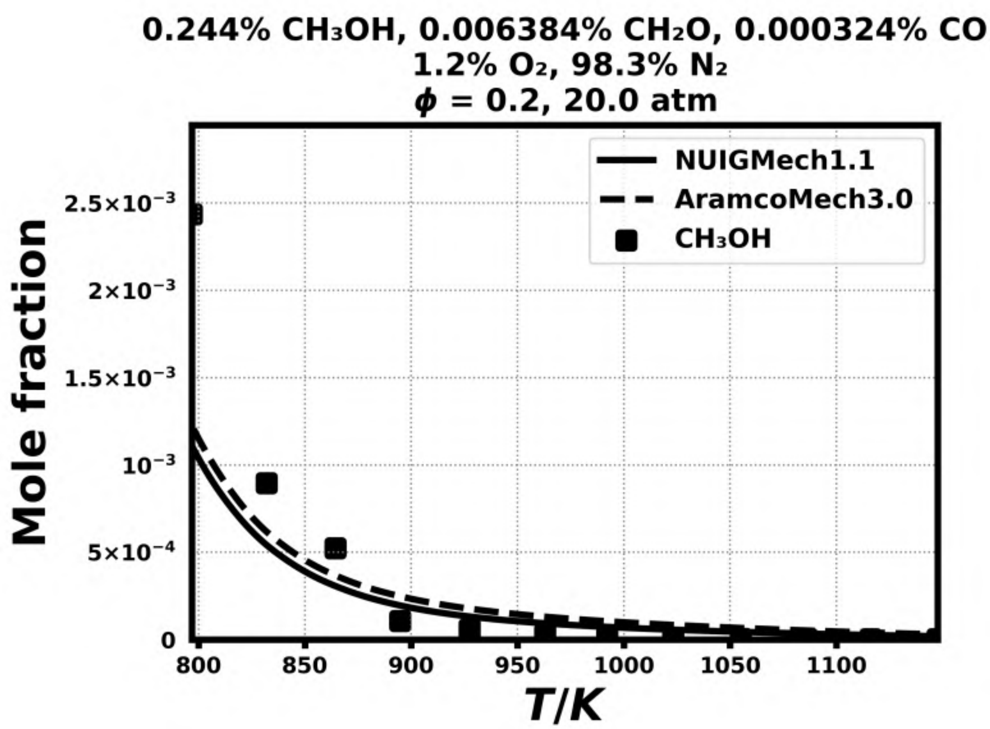


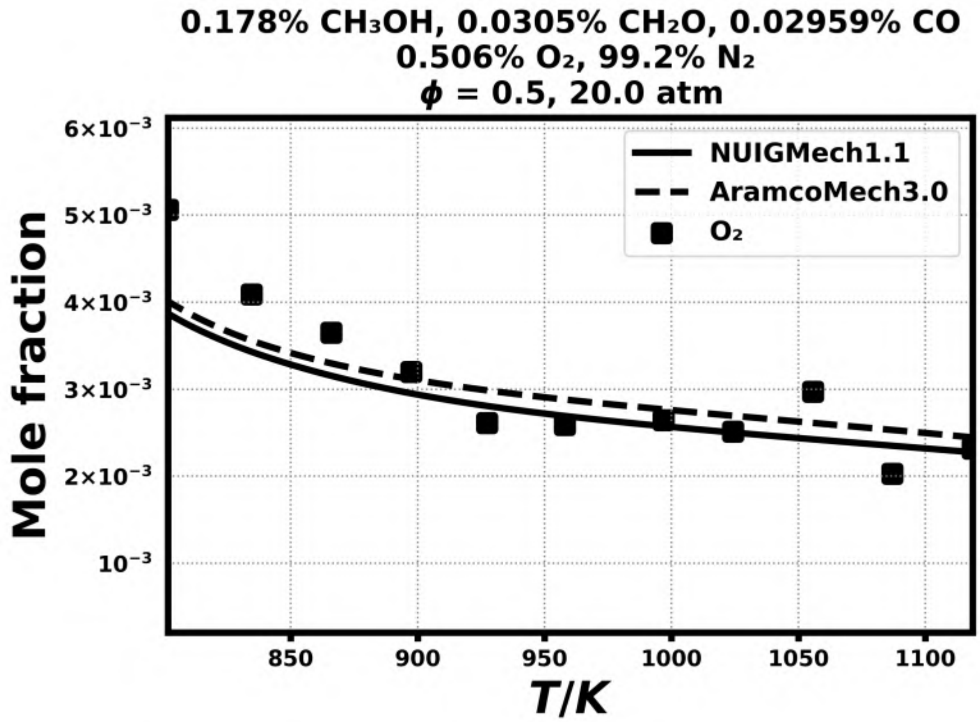
0.244% CH₃OH, 0.006384% CH₂O, 0.000324% CO
1.2% O₂, 98.3% N₂
ϕ = 0.2, 20.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
T/K

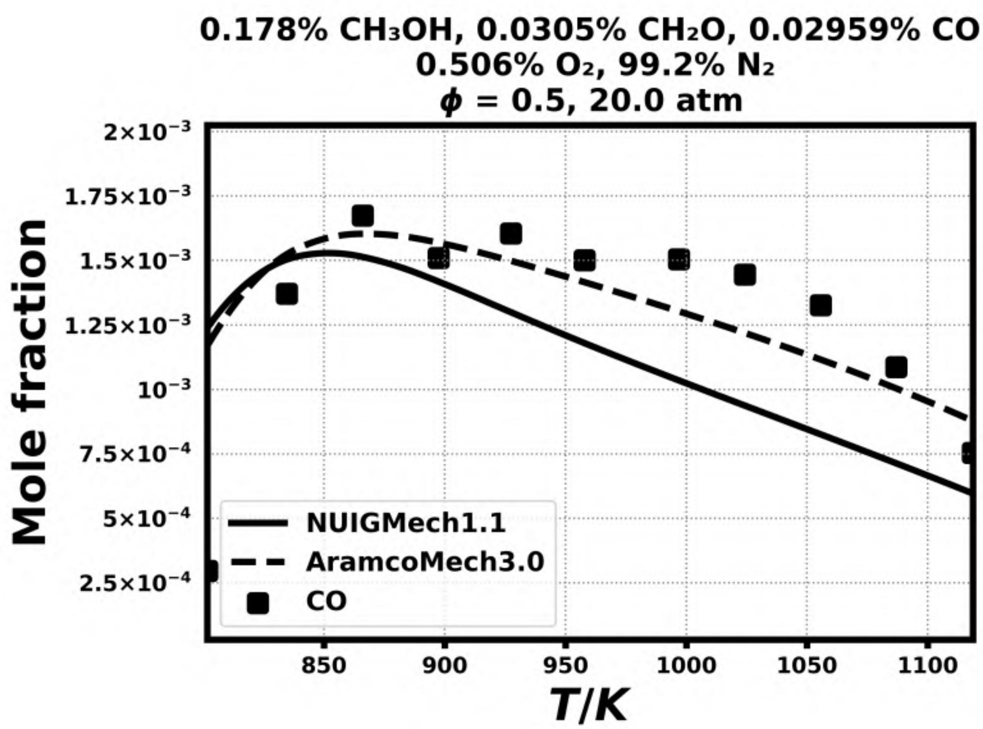


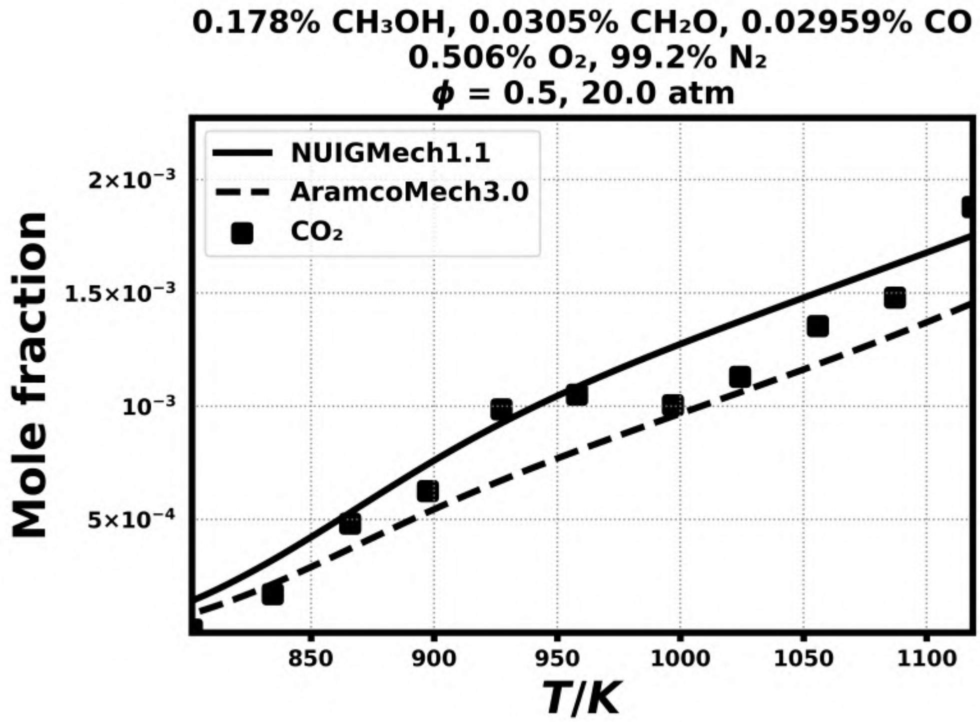
0.244% CH₃OH, 0.006384% CH₂O, 0.000324% CO
1.2% O₂, 98.3% N₂
ϕ = 0.2, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
T/K

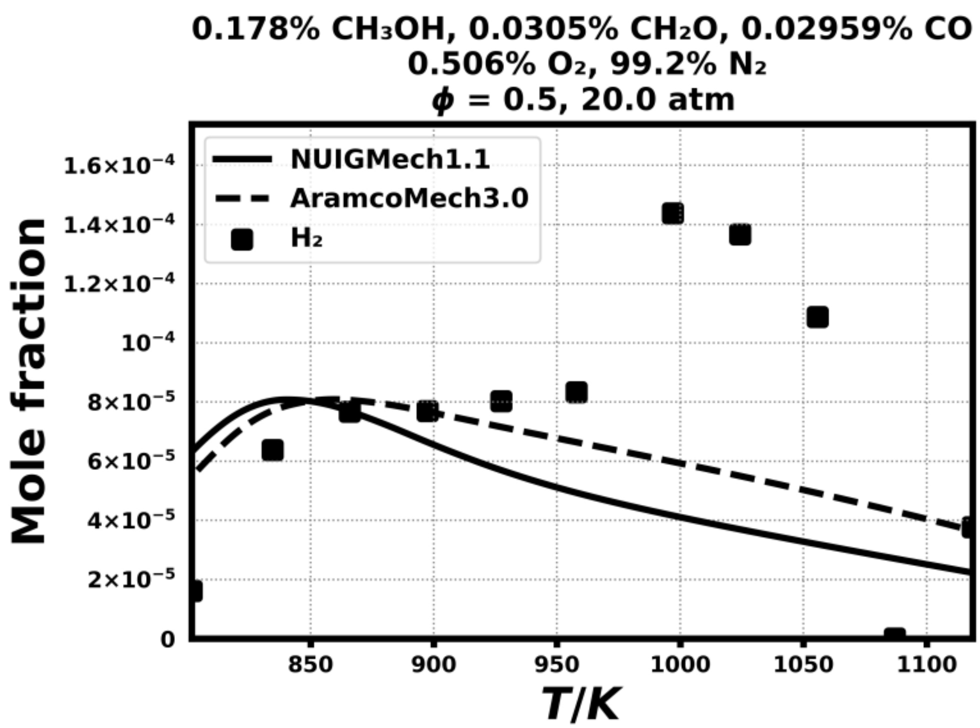

0.244% CH₃OH, 0.006384% CH₂O, 0.000324% CO
1.2% O₂, 98.3% N₂
ϕ = 0.2, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
T/K

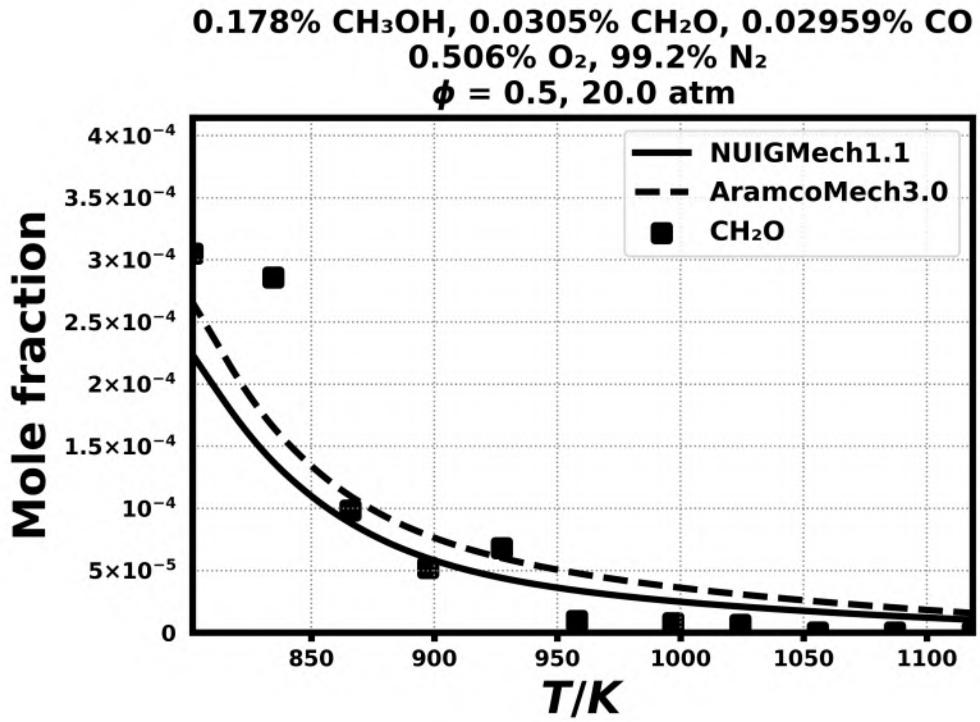

0.244% CH₃OH, 0.006384% CH₂O, 0.000324% CO
1.2% O₂, 98.3% N₂
ϕ = 0.2, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CH₃OH
Mole fraction
T/K

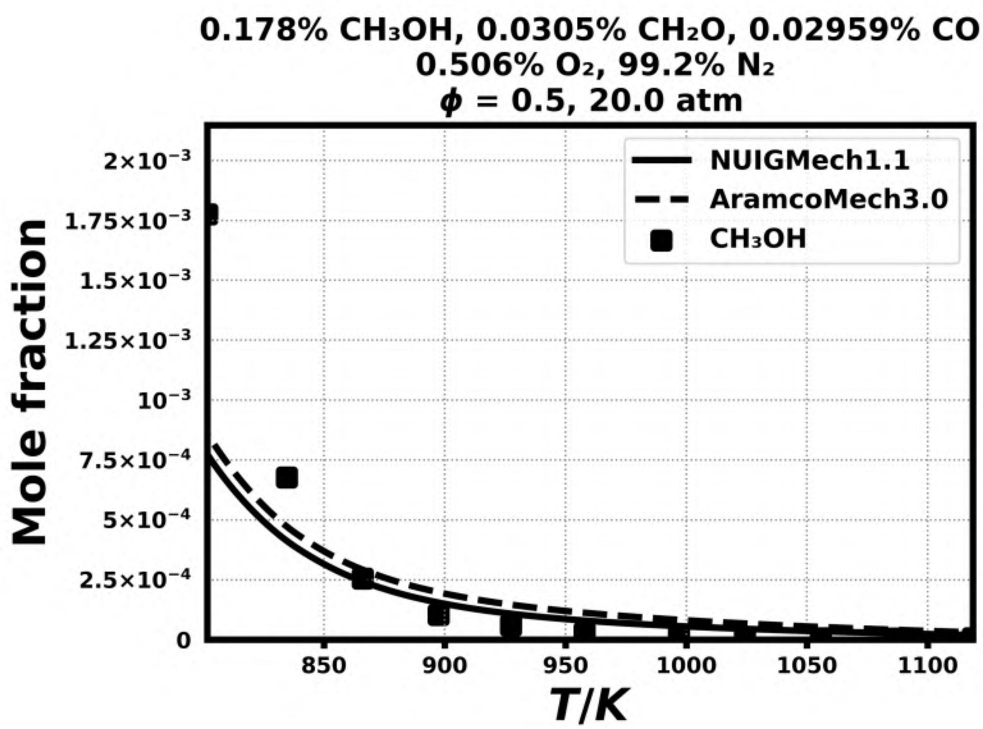

0.178% CH₃OH, 0.0305% CH₂O, 0.02959% CO
0.506% O₂, 99.2% N₂
ϕ = 0.5, 20.0 atm
Mole fraction
6×10⁻³
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
850
900
950
1000
1050
1100
T/K
NUIGMech1.1
AramcoMech3.0
O₂

