

Supplemental Material

to

Combustion Kinetics of Alternative Fuels, Part-IV: Extending Reaction Mechanism “DLR Concise” to include oxygenates for Transportation Fuels

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Details of measurement data used for validation

Table S1: List of laminar burning velocities and flame speed measurements from literature used for validation.

Fuel	T _{preheat} (K)	Pressure (bar)	Ref.
DME	298	1	[Vries2011, Daly2001, Qin2005, Wang2009, Shrestha2020, Varghese2017, Yu2015, Huang2007, Zhao2004, Chen2009, Wang2018, Lavadera2022]
		3	[Shrestha2020]
		5	[Shrestha2020, Vries2011]
		10	[Qin2005, Vries2011]
	308, 323, 338	1	[Lavadera2022]
OME1	298	1,3,5	[Shrestha2020]
	328, 358	1	[Gillespie2014]
	443	1,3	[Shrestha2022]
	473	1,3,6	In-house [Ngugi2022]
OME2	383	1	[Eckart2021]
	388	1	[Eckart2021]
	393	1	[Eckart2021]
		3,5	[Shrestha2022]
	401	1	[Eckart2021]
	443	1,3	[Shrestha2022]
	473	1,3,6	In-house [Ngugi2021]
OME3	363	1	[Wang2021]
	393	1	[Wang2021]
	408	1	[Sun2017-OME3]
	423	1	[Wang2021]
	443	1,3	[Shrestha2022]
OME4	473	1,3,6	In-house [Richter2021]
PRF90	473	1,3,6	In-house [Richter2019, Ngugi2022]
PRF90+40%nC ₄ H ₉ OH	473	1,3,6	In-house [Richter2019]
PRF90+30%OME1	473	1,3,6	In-house [Ngugi2022]
DME+CH ₄	298	1	[Chen2007]

Diesel Surrogate	473	1,3,6	In-house [Richter2021]
OME4+70%Diesel Surrogate	473	1,3,6	In-house [Richter2021]

Table S2: List of ignition delay times measurements data from literature used for validation.

Fuel	Ref	Conditions
DME	Burke2015	$\phi = 0.3$: 2.06%DME + 20.58%O ₂ + 77.37% N ₂ ; 12, 25 atm (ST) $\phi = 0.5$: 3.38%DME + 20.3%O ₂ + 76.32% N ₂ ; 12, 25 atm (ST) $\phi = 1.0$: 6.55%DME + 19.6%O ₂ + 73.82% N ₂ ; 12, 25 atm (ST) $\phi = 2.0$: 12.3%DME + 18.43%O ₂ + 69.29% N ₂ ; 12, 25 atm (ST)
DME	Ngugi2023	$\phi = 1.0$: 1.3%DME + 3.93%O ₂ + 94.76% N ₂ ; 1, 4, 16 bar (ST)
DME DME+60%CH ₄ DME+80%CH ₄ CH ₄	Burke2015	$\phi = 1.0$: 6.55%DME + 19.6%O ₂ + 73.82% N ₂ ; 25 atm (ST) $\phi = 1.0$: 3.22%DME + 4.83%CH ₄ + 19.3%O ₂ + 72.6% N ₂ ; 20 atm (ST) $\phi = 1.0$: 1.74%DME + 6.97%CH ₄ + 19.18%O ₂ + 72.11% N ₂ ; 20 atm (ST) $\phi = 1.0$: 9.5%CH ₄ + 19.0%O ₂ + 71.48% N ₂ ; 24 atm (ST)
OME1 OME1+95%CH ₄ OME1+80%CH ₄ CH ₄	Herzler2020	$\phi = 0.5$: 2.56%OME1 + 20.46% O ₂ + 76.98% N ₂ ; 30 bar (ST) $\phi = 1.0$: 4.99%OME1 + 19.95% O ₂ + 75.06% N ₂ ; 30 bar (ST) $\phi = 2.0$: 9.5%OME1 + 19.0% O ₂ + 71.49% N ₂ ; 30 bar (ST) $\phi = 2.0$: 0.83%OME1 + 15.83%CH ₄ + 17.5%O ₂ + 65.8% N ₂ ; 30 bar (ST) $\phi = 10.0$: 2.5%OME1 + 47.5%CH ₄ + 10.5% O ₂ + 39.5% N ₂ ; 30 bar (ST) $\phi = 2.0$: 2.98%OME1 + 11.9% CH ₄ + 17.87% O ₂ + 67.2% N ₂ ; 30 bar (ST) $\phi = 2.0$: 17.36% CH ₄ + 17.36% O ₂ + 65.29% N ₂ ; 30 bar (ST)
DME DME-30%NO ₂ DME-70%NO ₂	Ye2016	$\phi = 0.5$: 0.67%DME + 4%O ₂ + 95.3% Ar; 4, 10 atm (ST) $\phi = 0.5$: 0.67%DME + 0.2%NO ₂ + 4%O ₂ + 95.1% Ar; 4, 10 atm (ST) $\phi = 0.5$: 0.67%DME + 0.469%NO ₂ + 4%O ₂ + 94.8% Ar; 4, 10 atm (ST)
DME DME+26%Tol. DME+58%Tol. DME+76%Tol. Toluene	Zhang2017	$\phi = 1.0$: 6.54%DME + 19.63%O ₂ + 73.83% N ₂ ; 20, 40 atm (ST) $\phi = 1.0$: 3.27%DME + 1.14%C ₇ H ₈ + 20.1%O ₂ + 75.5% N ₂ ; 20, 40 atm (ST) $\phi = 1.0$: 1.31%DME + 1.82%C ₇ H ₈ + 20.3%O ₂ + 76.53% N ₂ ; 20, 40 atm (ST) $\phi = 1.0$: 0.65%DME + 2.05%C ₇ H ₈ + 20.43%O ₂ + 76.87% N ₂ ; 20, 40 atm (ST) $\phi = 1.0$: 2.28%C ₇ H ₈ + 20.52%O ₂ + 77.2% N ₂ ; 20, 40 atm (ST)
OME1	Zhang2014	$\phi = 1.0$: 0.5%OME1 + 2%O ₂ + Ar; 2.0 atm (ST) dilutions: Ar/O ₂ = 11.25, 23.75, 48.75
OME1	Ngugi2023	$\phi = 1.0$: 0.949%OME1 + 3.83%O ₂ + 95.22% N ₂ ; 1,4,16 bar (ST)
OME1	Jacobs2019	$\phi = 1.0$: 5%OME1 + 19.95%O ₂ + 75.06% N ₂ ; 10 bar (RCM) $\phi = 1.0$: 5%OME1 + 19.95%O ₂ + 75.06% N ₂ ; 20,40 bar (ST, RCM)
OME1	Gillespie2014	$\phi = 0.5$: 1%OME1 + 8%O ₂ + Ar; 1, 3.5 atm (ST) $\phi = 1.0$: 1%OME1 + 4%O ₂ + Ar; 1, 3.5 atm (ST) $\phi = 2.0$: 1%OME1+ 3%O ₂ + Ar; 1, 3.5 atm (ST) $\phi = 0.5$: 2.6%OME1 + 20.5%O ₂ + N ₂ ; 9 atm (ST) $\phi = 1.0$: 5.0%OME1 + 20.0%O ₂ + N ₂ ; 9 atm (ST) $\phi = 2.0$: 9.5%OME1 + 19.0%O ₂ + N ₂ ; 9 atm (ST/RCM)
OME1 OME1+20%n-C ₇ H ₁₆ OME1+80%n-C ₇ H ₁₆ n-C ₇ H ₁₆	Hu2017	$\phi = 1.0$: 0.998%OME1 + 3.99%O ₂ + 95%Ar; 2,10 atm (ST) $\phi = 1.0$: 0.6%OME1 + 0.15% n-C ₇ H ₁₆ + 4.04%O ₂ + 95.2%Ar; 2,10 atm (ST) $\phi = 1.0$: 0.086%OME1 + 0.342% n-C ₇ H ₁₆ + 4.112%O ₂ + 95.46%Ar; 2,10 atm (ST) $\phi = 1.0$: 0.375% n-C ₇ H ₁₆ + 4.123%O ₂ + 95.5%Ar; 2,10 atm (ST)
OME2	Cai2020	$\phi = 0.5$: 2.06%OME2 + 20.57%O ₂ + 77.38% N ₂ ; 20 bar (ST)