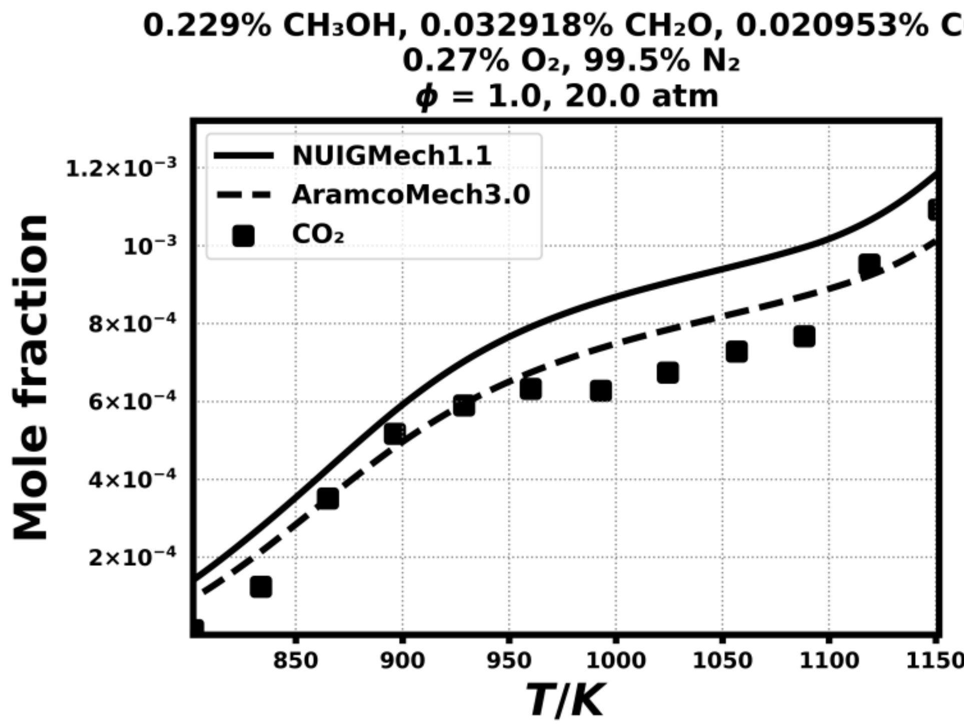

0.178% CH₃OH, 0.0305% CH₂O, 0.02959% CO
0.506% O₂, 99.2% N₂
ϕ = 0.5, 20.0 atm
Mole fraction
2×10⁻³
1.75×10⁻³
1.5×10⁻³
1.25×10⁻³
10⁻³
7.5×10⁻⁴
5×10⁻⁴
2.5×10⁻⁴
850
900
950
1000
1050
1100
T/K
NUIGMech1.1
AramcoMech3.0
CO


0.178% CH₃OH, 0.0305% CH₂O, 0.02959% CO
0.506% O₂, 99.2% N₂
ϕ = 0.5, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CO₂
Mole fraction
T/K

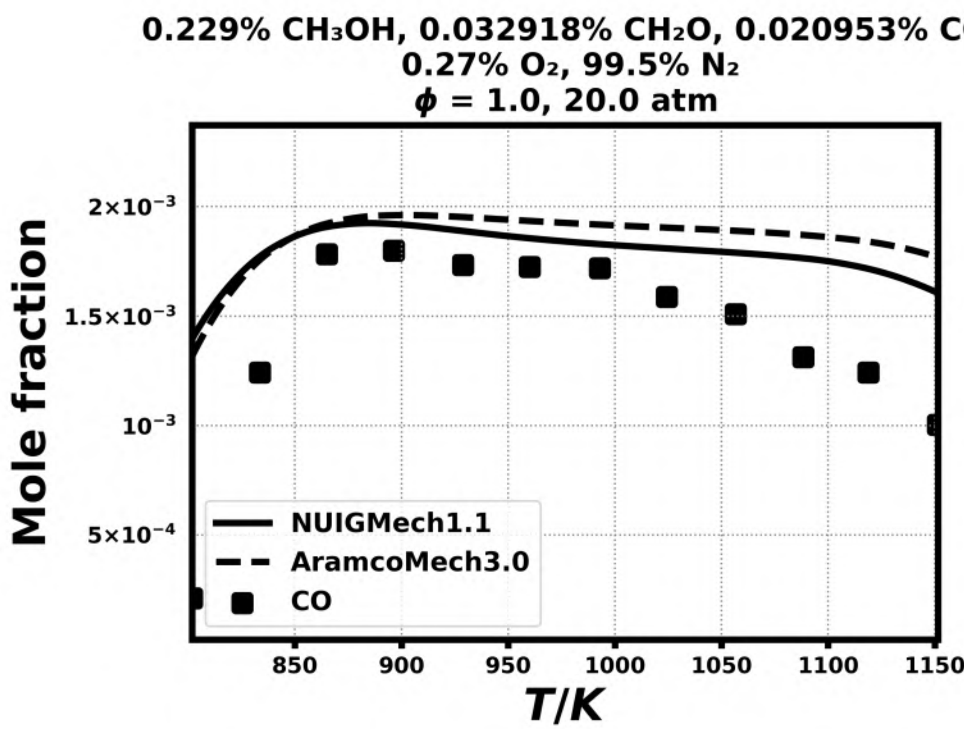

0.178% CH₃OH, 0.0305% CH₂O, 0.02959% CO
0.506% O₂, 99.2% N₂
ϕ = 0.5, 20.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K


0.178% CH₃OH, 0.0305% CH₂O, 0.02959% CO
0.506% O₂, 99.2% N₂
ϕ = 0.5, 20.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH₂O
4×10⁻⁴
3.5×10⁻⁴
3×10⁻⁴
2.5×10⁻⁴
2×10⁻⁴
1.5×10⁻⁴
10⁻⁴
5×10⁻⁵
0
850
900
950
1000
1050
1100

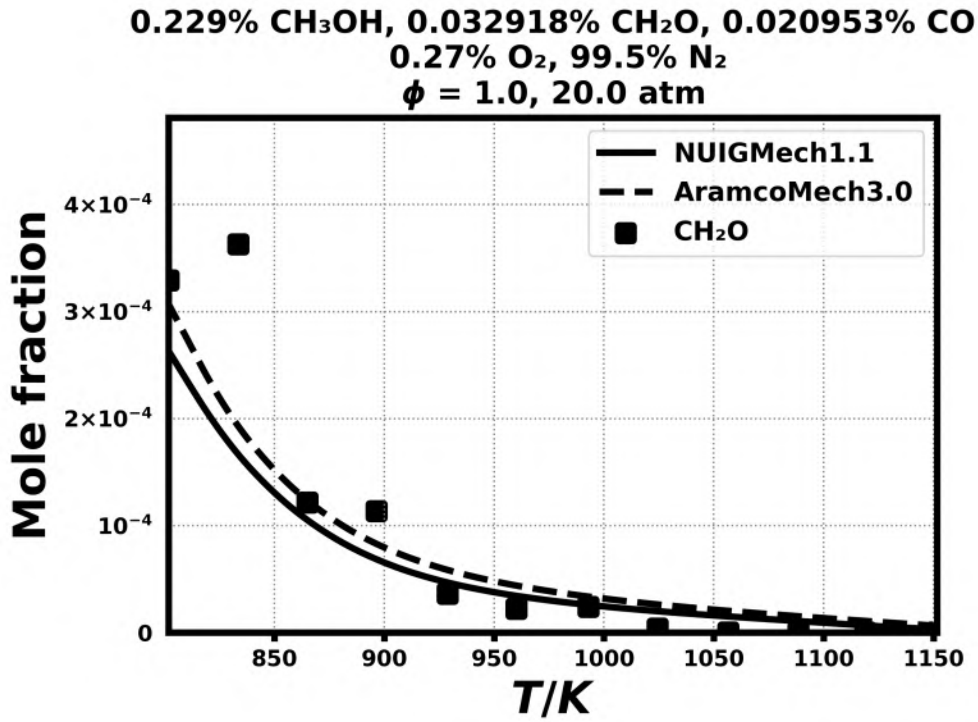

0.178% CH₃OH, 0.0305% CH₂O, 0.02959% CO
0.506% O₂, 99.2% N₂
ϕ = 0.5, 20.0 atm
Mole fraction
T/K
NUIGMech1.1
AramcoMech3.0
CH₃OH
2×10⁻³
1.75×10⁻³
1.5×10⁻³
1.25×10⁻³
10⁻³
7.5×10⁻⁴
5×10⁻⁴
2.5×10⁻⁴
0
850
900
950
1000
1050
1100

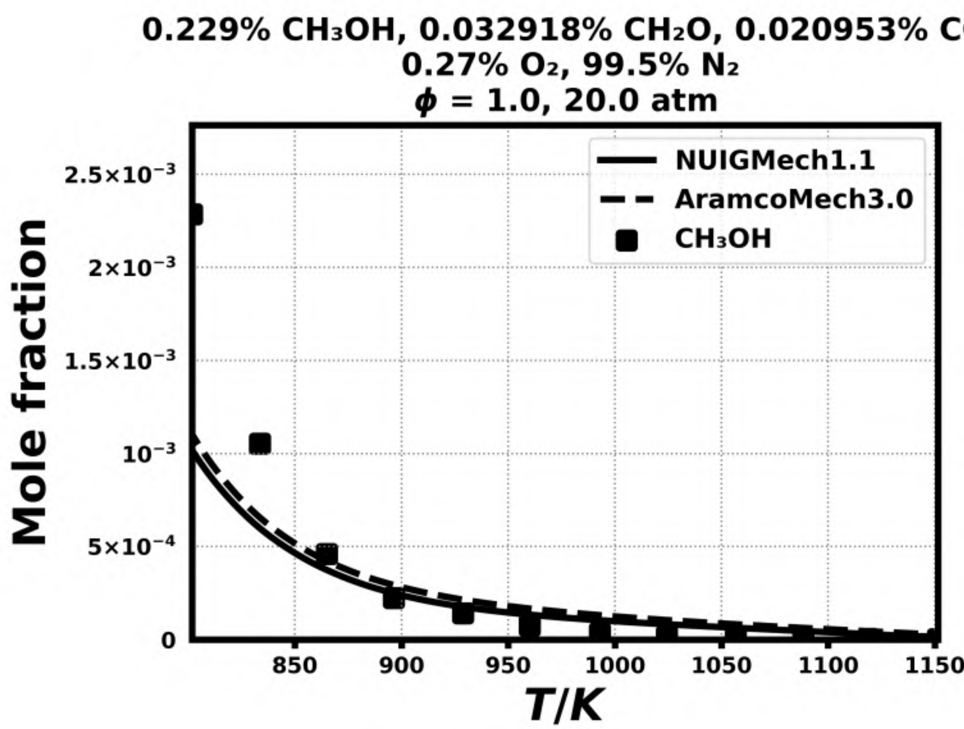


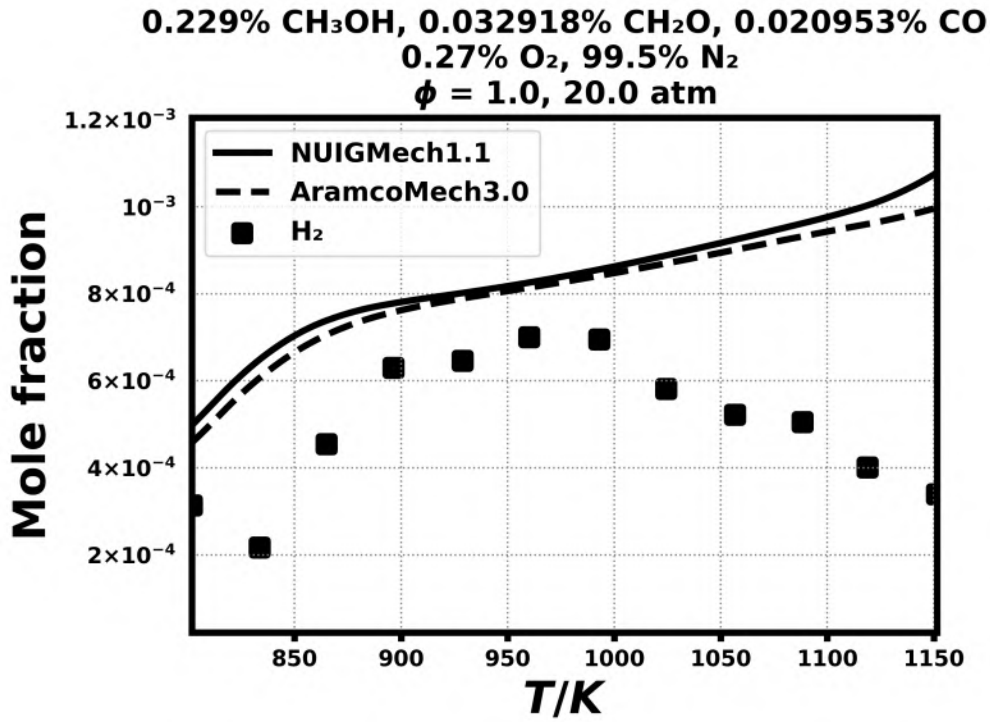
0.229% CH₃OH, 0.032918% CH₂O, 0.020953% CO
0.27% O₂, 99.5% N₂
ϕ = 1.0, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CO₂
Mole fraction
T/K
1.2×10⁻³
10⁻³
8×10⁻⁴
6×10⁻⁴
4×10⁻⁴
2×10⁻⁴
850
900
950
1000
1050
1100
1150



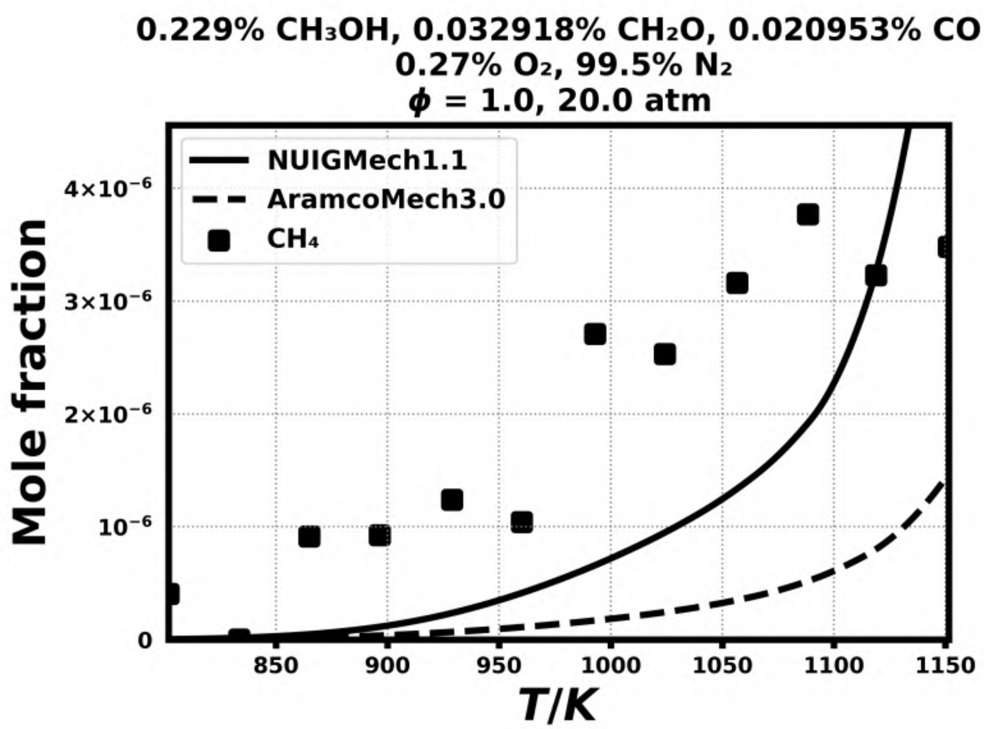
0.229% CH₃OH, 0.032918% CH₂O, 0.020953% CO
0.27% O₂, 99.5% N₂
ϕ = 1.0, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
T/K
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
850
900
950
1000
1050
1100
1150


0.229% CH3OH, 0.032918% CH2O, 0.020953% CO
0.27% O2, 99.5% N2
ϕ = 1.0, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CH2O
Mole fraction
4×10⁻⁴
3×10⁻⁴
2×10⁻⁴
10⁻⁴
0
850
900
950
1000
1050
1100
1150
T/K


0.229% CH3OH, 0.032918% CH2O, 0.020953% CO
0.27% O2, 99.5% N2
ϕ = 1.0, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CH3OH
Mole fraction
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
0
850
900
950
1000
1050
1100
1150
T/K



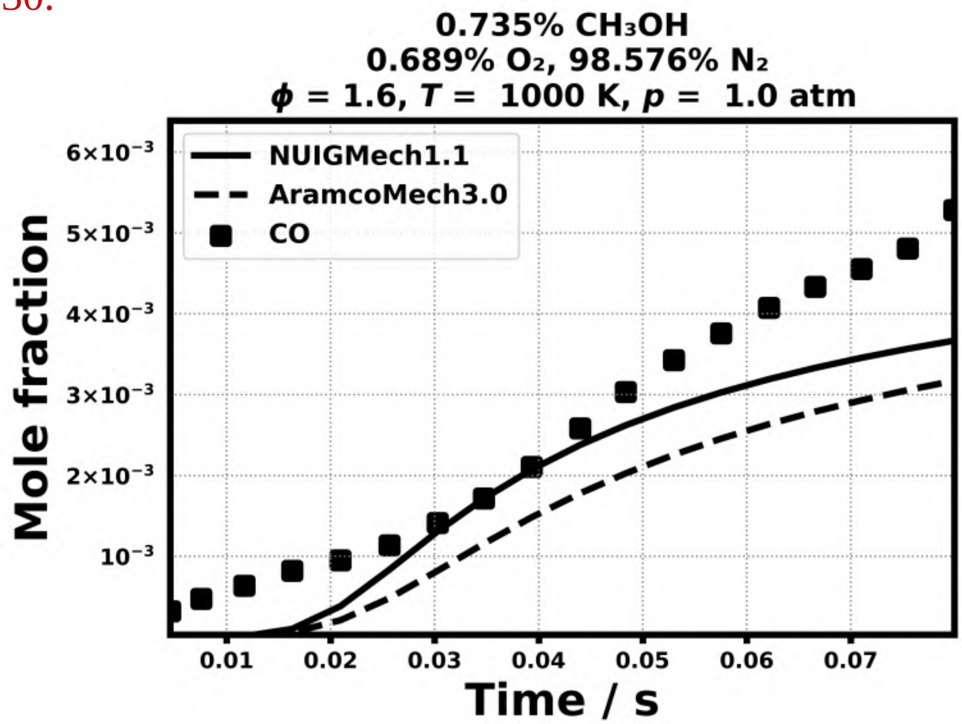
0.229% CH₃OH, 0.032918% CH₂O, 0.020953% CO
0.27% O₂, 99.5% N₂
ϕ = 1.0, 20.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
T/K

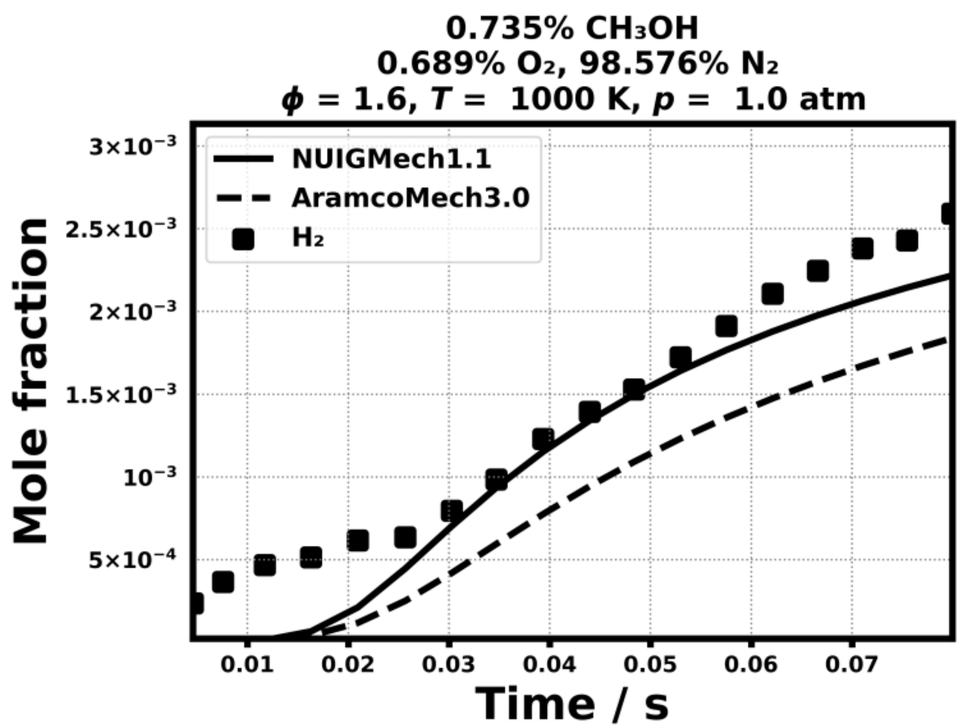


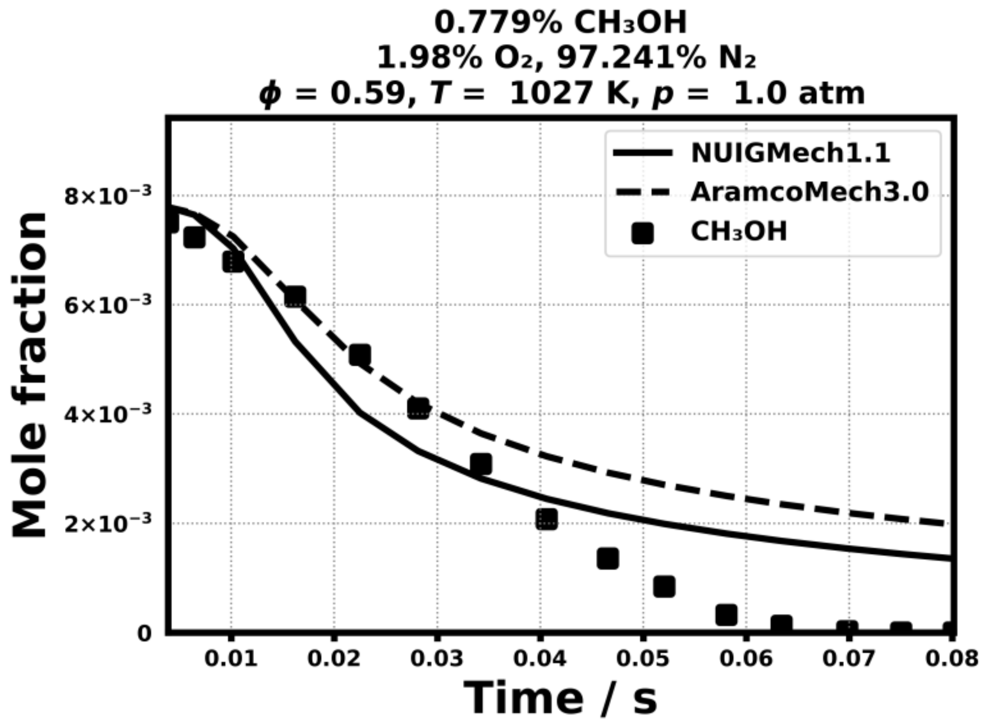
0.229% CH₃OH, 0.032918% CH₂O, 0.020953% CO
0.27% O₂, 99.5% N₂
ϕ = 1.0, 20.0 atm
NUIGMech1.1
AramcoMech3.0
CH₄
Mole fraction
T/K

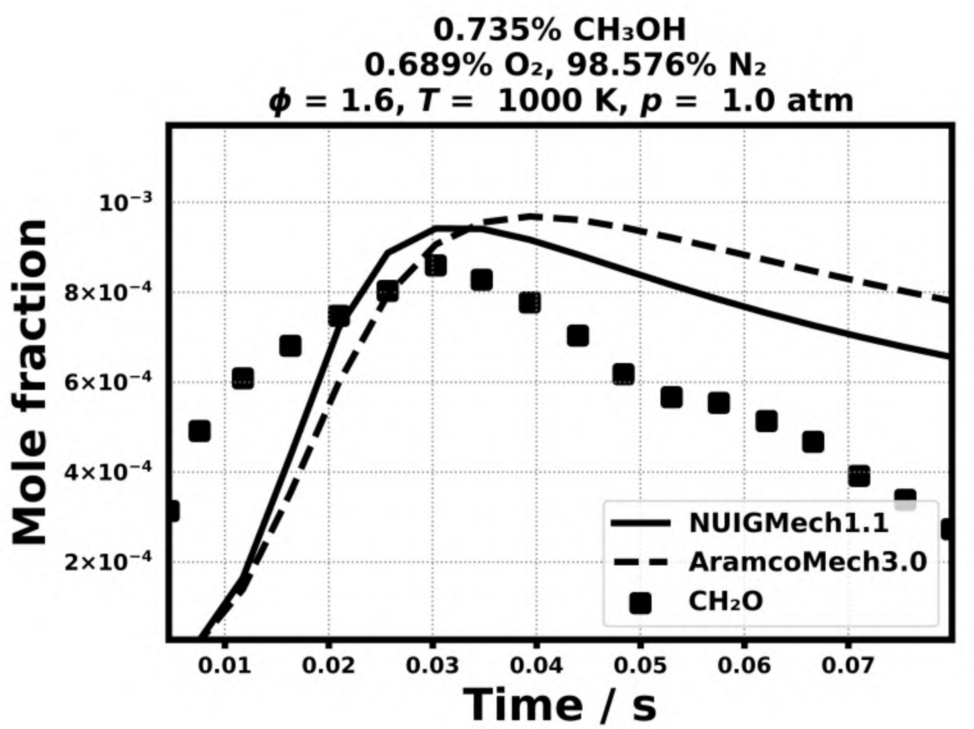
Speciation in Flow reactor

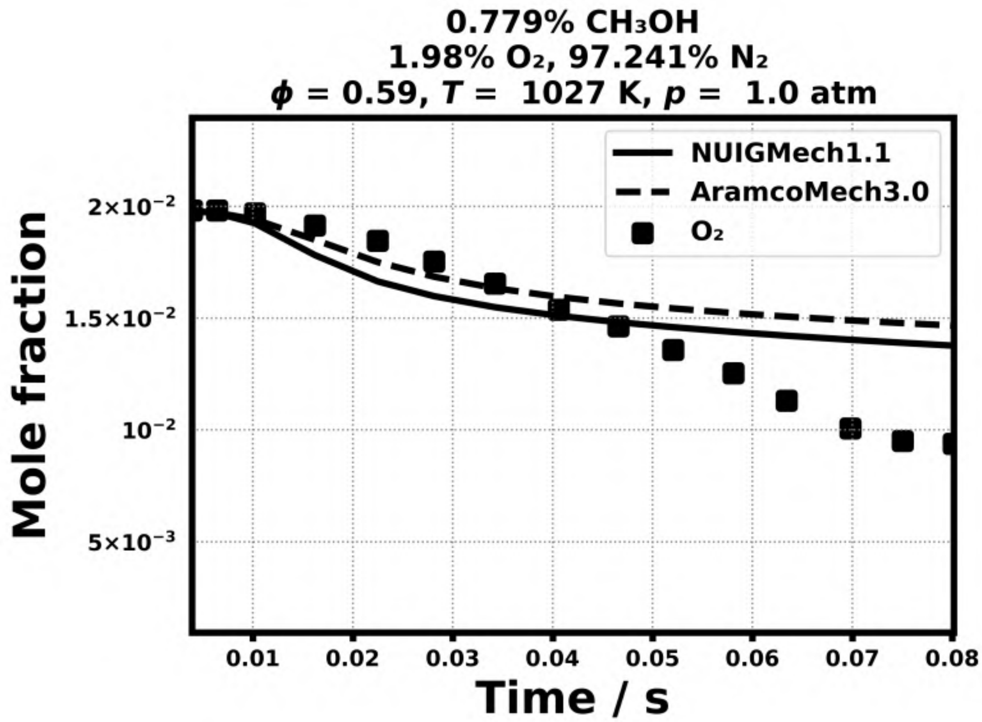
4.9) Held, T. J., & Dryer, F. L., International Journal of Chemical Kinetics, 30(11) (1998) 805-830.