		$\phi = 1.0$: 2.6%OME2 + 20.5%O ₂ + 77% N ₂ ; 10 bar (ST) $\phi = 1.0$: 2.6%OME2 + 20.5%O ₂ + 77% N ₂ ; 20 bar (ST)
OME2	Ngugi2023	$\phi = 1.0$: 0.78%OME2 + 3.85%O ₂ + 95.37% N ₂ ; 1,4,16 bar (ST)
OME3	Cai2020	$\phi = 1.0$: 3.4%OME3 + 20.3%O ₂ + 76.3% N ₂ ; 10 bar (ST) $\phi = 0.5$: 1.7%OME3 + 20.6%O ₂ + 77.6% N ₂ ; 20 bar (ST) $\phi = 1.0$: 3.4%OME3 + 20.3%O ₂ + 76.3% N ₂ ; 20 bar (ST) $\phi = 2.0$: 6.5%OME3 + 19.6%O ₂ + 73.4% N ₂ ; 20 bar (ST)
OME4	Ngugi2023	$\phi = 1.0$: 0.79%OME4 + 3.88%O ₂ + 95.32% N ₂ ; 1,4,16 bar (ST)
OME4	Cai2020	$\phi = 1.0$: 2.9%OME4 + 20.4%O ₂ + 76.7% N ₂ ; 10 bar (ST) $\phi = 1.0$: 2.9%OME4 + 20.4%O ₂ + 76.7% N ₂ ; 20 bar (ST)
PRF90	Ngugi2022	$\phi = 1.0$: 0.032% n-C ₇ H ₁₆ + 0.287% I-C ₈ H ₁₈ + 3.929%O ₂ + 95.75% N ₂ ; 1,4,16 bar (ST)
	Richter2019	$\phi = 1.0$: 0.037% n-C ₇ H ₁₆ + 0.297% I-C ₈ H ₁₈ + 4.128%O ₂ + 95.54% Ar; 1,4,16 bar (ST)
PRF90 + 70% OME1	Ngugi2022	$\phi = 1.0$: 0.418%OME1 + 0.018% n-C ₇ H ₁₆ + 0.161% I-C ₈ H ₁₈ + 3.85%O ₂ + 95.55% N ₂ ; 1,4,16 bar (ST)
PRF90+20%n-C ₄ H ₉ OH	Richter2019	$\phi = 1.0$: 0.031%n-C ₇ H ₁₆ + 0.246% I-C ₈ H ₁₈ + 0.123% nC ₄ H ₉ OH + 4.11%O ₂ + 95.49% Ar; 1,4,16 bar (ST)
PRF90+40%n-C ₄ H ₉ OH		$\phi = 1.0$: 0.024%n-C ₇ H ₁₆ + 0.188% I-C ₈ H ₁₈ + 0.25% nC ₄ H ₉ OH + 4.103%O ₂ + 95.435% Ar; 1,4,16 bar (ST)
n-C ₇ H ₁₆	Gauthier2004	$\phi = 1.0$: 1.87%n-C ₇ H ₁₆ + 20.6%O ₂ + 77.5% N ₂ ; 13,20,55 atm (ST)
I-C ₈ H ₁₈	Fang2020	$\phi = 0.7$: 1.163%I-C ₈ H ₁₈ + 20.764%O ₂ + 78.073% N ₂ ; 20 bar (RCM)
	Fang2020, Shen2008, Atef2017	$\phi = 1.0$: 1.653%I-C ₈ H ₁₈ + 20.661%O ₂ + 77.686% N ₂ ; 20 bar (ST, RCM)
	Fang2020	$\phi = 2.0$: 3.252%I-C ₈ H ₁₈ + 20.325%O ₂ + 76.423% N ₂ ; 20 bar (RCM)
DF-2 diesel	Haylett2009	$\phi = 0.5$: 0.56%Diesel + 21%O ₂ + 78.5% Ar; 6,7atm (ST)
Gasoline Surrogate	Davidson2019	$\phi = 1.0$: 20.43% 1-C ₆ H ₁₂ + 79.57% C ₇ H ₈ in air 60 atm (ST)
	Javed2016	$\phi = 1.0$: TPRF 70 = 36.5%iC ₈ H ₁₈ + 35%n-C ₇ H ₁₆ + 28.5%C ₇ H ₈ in air; 20 bar (ST, RCM) $\phi = 1.0$: TPRF 80 = 33%iC ₈ H ₁₈ + 27%n-C ₇ H ₁₆ + 40%C ₇ H ₈ in air; 20 bar (ST, RCM) $\phi = 1.0$: TPRF 91 = 29%iC ₈ H ₁₈ + 17%n-C ₇ H ₁₆ + 54%C ₇ H ₈ in air; 20 bar (ST, RCM) $\phi = 1.0$: TPRF 97.5 = 8%iC ₈ H ₁₈ + 14.5%n-C ₇ H ₁₆ + 77.5%C ₇ H ₈ in air; 20 bar (ST, RCM)

Shock-tube: ST, Rapid Compression Machine: RCM

Table S3: List of burner-stabilized laminar flame measurements from literature used for validation.

Fuel	Ref	Conditions
DME	Cool2007	$\phi = 1.2$: 8.5%DME + 21.2 %O ₂ + 70.3% Ar; 0.04 bar flow rate = 0.0052 g/sec.cm ² , burner diameter 6 cm
DME	Zeng2017	$\phi = 1.84$: 19.03%DME + 30.98%O ₂ + 50%Ar; 0.04 bar 6.5 cm diameter, 0.1111 g/s
Methyl formate	Dooley2011	$\phi = 1.0$, 25.2%MF + 50.2%O ₂ + 24.6%Ar; 0.029 bar, flow rate = 3.52e-3 g/sec.cm ² , burner diameter 6 cm
OME1	Sun2017-OME3 Sun2017-OME1	$\phi = 1.0$: 15%OME1 + 60%O ₂ + 25%Ar; 0.033 bar, flow rate = 0.00427 g/sec.cm ² , burner diameter = 6 cm $\phi = 2.0$: 25%OME1 + 50%O ₂ + 25%Ar; 0.04 bar, flow rate = 0.1339 g/sec, burner diameter = 6 cm
OME1 OME1+50%CH ₄	Hao-Zhang2022	$\phi = 1.7$: 14.9%OME1 + 35.1%O ₂ + 50%Ar; 0.04 bar 0.1199 g/s, burner diameter = 6.882 cm $\phi = 1.7$: 9.05%OME1 + 9.03%CH ₄ + 31.98%O ₂ + 50%Ar; 0.04 bar

OME1+80%CH4		0.1086 g/s, burner diameter = 6.882 cm $\phi = 1.7$: 3.7%OME1 + 14.76%CH ₄ + 31.62%O ₂ + 50%Ar; 0.04 bar 0.0994 g/s, burner diameter = 6.882 cm
OME3	Sun2017-OME3	$\phi = 1.0$: 7.15%OME3 + 42.85%O ₂ + 50% Ar; 0.033 bar flow rate = 0.00427 g/sec.cm ² , burner diameter = 6 cm
DME	Gaiser2022C	$\phi = 1.7$: 18%DME + 32%O ₂ + 50%Ar; 0.04 bar, flow rate = 3.4E-3 g/sec.cm ² , burner diameter = 6.382 cm
OME1		$\phi = 1.7$: 15%OME1 + 35%O ₂ + 50%Ar; 0.04 bar, flow rate = 3.76E-3 g/sec.cm ² , burner diameter = 6.382 cm
OME2		$\phi = 1.7$: 13%OME2 + 37%O ₂ + 50%Ar; 0.04 bar, flow rate = 4.02E-3 g/sec.cm ² , burner diameter = 6.382 cm
OME3		$\phi = 1.7$: 11% OME3 + 39%O ₂ + 50%Ar; 0.04 bar flow rate = 4.2E-3. g/sec.cm ² , burner diameter = 6.382 cm

Table S4: List of flow reactor measurements from literature used for validation.