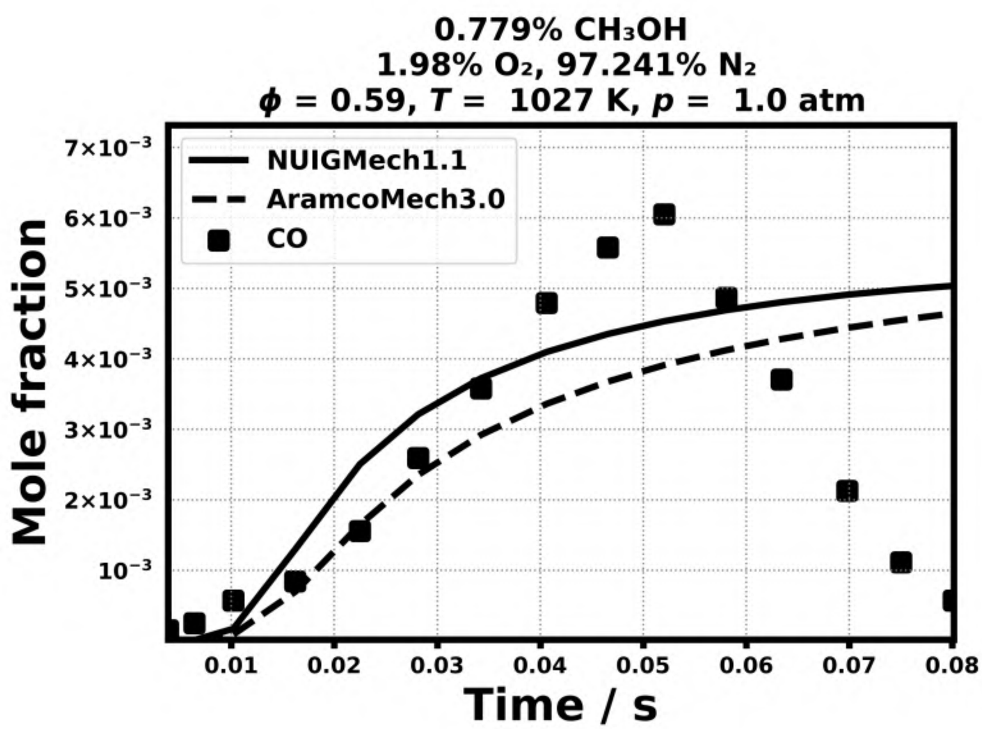


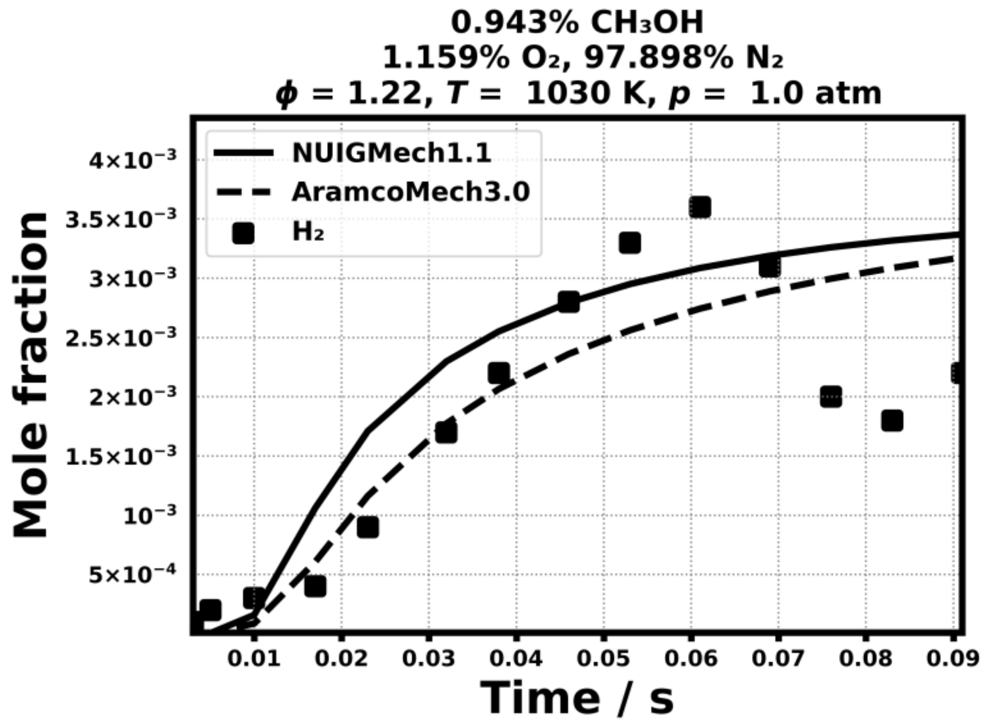


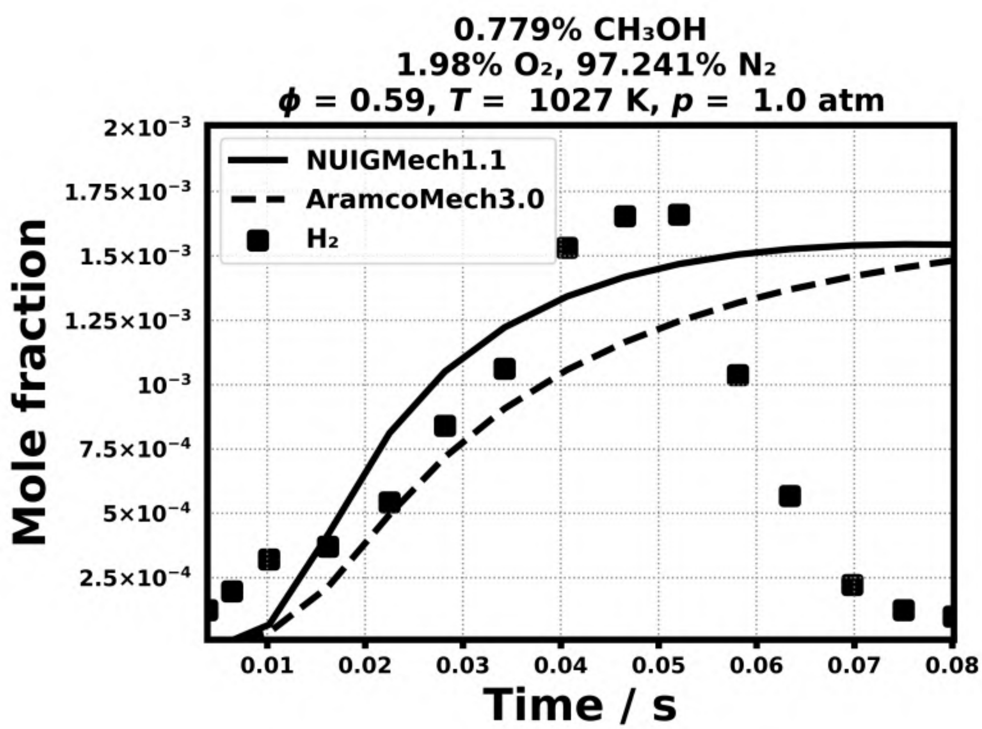

0.779% CH₃OH
1.98% O₂, 97.241% N₂
ϕ = 0.59, T = 1027 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₃OH
Mole fraction
Time / s

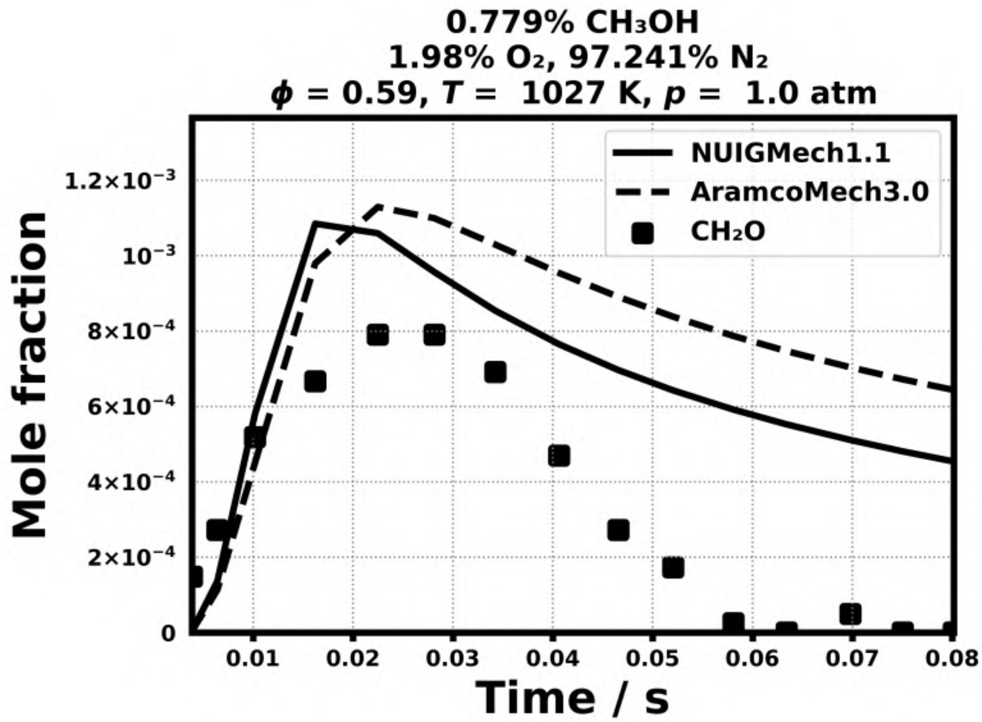

0.735% CH₃OH
0.689% O₂, 98.576% N₂
ϕ = 1.6, T = 1000 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
Time / s

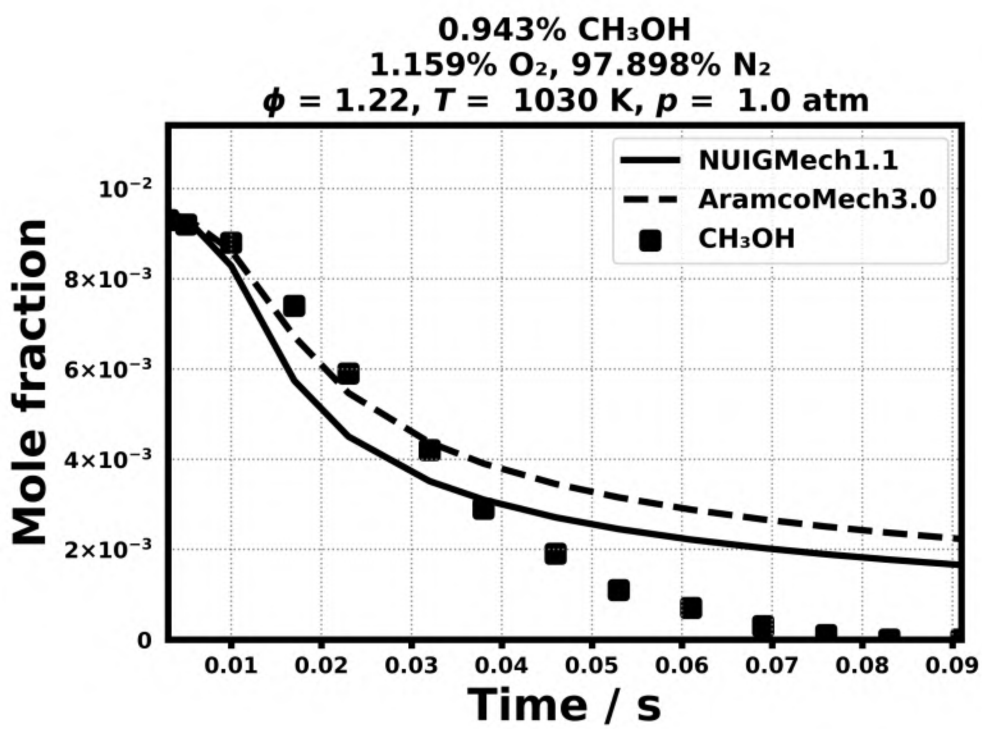

0.779% CH₃OH
1.98% O₂, 97.241% N₂
ϕ = 0.59, T = 1027 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
Time / s

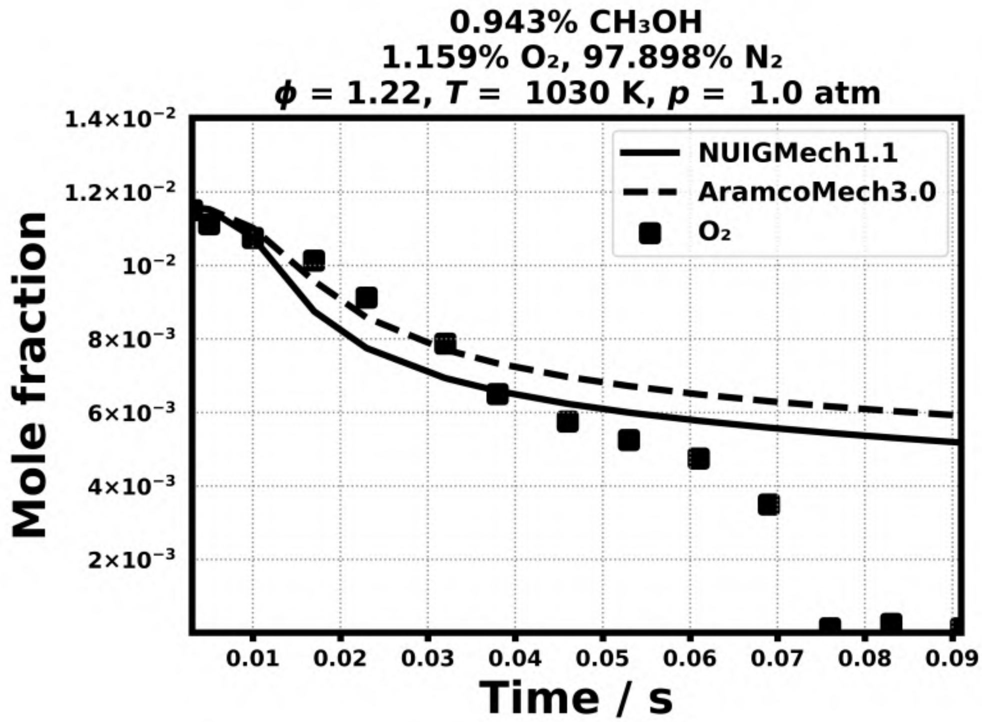

0.779% CH₃OH
1.98% O₂, 97.241% N₂
ϕ = 0.59, T = 1027 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
Time / s

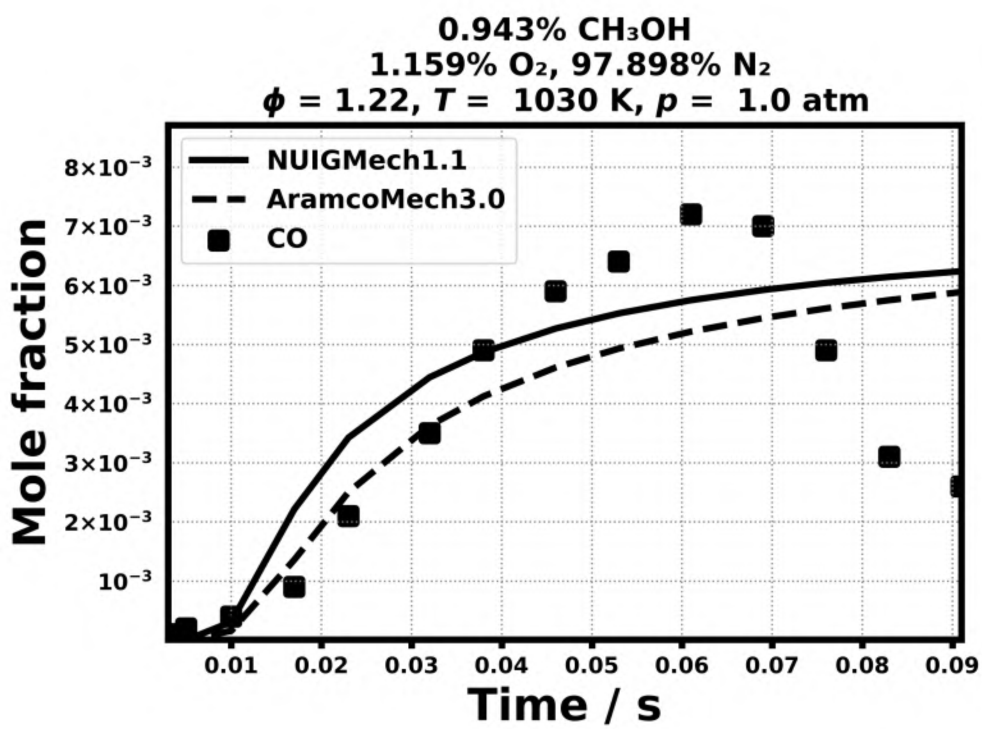

0.943% CH₃OH
1.159% O₂, 97.898% N₂
ϕ = 1.22, T = 1030 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
Time / s
4×10⁻³
3.5×10⁻³
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09

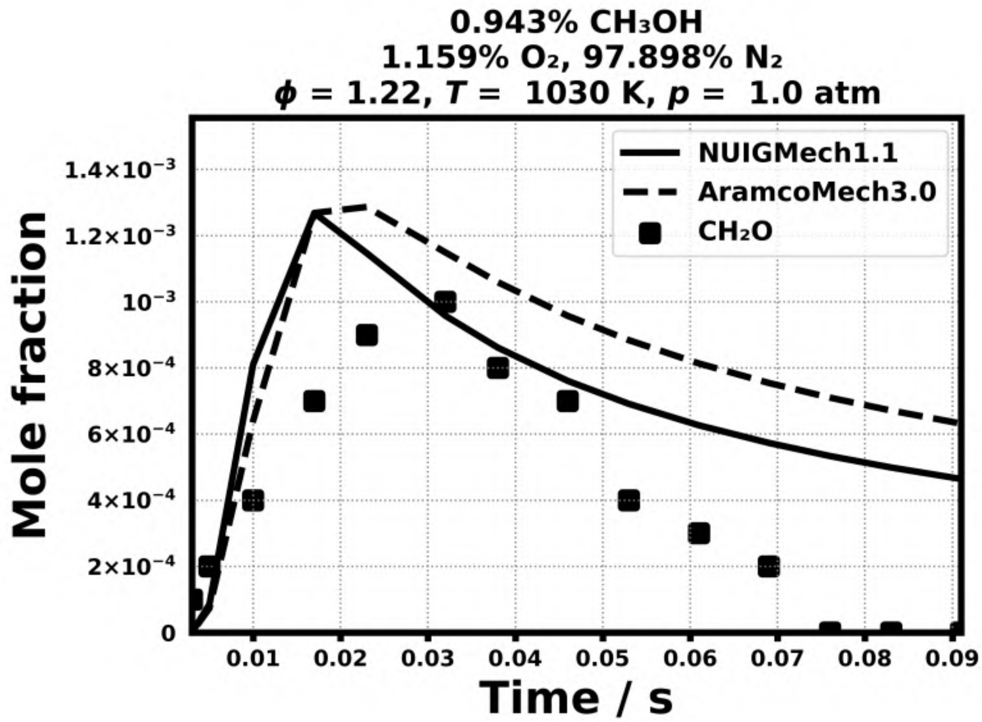

0.779% CH₃OH
1.98% O₂, 97.241% N₂
ϕ = 0.59, T = 1027 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
Time / s
2×10⁻³
1.75×10⁻³
1.5×10⁻³
1.25×10⁻³
10⁻³
7.5×10⁻⁴
5×10⁻⁴
2.5×10⁻⁴
0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08