Fuel	Ref	Conditions
DME DME+1000NO DME+2000NO	Zhang2021	$\phi = 0.8$: 1.5%DME + 5.5%O ₂ + 93% Ar; 0.970 bar $\phi = 0.8$: 1.5%DME + 0.1%NO+ 5.5%O ₂ + 92.9% Ar; 0.970 bar $\phi = 0.8$: 1.5%DME + 0.2%NO+ 5.5%O ₂ + 92.8% Ar; 0.970 bar 430-950K
OME1 OME1+1000NO OME1+2000NO	Zhang2021	$\phi = 0.8$: 1.2%OME1 + 5.8%O ₂ + 93% Ar; 0.970 bar $\phi = 0.8$: 1.2%OME1 + 0.1%NO+ 5.8%O ₂ + 92.9% Ar; 970 mbar $\phi = 0.8$: 1.2%OME1 + 0.2%NO+ 5.8%O ₂ + 92.8% Ar; 970 mbar 430-950K
DME OME1 OME2 OME3 OME4 OME5	Gaiser2022F	$\phi = 0.8$: 0.25%DME + 0.936%O ₂ + 98.8% Ar; 1bar $\phi = 1.2$: 0.25%DME + 0.626%O ₂ + 99.1% Ar; 1bar $\phi = 2.0$: 0.25%DME + 0.376%O ₂ + 99.4% Ar; 1bar $\phi = 0.8$: 0.17%OME1 + 0.833%O ₂ + 99% Ar; 1bar $\phi = 1.2$: 0.17%OME1 + 0.557%O ₂ + 99.3% Ar; 1bar $\phi = 2.0$: 0.17%OME1 + 0.335%O ₂ + 99.5% Ar; 1bar $\phi = 0.8$: 0.125%OME2 + 0.782%O ₂ + 99.1% Ar; 1bar $\phi = 1.2$: 0.125%OME2 + 0.523%O ₂ + 99.3% Ar; 1bar $\phi = 2.0$: 0.126%OME2 + 0.283%O ₂ + 99.6% Ar; 1bar $\phi = 0.8$: 0.10%OME3 + 0.751%O ₂ + 99.1% Ar; 1bar $\phi = 1.2$: 0.10%OME3 + 0.502%O ₂ + 99.4% Ar; 1bar $\phi = 2.0$: 0.10%OME3 + 0.302%O ₂ + 99.6% Ar; 1bar $\phi = 0.8$: 0.08%OME4 + 0.731%O ₂ + 99.2% Ar; 1bar $\phi = 1.2$: 0.08%OME4 + 0.488%O ₂ + 99.4% Ar; 1bar $\phi = 2.0$: 0.08%OME4 + 0.294%O ₂ + 99.6% Ar; 1bar $\phi = 0.8$: 0.07%OME5 + 0.715%O ₂ + 99.2% Ar; 1bar $\phi = 1.2$: 0.07%OME5 + 0.478%O ₂ + 99.5% Ar; 1bar $\phi = 2.0$: 0.07%OME5 + 0.287%O ₂ + 99.4% Ar; 1bar 750-1250K
PRF90	Present work	$\phi = 0.8$: 0.007%n-C ₇ H ₁₆ + 0.056% I-C ₈ H ₁₈ + 0.98%O ₂ + 98.96% Ar; 1bar $\phi = 1.2$: 0.007%n-C ₇ H ₁₆ + 0.057% I-C ₈ H ₁₈ + 0.653%O ₂ + 99.283% Ar; 1bar $\phi = 1.43$: 0.007%n-C ₇ H ₁₆ + 0.057% I-C ₈ H ₁₈ + 0.55%O ₂ + 99.386% Ar; 1bar $\phi = 2.0$: 0.007%n-C ₇ H ₁₆ + 0.057% I-C ₈ H ₁₈ + 0.393%O ₂ + 99.543% Ar; 1bar 750-1350K
Methanol	Present work	$\phi = 0.8$: 0.5%CH ₃ OH + 0.933%O ₂ + 98.57% Ar; 1bar

		$\phi = 1.2: 0.5\% \text{CH}_3\text{OH} + 0.624\% \text{O}_2 + 98.88\% \text{Ar}; 1\text{bar}$ $\phi = 2.0: 0.5\% \text{CH}_3\text{OH} + 0.500\% \text{O}_2 + 99.00\% \text{Ar}; 1\text{bar}$ 750-1250K
Ethanol	Present work	$\phi = 0.8: 0.25\% \text{C}_2\text{H}_5\text{OH} + 0.935\% \text{O}_2 + 98.8\% \text{Ar}; 1\text{bar}$ $\phi = 1.2: 0.25\% \text{C}_2\text{H}_5\text{OH} + 0.636\% \text{O}_2 + 99.1\% \text{Ar}; 1\text{bar}$ $\phi = 2.0: 0.25\% \text{C}_2\text{H}_5\text{OH} + 0.501\% \text{O}_2 + 99.3\% \text{Ar}; 1\text{bar}$ 750-1250K
n-Butanol	Present work	$\phi = 0.8: 0.125\% \text{n-C}_4\text{H}_9\text{OH} + 0.937\% \text{O}_2 + 98.9\% \text{Ar}; 1\text{bar}$ $\phi = 1.2: 0.125\% \text{n-C}_4\text{H}_9\text{OH} + 0.627\% \text{O}_2 + 99.3\% \text{Ar}; 1\text{bar}$ $\phi = 2.0: 0.125\% \text{n-C}_4\text{H}_9\text{OH} + 0.502\% \text{O}_2 + 99.4\% \text{Ar}; 1\text{bar}$ 750-1250K

Table S5: List of jet-stirred reactor measurements from literature used for validation.

Fuel	Ref	Conditions
DME	Moshhammer2016	$\phi = 0.35: 2.3\% \text{DME} + 19.7\% \text{O}_2 + 78\% \text{Ar}; 1 \text{ atm}; \tau = 4\text{s}, 460\text{-}900\text{K}$
DME	Rodriguez2015	$\phi = 1.0: 2\% \text{DME} + 6\% \text{O}_2 + 92\% \text{He}; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}1100\text{K}$ $\phi = 2.0: 2\% \text{DME} + 3\% \text{O}_2 + 95\% \text{He}; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}1100\text{K}$
OME1	Sun2017-OME1	$\phi = 0.2: 0.1\% \text{OME1} + 2\% \text{O}_2 + 97.9\% \text{N}_2; 10 \text{ atm}; \tau = 0.7\text{s}, 500\text{-}1200\text{K}$
OME1	Vermeire2018	$\phi = 0.25, 1.0, 2.0: 1\% \text{OME1} + 4\% \text{O}_2 + 95\% \text{He}; 1\text{atm}; \tau = 2.83\text{s}, 500\text{-}1100\text{K}$
OME1 pyrolysis	Vermeire2018	$\phi = -: 1\% \text{OME1} + 99\% \text{He}; 1\text{atm}; \tau = 2.83\text{s}, 800\text{-}1200\text{K}$
OME1	Wang2022	$\phi = 0.5: 0.8\% \text{OME1} + 6.4\% \text{O}_2 + 92.8\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$ $\phi = 1.0: 0.8\% \text{OME1} + 3.2\% \text{O}_2 + 96.0\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$ $\phi = 2.0: 0.8\% \text{OME1} + 1.6\% \text{O}_2 + 97.6\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$
OME2	Wang2022	$\phi = 0.5: 0.8\% \text{OME2} + 8\% \text{O}_2 + 91.2\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$ $\phi = 1.0: 0.8\% \text{OME2} + 4\% \text{O}_2 + 95.2\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$ $\phi = 2.0: 0.8\% \text{OME2} + 2\% \text{O}_2 + 97.2\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$
OME3	Wang2022	$\phi = 0.5: 0.8\% \text{OME3} + 9.6\% \text{O}_2 + 89.6\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$ $\phi = 1.0: 0.8\% \text{OME3} + 4.8\% \text{O}_2 + 94.4\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$ $\phi = 2.0: 0.8\% \text{OME3} + 2.4\% \text{O}_2 + 96.8\% \text{He}; 1\text{atm}; \tau = 2\text{s}, 400\text{-}1150\text{K}$
OME1 pyrolysis	Zhong2021	$\phi = -: 1\% \text{OME1} + 99\% \text{Ar}; 1 \text{ atm}; \tau = 2\text{s}, 450\text{-}1100\text{K}$
OME2 pyrolysis	Zhong2021	$\phi = -: 1\% \text{OME2} + 99\% \text{Ar}; 1 \text{ atm}; \tau = 2\text{s}, 450\text{-}1100\text{K}$
OME3 pyrolysis	Zhong2021	$\phi = -: 1\% \text{OME3} + 99\% \text{Ar}; 1 \text{ atm}; \tau = 2\text{s}, 450\text{-}1100\text{K}$
OME3	Qiu2022	$\phi = 0.5: 0.5\% \text{OME3} + 6\% \text{O}_2 + 93.5\% \text{N}_2; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}950\text{K}$ $\phi = 1.0: 0.5\% \text{OME3} + 3\% \text{O}_2 + 96.5\% \text{N}_2; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}950\text{K}$ $\phi = 2.0: 0.5\% \text{OME3} + 1.5\% \text{O}_2 + 98\% \text{N}_2; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}950\text{K}$
OME1 OME1-50%n-C ₇ H ₁₆ OME1-75%n-C ₇ H ₁₆ n-C ₇ H ₁₆	Gao2019	$\phi = 2.0: 0.5\% \text{OME1} + 1\% \text{O}_2 + 98.5\% \text{Ar}; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}1100\text{K}$ $\phi = 2.0: 0.25\% \text{OME1} + 0.25\% \text{n-C}_7\text{H}_{16} + 1.875\% \text{O}_2 + 97.625\% \text{Ar}; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}1100\text{K}$ $\phi = 2.0: 0.125\% \text{OME1} + 0.375\% \text{n-C}_7\text{H}_{16} + 2.312\% \text{O}_2 + 97.19\% \text{Ar}; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}1100\text{K}$ $\phi = 2.0: 0.5\% \text{n-C}_7\text{H}_{16} + 2.75\% \text{O}_2 + 96.75\% \text{Ar}; 1 \text{ atm}; \tau = 2\text{s}, 500\text{-}1100\text{K}$

PRF90	Dagaut1994	$\phi = 1.0$: 0.012% n-C ₇ H ₁₆ + 0.093% i-C ₈ H ₁₈ + 1.295% O ₂ + 98.6% N ₂ ; 10 atm; $\tau = 1$ s, 550-1150K
Diesel fuel surrogate	Mati2007	$\phi = 2.0$: 0.01161% n-C ₁₆ H ₃₄ + 0.00937% i-C ₈ H ₁₈ + 0.01332% cyC ₉ H ₁₈ + 0.01133% cyC ₉ H ₁₂ + 0.00394% A ₂ CH ₃ + 0.345% O ₂ + 99.6% Ar; 10 atm; $\tau = 0.5$ s, 800-1300K

(S1) Validation of DLR Concise

In this section model predictions of DLR Concise is presented for different combustion characteristics. In all figures, experiments are shown by symbols and model predictions by curves.

(1.2) Ignition delay times

DLR Concise model predictions of ignition delay times of OMEs, fuel surrogates and their blends are presented here.