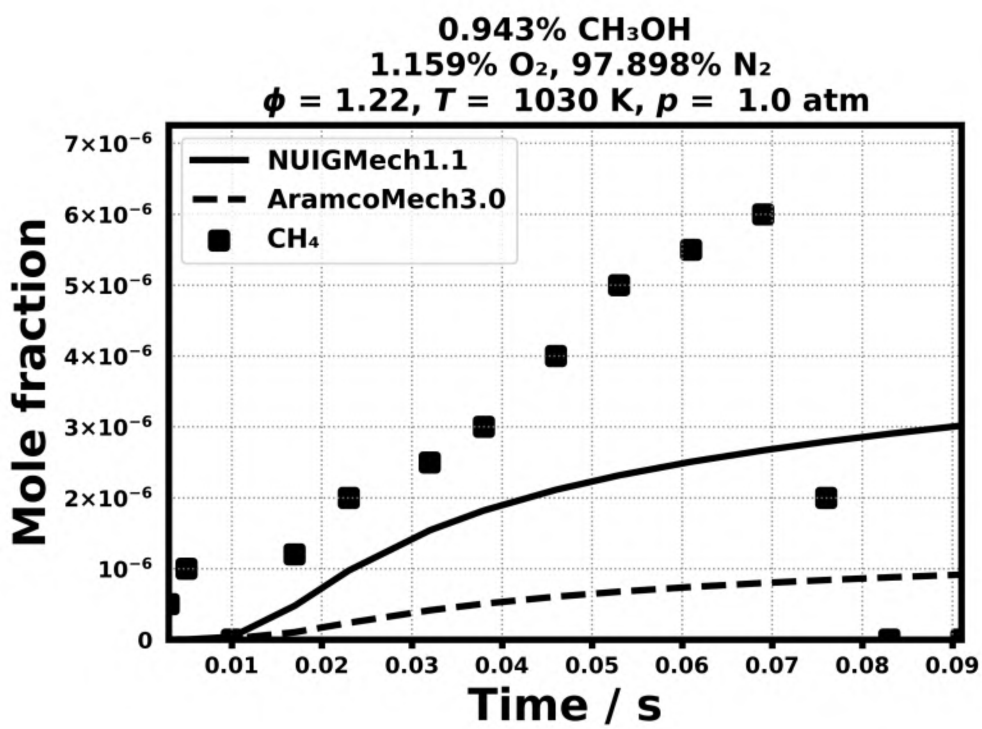

0.779% CH₃OH
1.98% O₂, 97.241% N₂
ϕ = 0.59, T = 1027 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
Time / s

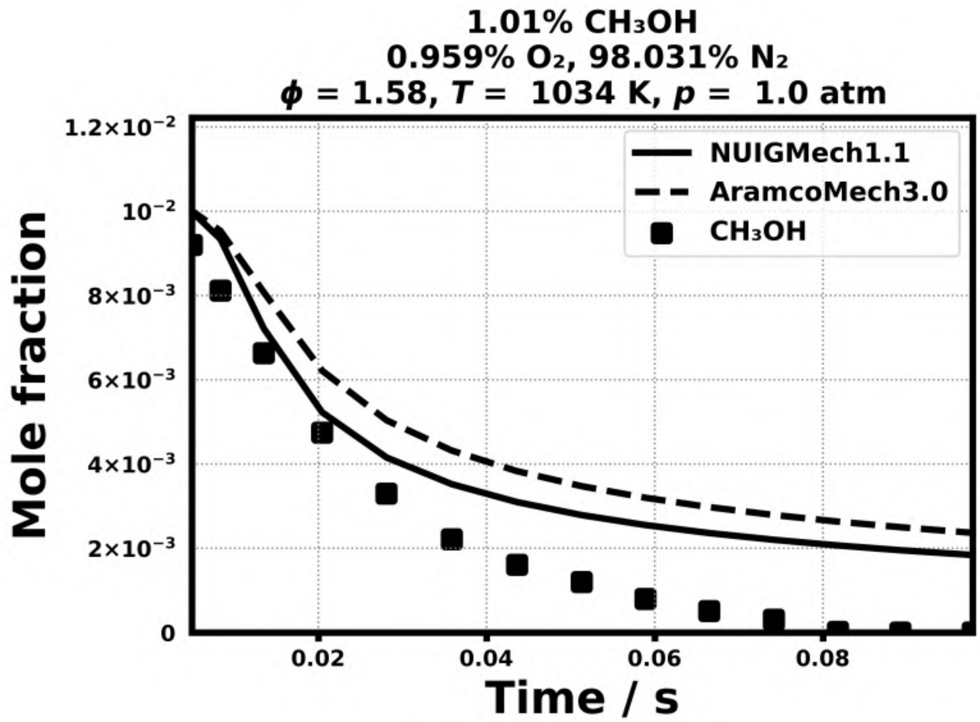

0.943% CH₃OH
1.159% O₂, 97.898% N₂
ϕ = 1.22, T = 1030 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₃OH
Mole fraction
Time / s

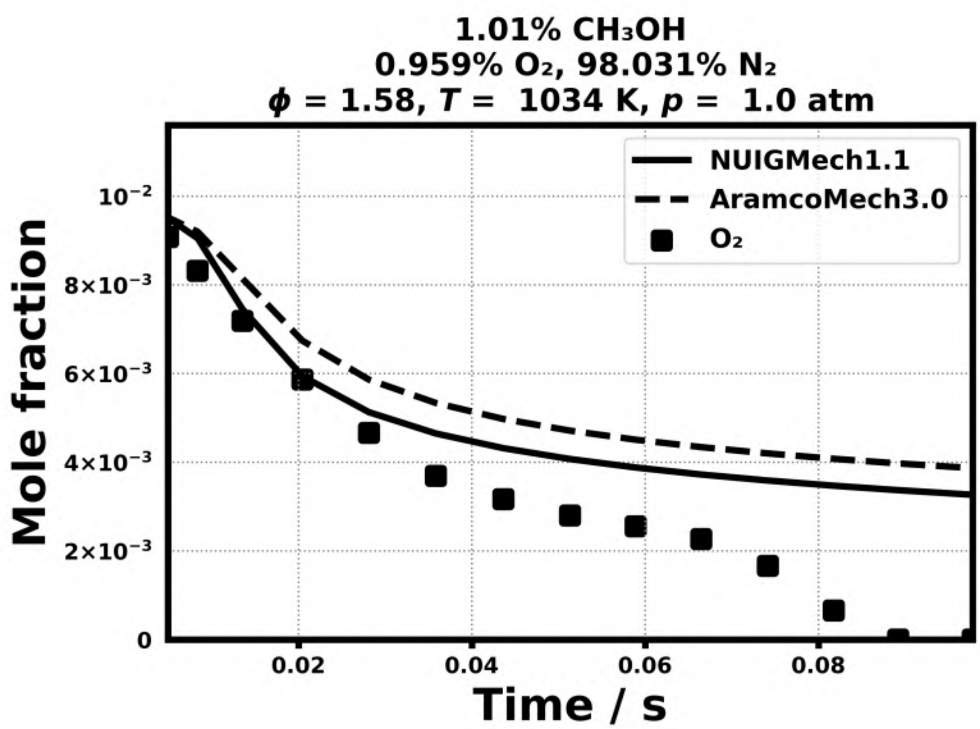

0.943% CH₃OH
1.159% O₂, 97.898% N₂
ϕ = 1.22, T = 1030 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
Time / s
1.4×10⁻²
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09

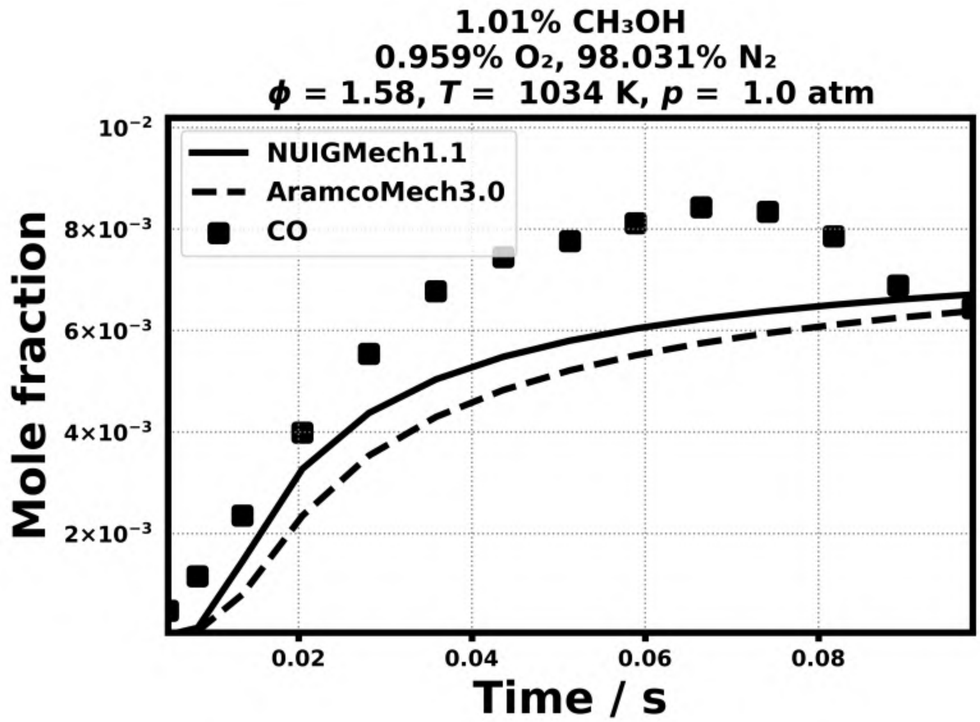

0.943% CH₃OH
1.159% O₂, 97.898% N₂
ϕ = 1.22, T = 1030 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
Time / s
8×10⁻³
7×10⁻³
6×10⁻³
5×10⁻³
4×10⁻³
3×10⁻³
2×10⁻³
10⁻³
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09

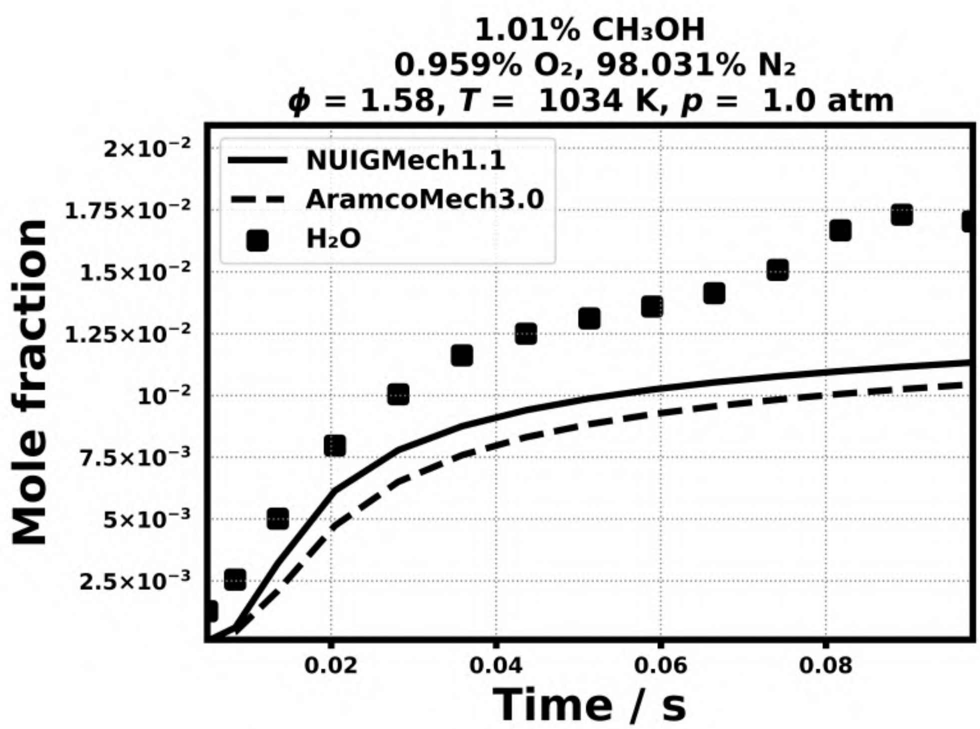

0.943% CH₃OH
1.159% O₂, 97.898% N₂
ϕ = 1.22, T = 1030 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
Time / s

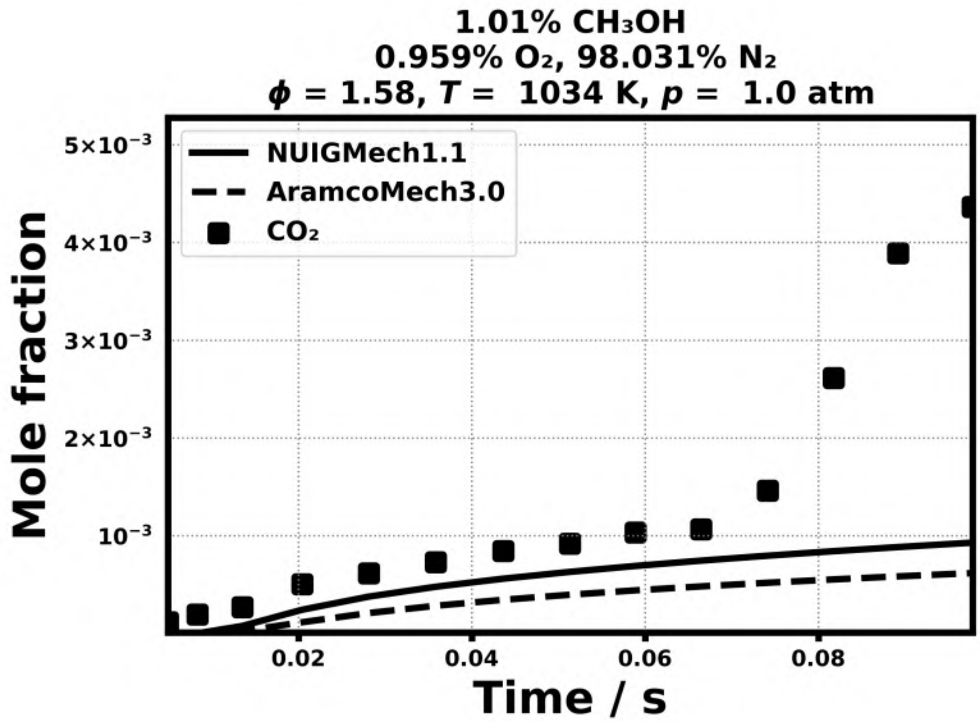

0.943% CH₃OH
1.159% O₂, 97.898% N₂
ϕ = 1.22, T = 1030 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₄
Mole fraction
Time / s


1.01% CH3OH
0.959% O2, 98.031% N2
ϕ = 1.58, T = 1034 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH3OH
Mole fraction
Time / s
1.2×10⁻²
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
0
0.02
0.04
0.06
0.08