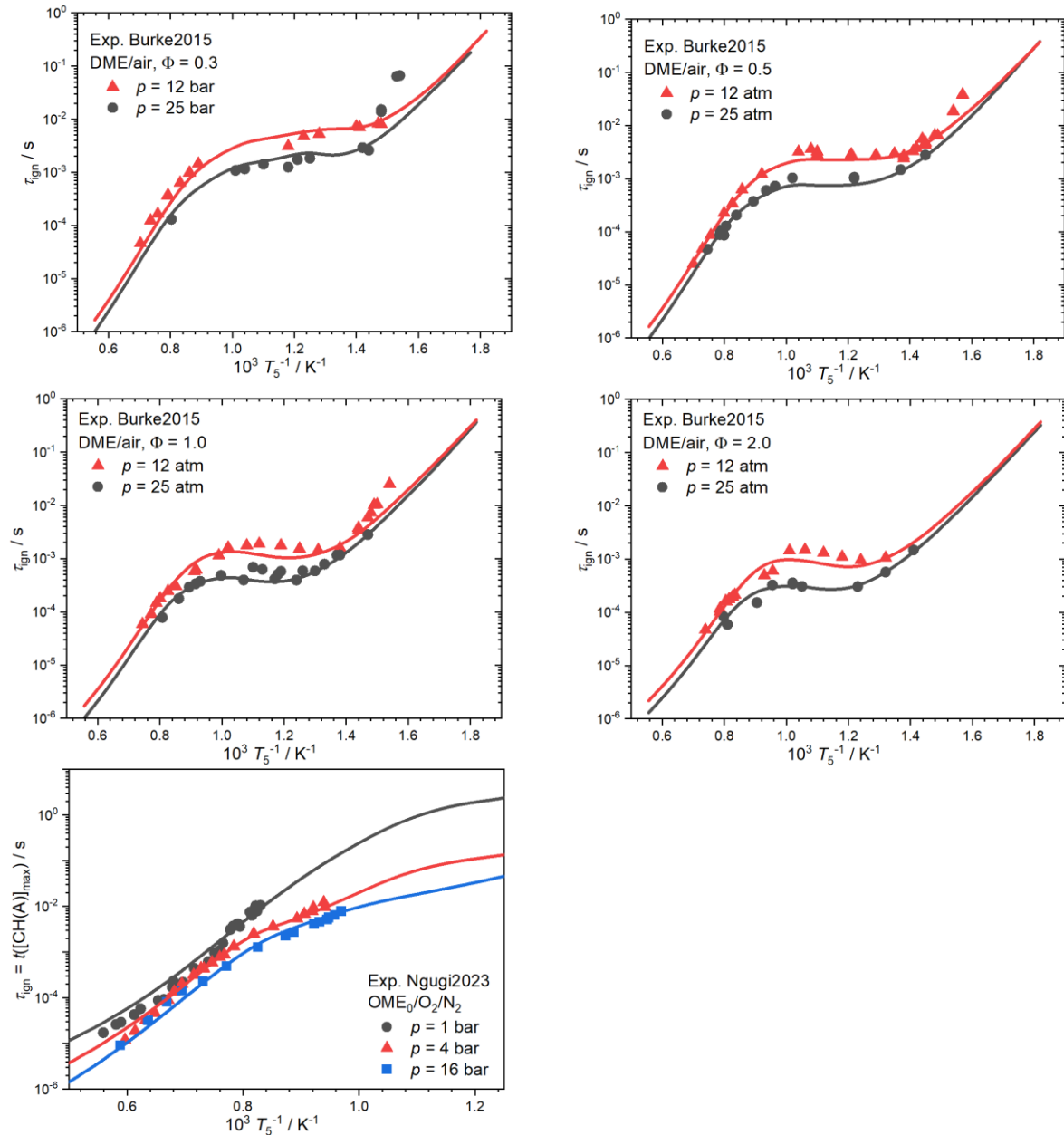


Fig. S1: DLR Concise model predictions of ignition delay times of DME [Burke2015, Ngugi2023].

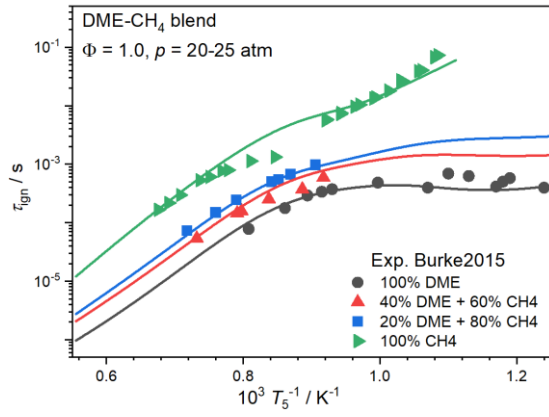


Fig. S2: DLR Concise model predictions of ignition delay times of DME-CH₄ blends [Burke2015].

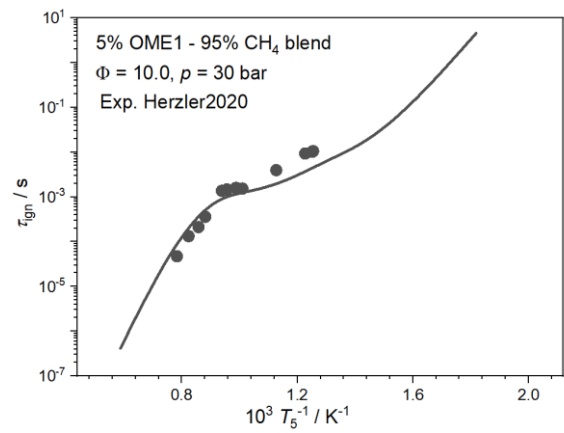
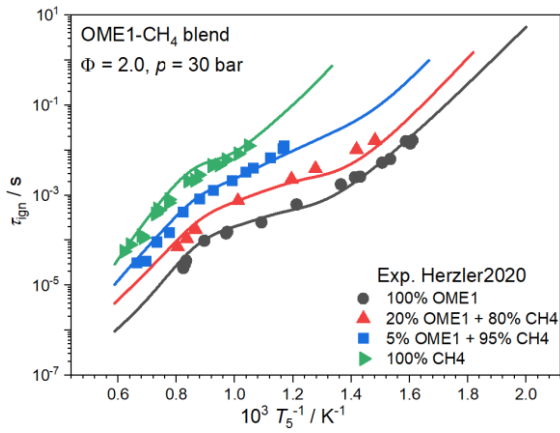


Fig. S3: DLR Concise model predictions of ignition delay times of OME1-CH₄ blends [Herzler2020].

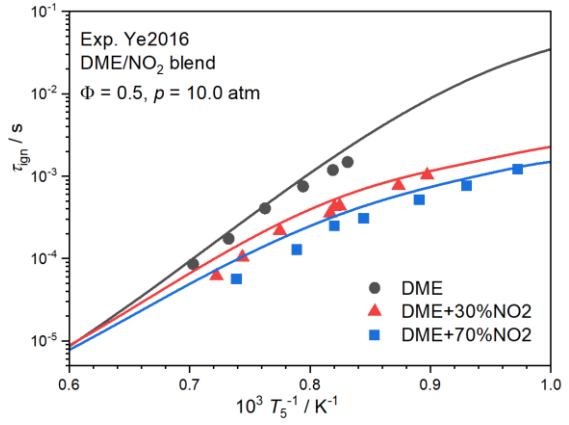
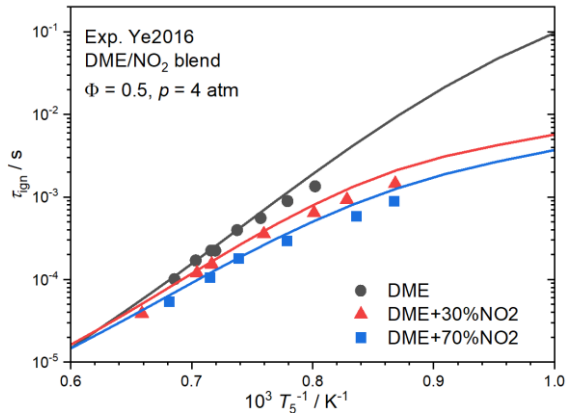


Fig. S4: DLR Concise model predictions of ignition delay times of DME-NO₂ blends [Ye2016].

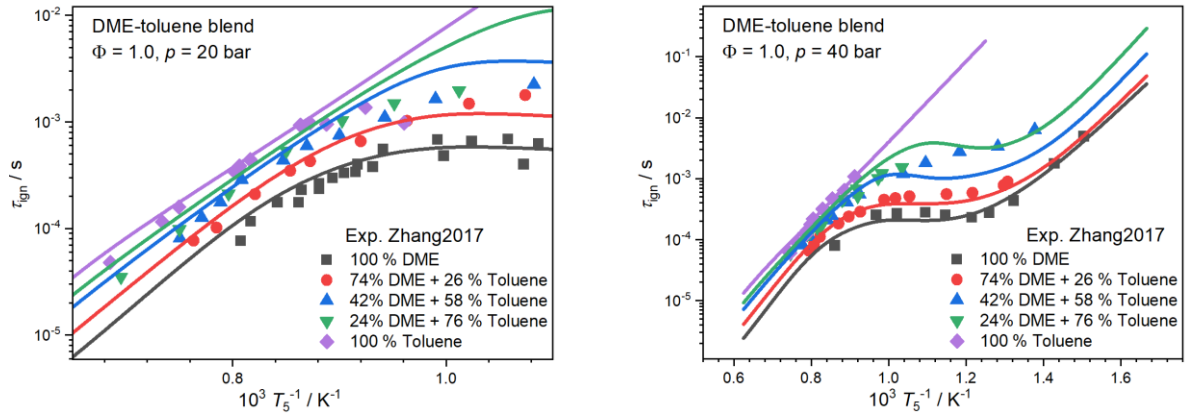


Fig. S5: DLR Concise model predictions of ignition delay times of DME-toluene blends [Zhang2017].