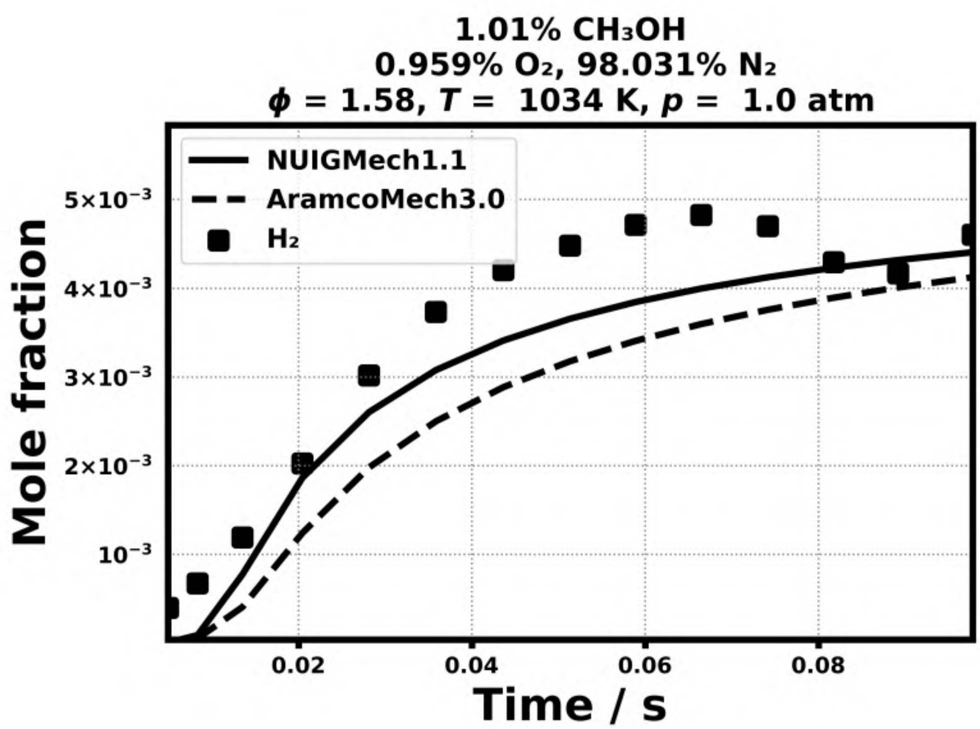

1.01% CH3OH
0.959% O2, 98.031% N2
ϕ = 1.58, T = 1034 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
O2
Mole fraction
Time / s
10⁻²
8×10⁻³
6×10⁻³
4×10⁻³
2×10⁻³
0
0.02
0.04
0.06
0.08


1.01% CH3OH
0.959% O2, 98.031% N2
ϕ = 1.58, T = 1034 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
Time / s
10−2
8×10−3
6×10−3
4×10−3
2×10−3
0.02
0.04
0.06
0.08

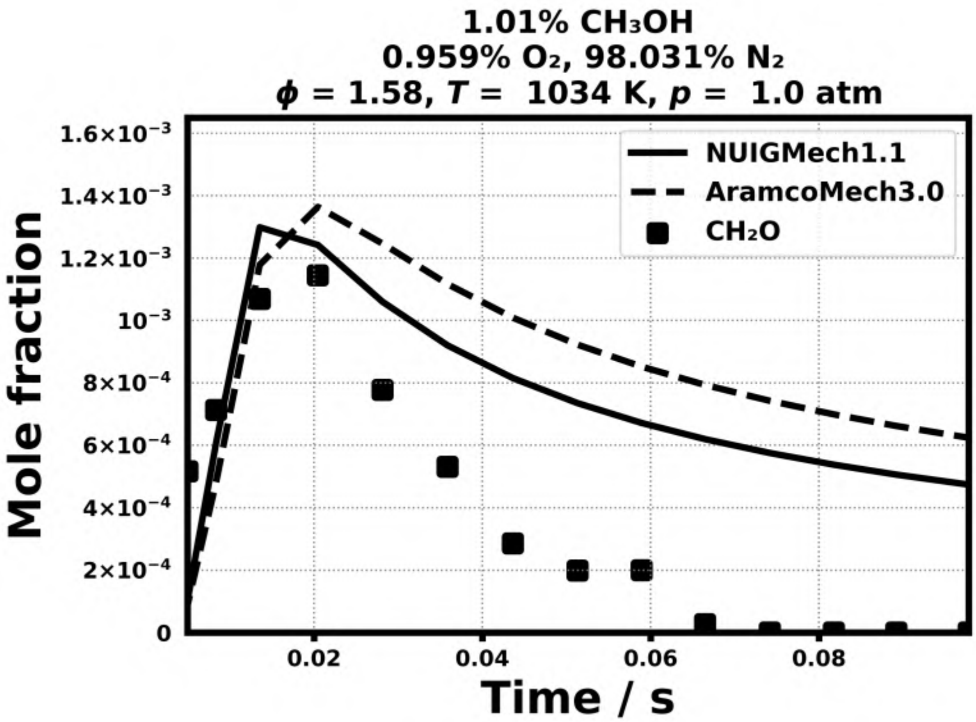

1.01% CH3OH
0.959% O2, 98.031% N2
ϕ = 1.58, T = 1034 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
H2O
Mole fraction
Time / s
2×10−2
1.75×10−2
1.5×10−2
1.25×10−2
10−2
7.5×10−3
5×10−3
2.5×10−3
0.02
0.04
0.06
0.08



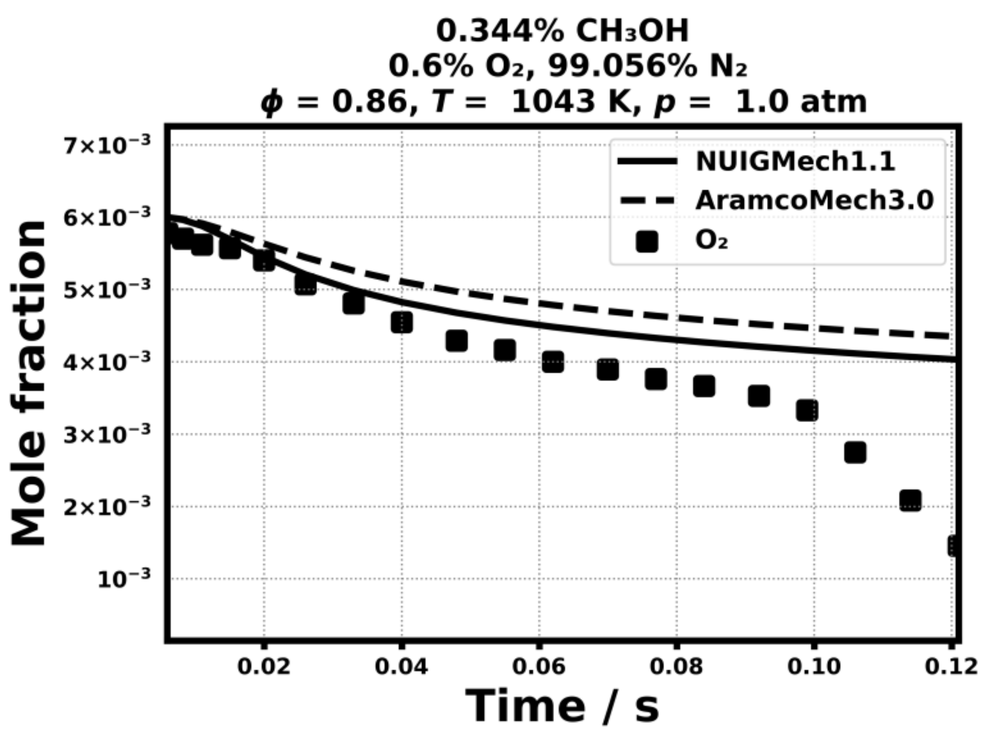
1.01% CH3OH
0.959% O2, 98.031% N2
ϕ = 1.58, T = 1034 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO2
Mole fraction
Time / s



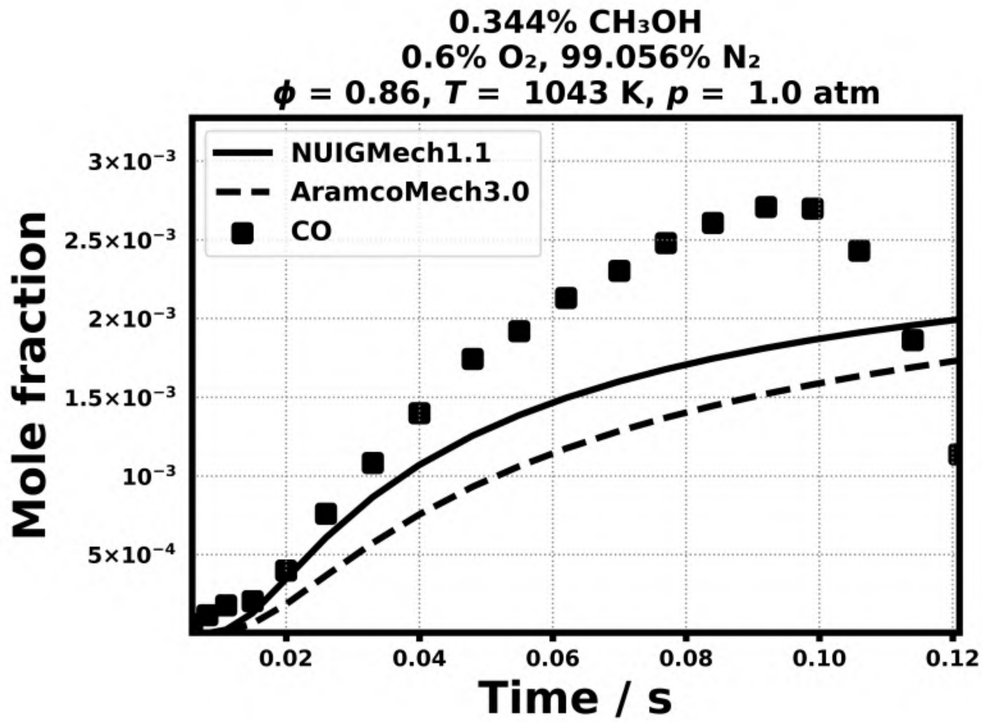
1.01% CH3OH
0.959% O2, 98.031% N2
ϕ = 1.58, T = 1034 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
H2
Mole fraction
Time / s



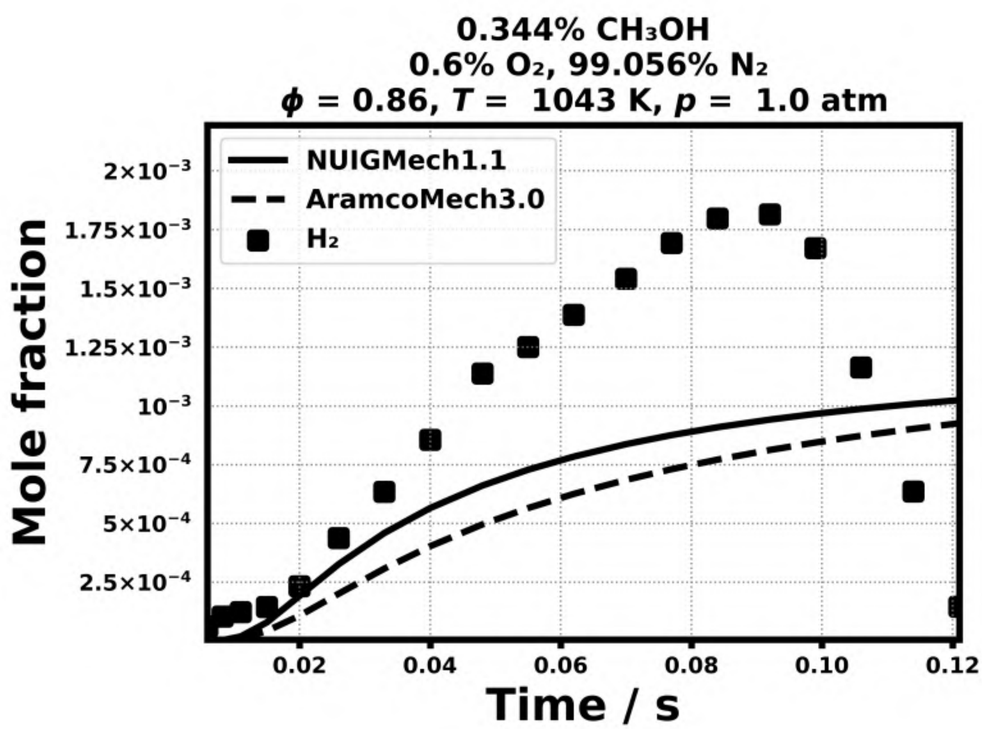
1.01% CH₃OH
0.959% O₂, 98.031% N₂
ϕ = 1.58, T = 1034 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
Time / s



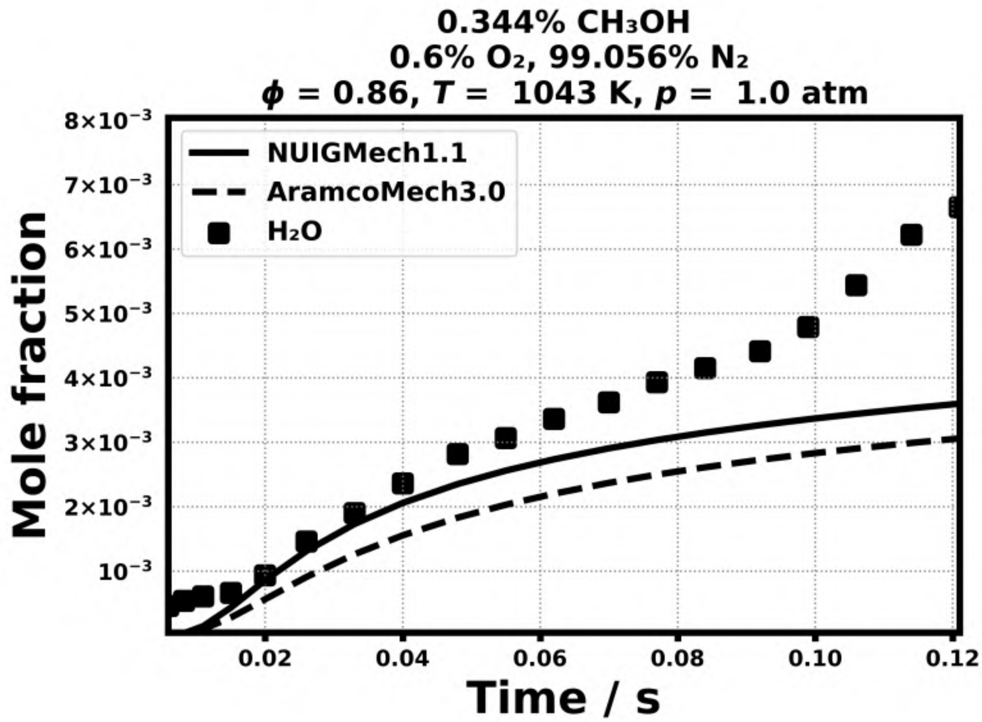
0.344% CH₃OH
0.6% O₂, 99.056% N₂
ϕ = 0.86, T = 1043 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
O₂
Mole fraction
Time / s

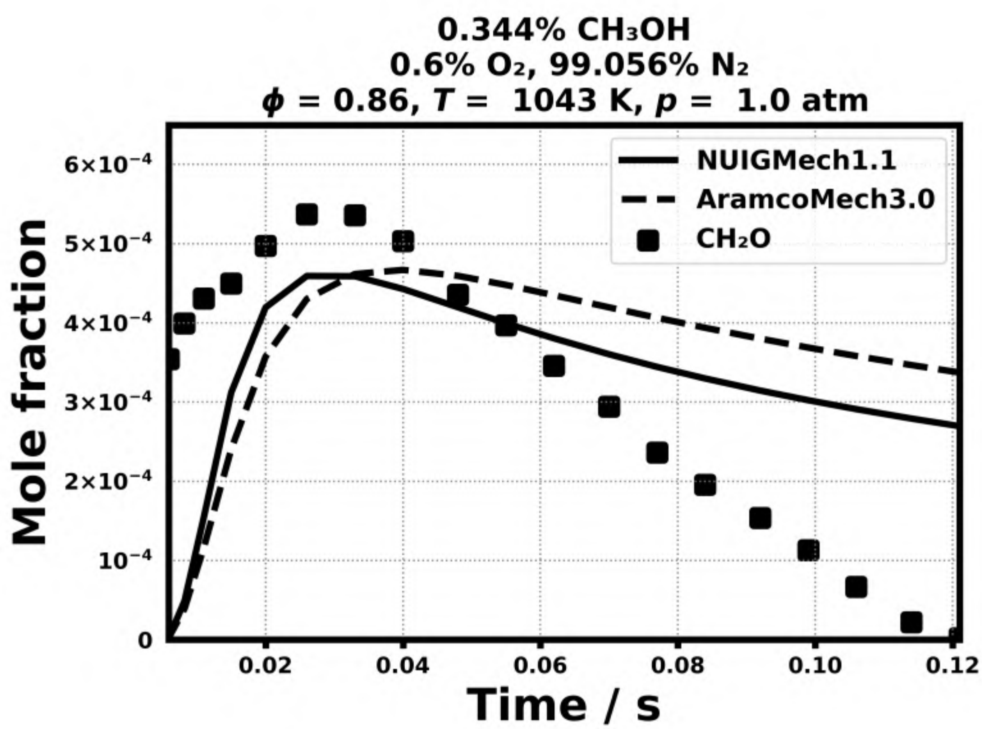


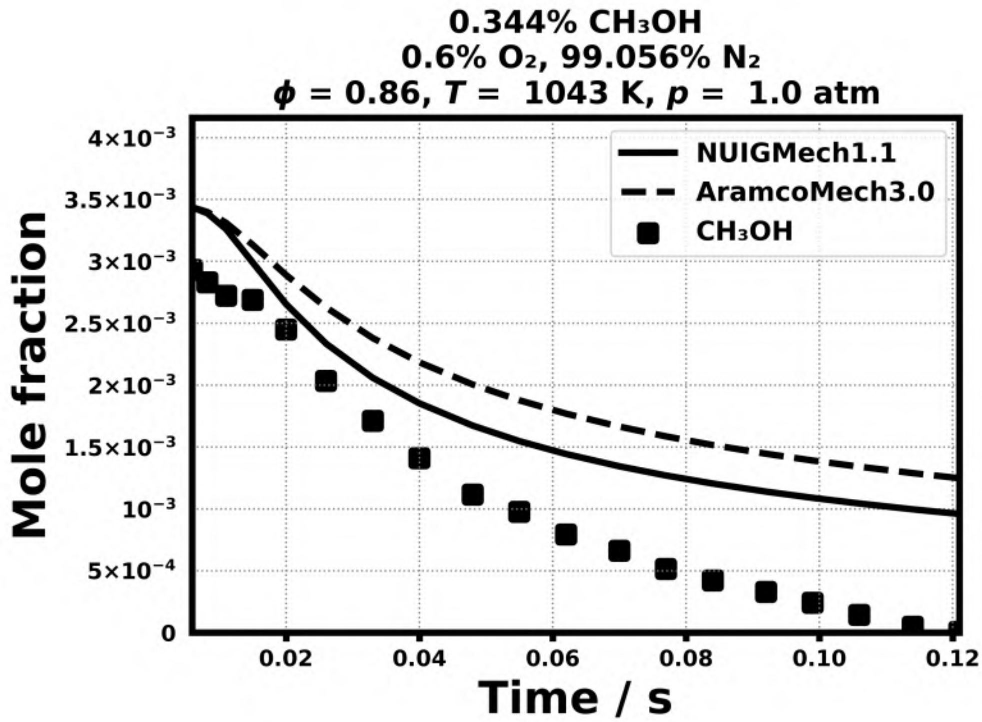
0.344% CH3OH
0.6% O2, 99.056% N2
ϕ = 0.86, T = 1043 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

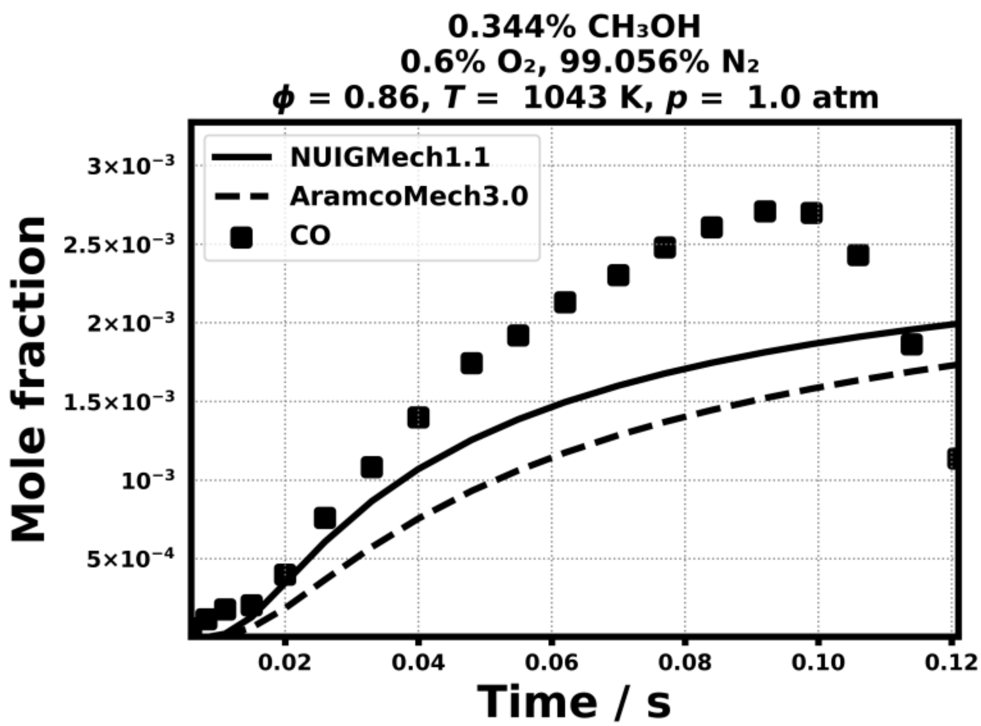


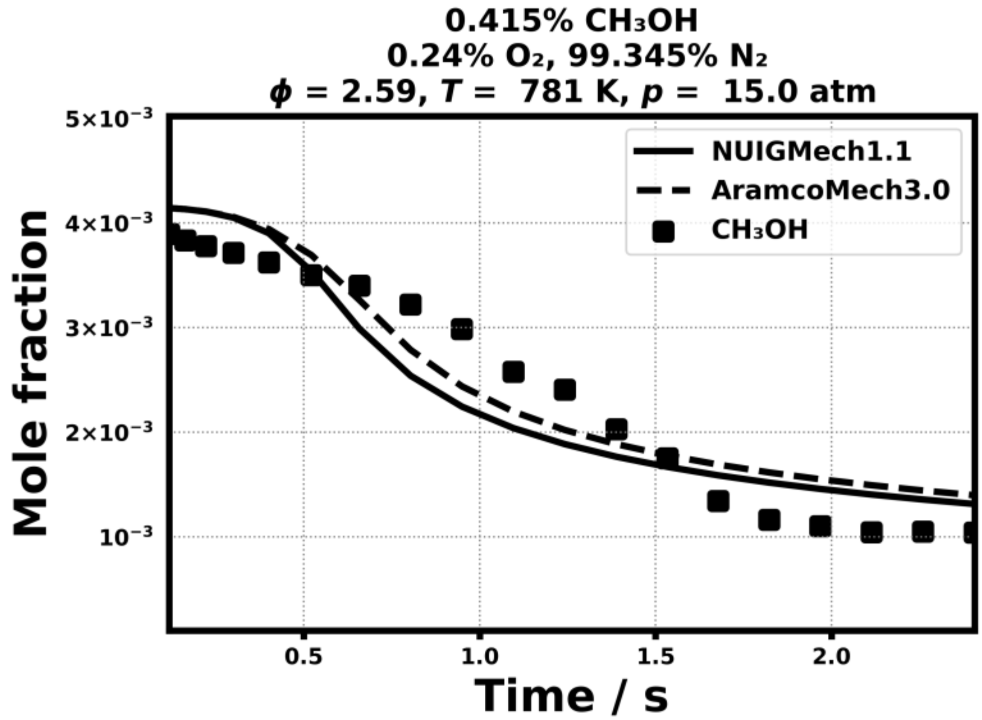
0.344% CH3OH
0.6% O2, 99.056% N2
ϕ = 0.86, T = 1043 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
H2
Mole fraction
2×10⁻³
1.75×10⁻³
1.5×10⁻³
1.25×10⁻³
10⁻³
7.5×10⁻⁴
5×10⁻⁴
2.5×10⁻⁴
0.02
0.04
0.06
0.08
0.10
0.12
Time / s

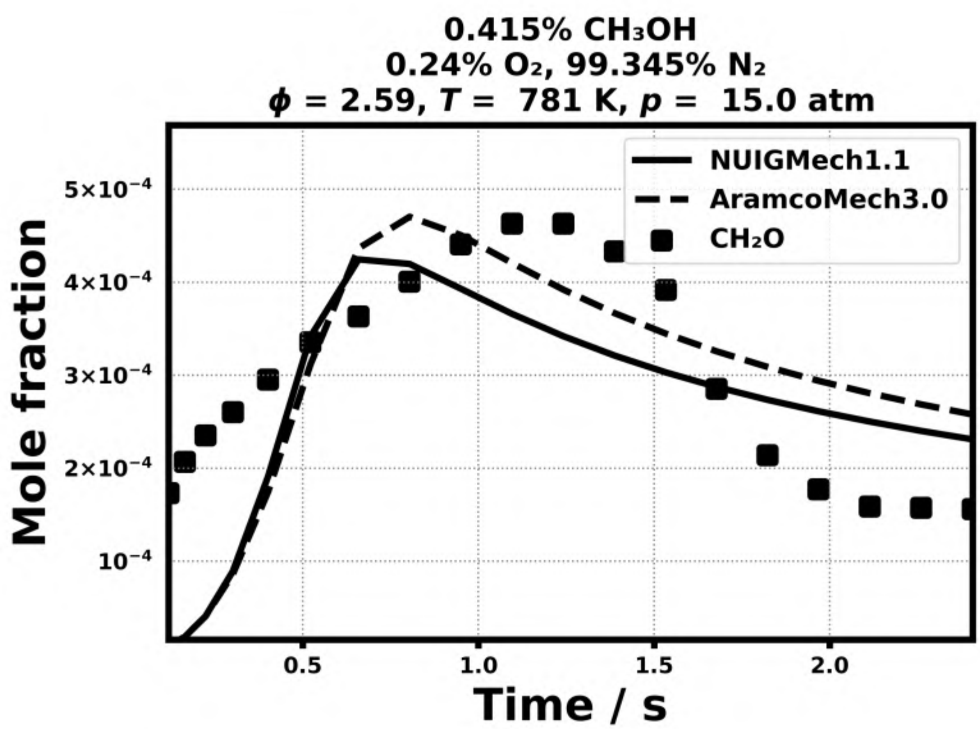

0.344% CH3OH
0.6% O2, 99.056% N2
ϕ = 0.86, T = 1043 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
H2O
Mole fraction
Time / s

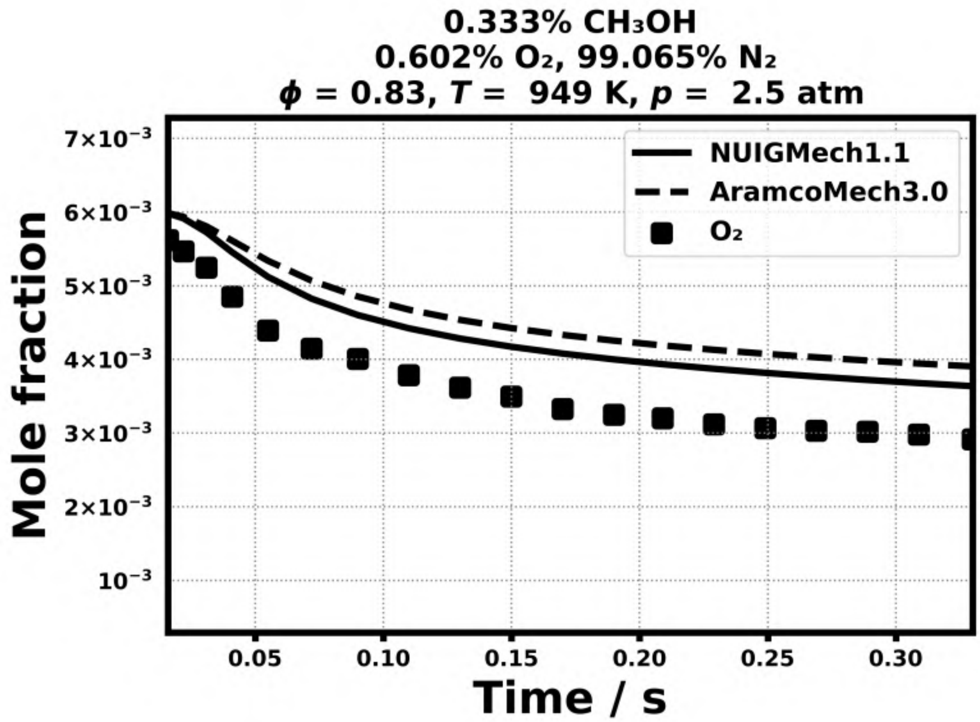

0.344% CH3OH
0.6% O2, 99.056% N2
ϕ = 0.86, T = 1043 K, p = 1.0 atm
NUIGMech1.1
AramcoMech3.0
CH2O
Mole fraction
Time / s

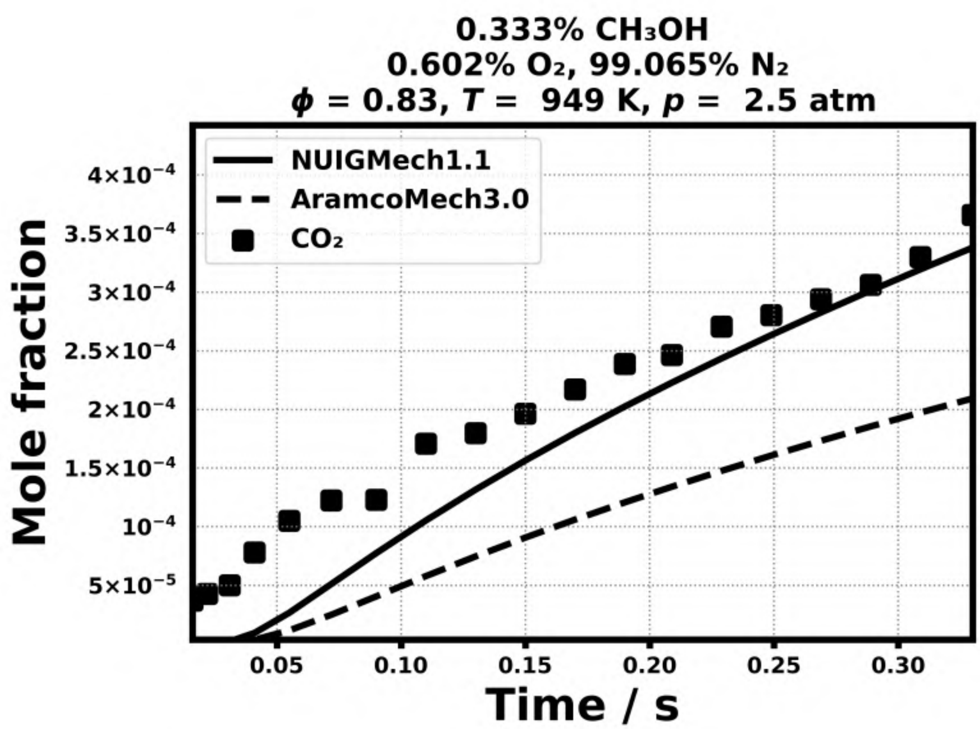

0.344% CH₃OH
0.6% O₂, 99.056% N₂
ϕ = 0.86, T = 1043 K, p = 1.0 atm
Mole fraction
Time / s
NUIGMech1.1
AramcoMech3.0
CH₃OH
4×10⁻³
3.5×10⁻³
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
0
0.02
0.04
0.06
0.08
0.10
0.12

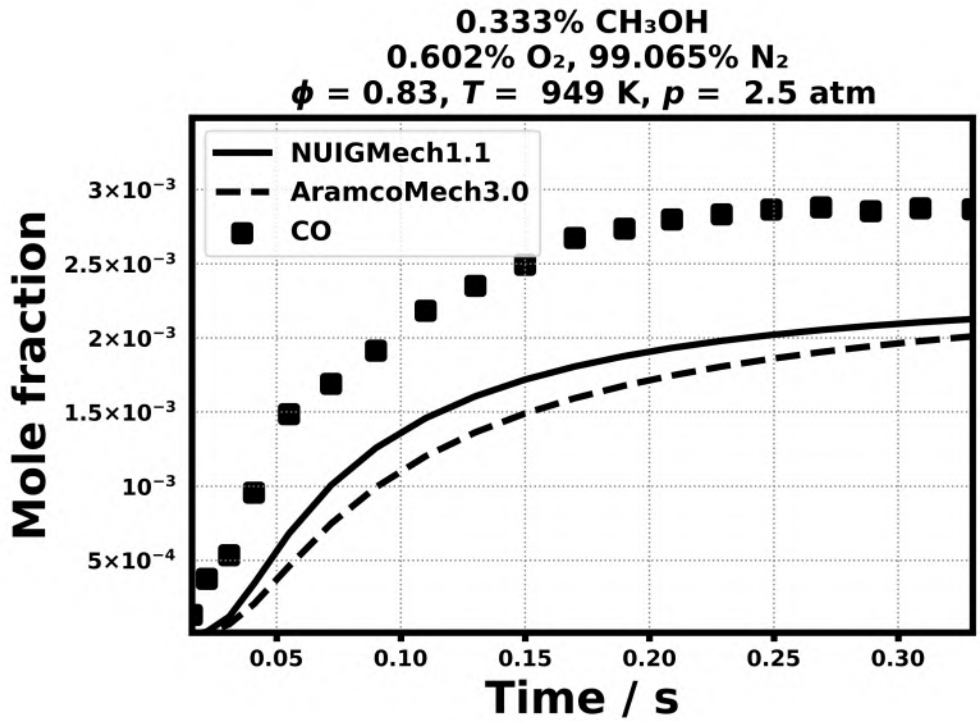

0.344% CH₃OH
0.6% O₂, 99.056% N₂
ϕ = 0.86, T = 1043 K, p = 1.0 atm
Mole fraction
Time / s
NUIGMech1.1
AramcoMech3.0
CO
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
0.02
0.04
0.06
0.08
0.10
0.12


0.415% CH₃OH
0.24% O₂, 99.345% N₂
ϕ = 2.59, T = 781 K, p = 15.0 atm
NUIGMech1.1
AramcoMech3.0
CH₃OH
Mole fraction
Time / s

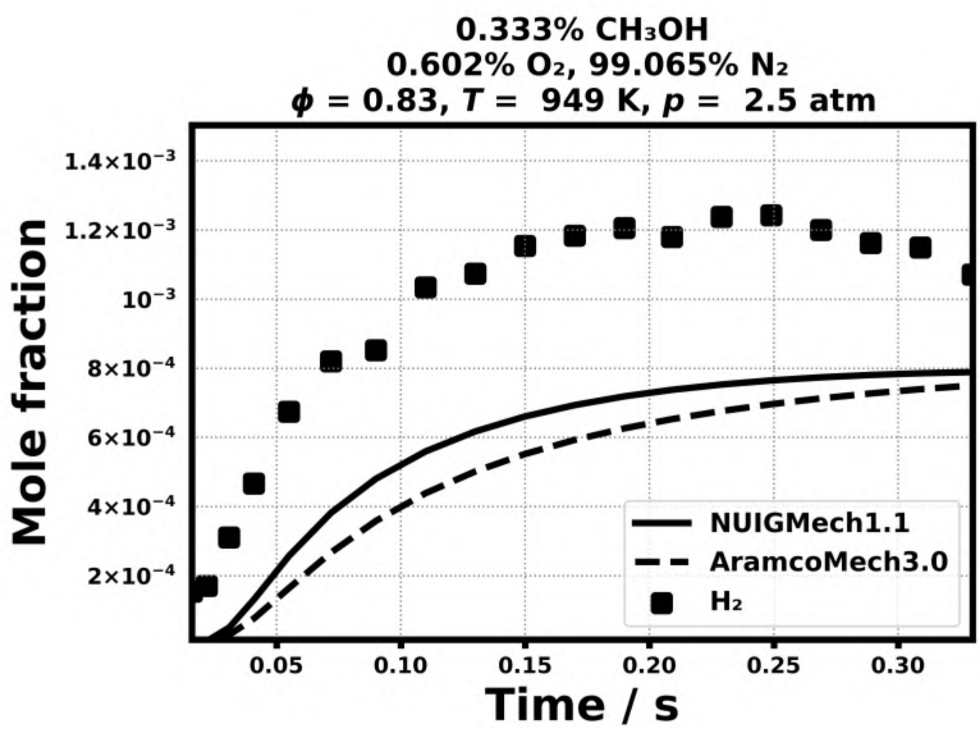

0.415% CH₃OH
0.24% O₂, 99.345% N₂
ϕ = 2.59, T = 781 K, p = 15.0 atm
NUIGMech1.1
AramcoMech3.0
CH₂O
Mole fraction
Time / s


0.333% CH3OH
0.602% O2, 99.065% N2
ϕ = 0.83, T = 949 K, p = 2.5 atm
NUIGMech1.1
AramcoMech3.0
O2
Mole fraction
Time / s

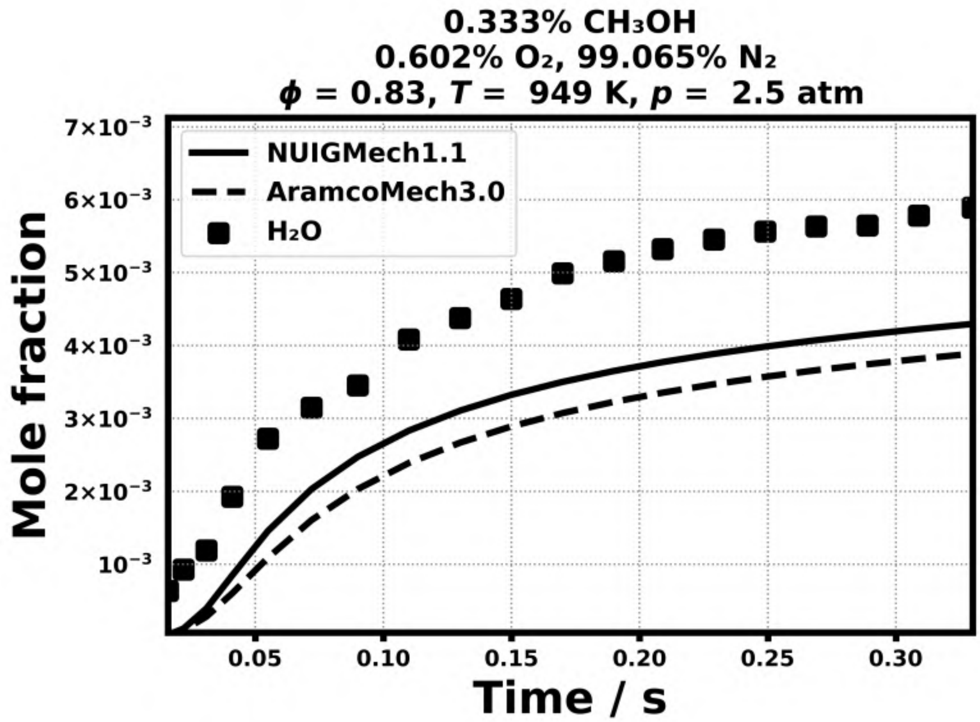

0.333% CH3OH
0.602% O2, 99.065% N2
ϕ = 0.83, T = 949 K, p = 2.5 atm
NUIGMech1.1
AramcoMech3.0
CO2
Mole fraction
Time / s

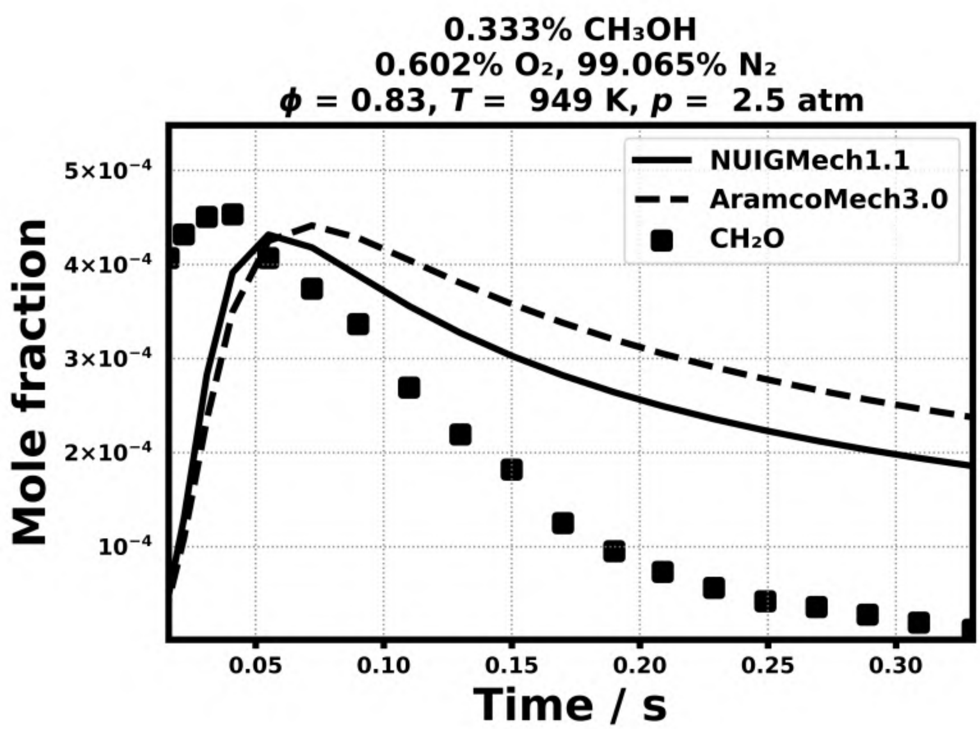


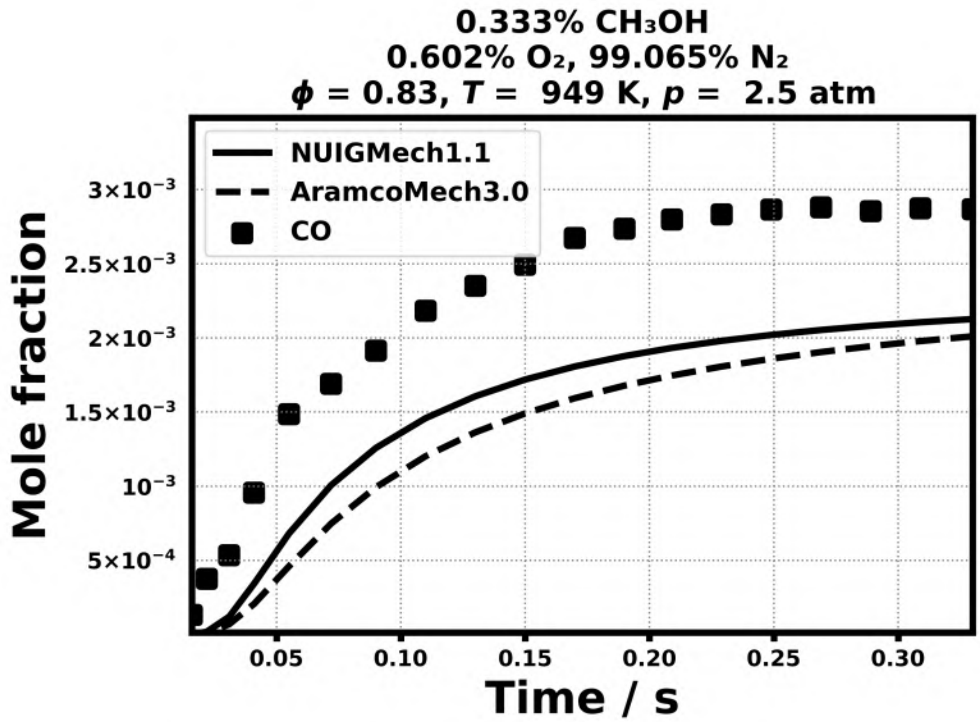
0.333% CH₃OH
0.602% O₂, 99.065% N₂
ϕ = 0.83, T = 949 K, p = 2.5 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
Time / s

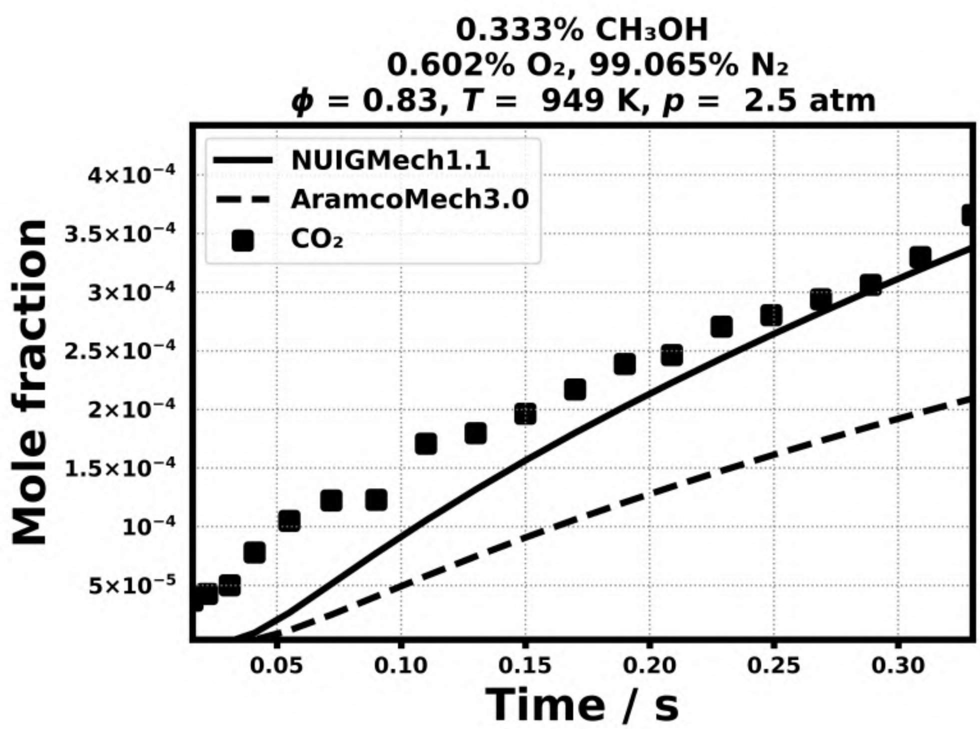


0.333% CH₃OH
0.602% O₂, 99.065% N₂
ϕ = 0.83, T = 949 K, p = 2.5 atm
NUIGMech1.1
AramcoMech3.0
H₂
Mole fraction
Time / s


0.333% CH₃OH
0.602% O₂, 99.065% N₂
ϕ = 0.83, T = 949 K, p = 2.5 atm
Mole fraction
Time / s
NUIGMech1.1
AramcoMech3.0
H₂O


0.333% CH₃OH
0.602% O₂, 99.065% N₂
ϕ = 0.83, T = 949 K, p = 2.5 atm
Mole fraction
Time / s
NUIGMech1.1
AramcoMech3.0
CH₂O


0.333% CH₃OH
0.602% O₂, 99.065% N₂
ϕ = 0.83, T = 949 K, p = 2.5 atm
NUIGMech1.1
AramcoMech3.0
CO
Mole fraction
3×10⁻³
2.5×10⁻³
2×10⁻³
1.5×10⁻³
10⁻³
5×10⁻⁴
0.05
0.10
0.15
0.20
0.25
0.30
Time / s


0.333% CH₃OH
0.602% O₂, 99.065% N₂
ϕ = 0.83, T = 949 K, p = 2.5 atm
NUIGMech1.1
AramcoMech3.0
CO₂
Mole fraction
4×10⁻⁴
3.5×10⁻⁴
3×10⁻⁴
2.5×10⁻⁴
2×10⁻⁴
1.5×10⁻⁴
10⁻⁴
5×10⁻⁵
0.05
0.10
0.15
0.20
0.25
0.30
Time / s

Laminar flame speed

4.10) Veloo, P. S., Wang, Y. L., Egolfopoulos, F. N., & Westbrook, C. K., Combustion and Flame, 157(10), (2010) 1989-2004.
4.11) Vancoillie, J., Christensen, M., Nilsson, E. J. K., Verhelst, S., & Konnov, A. A., Energy & fuels, 26 (2012) 1557-1564.
4.12) Sileghem, L., Alekseev, V.A., Vancoillie, J., Nilsson, E.J.K., Verhelst, S. and Konnov, A.A., Fuel, 115 (2014) 32-40.