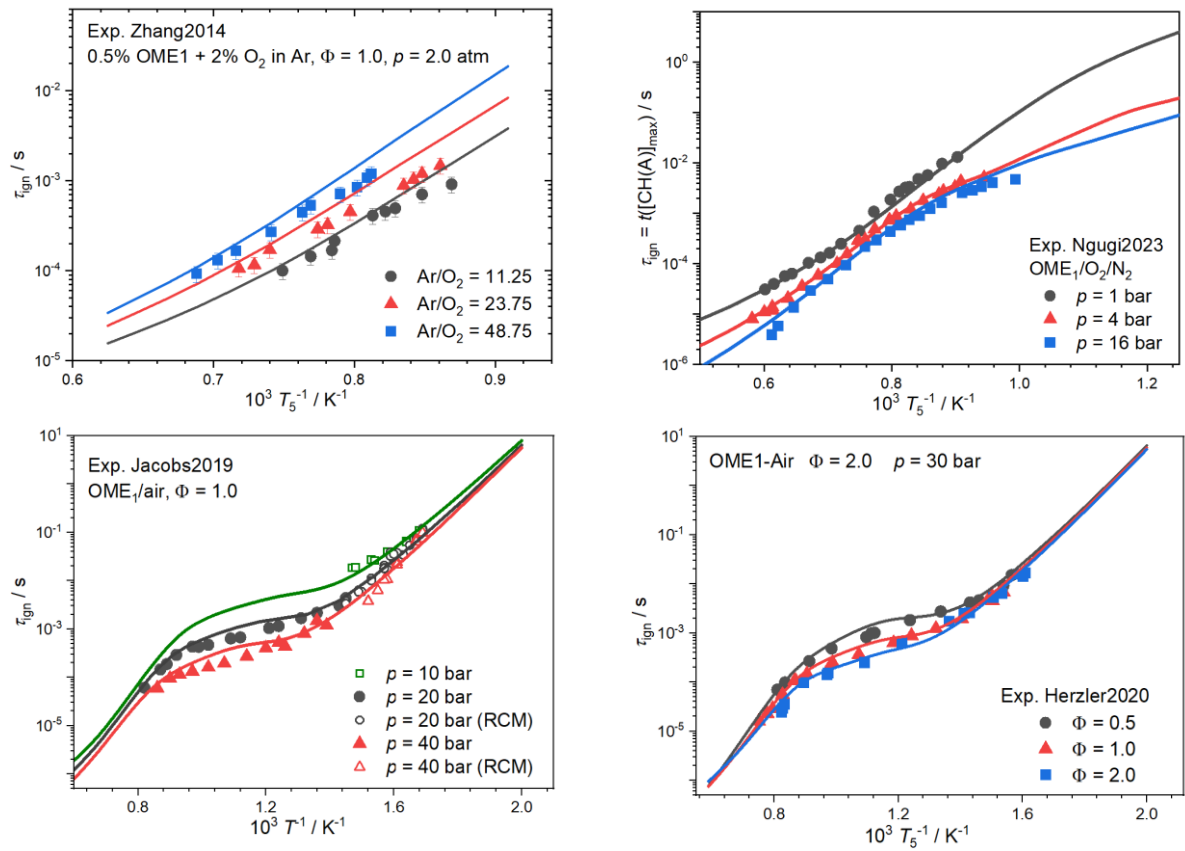


Fig. S6: DLR Concise model predictions of ignition delay times of OME1 [Zhang2017, Ngugi2023, Jacobs2019, Herzler2020].

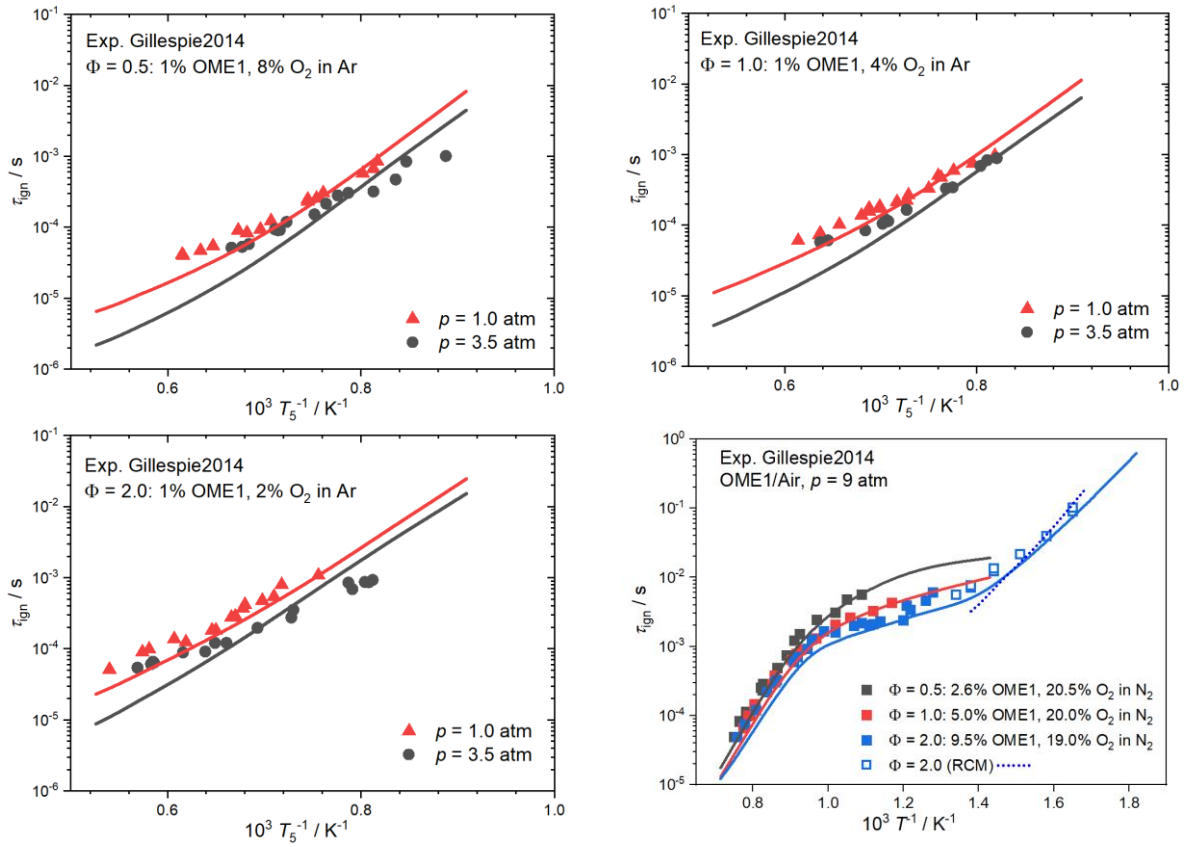


Fig. S7: DLR Concise model predictions of ignition delay times of OME1 [Gillespie2014].

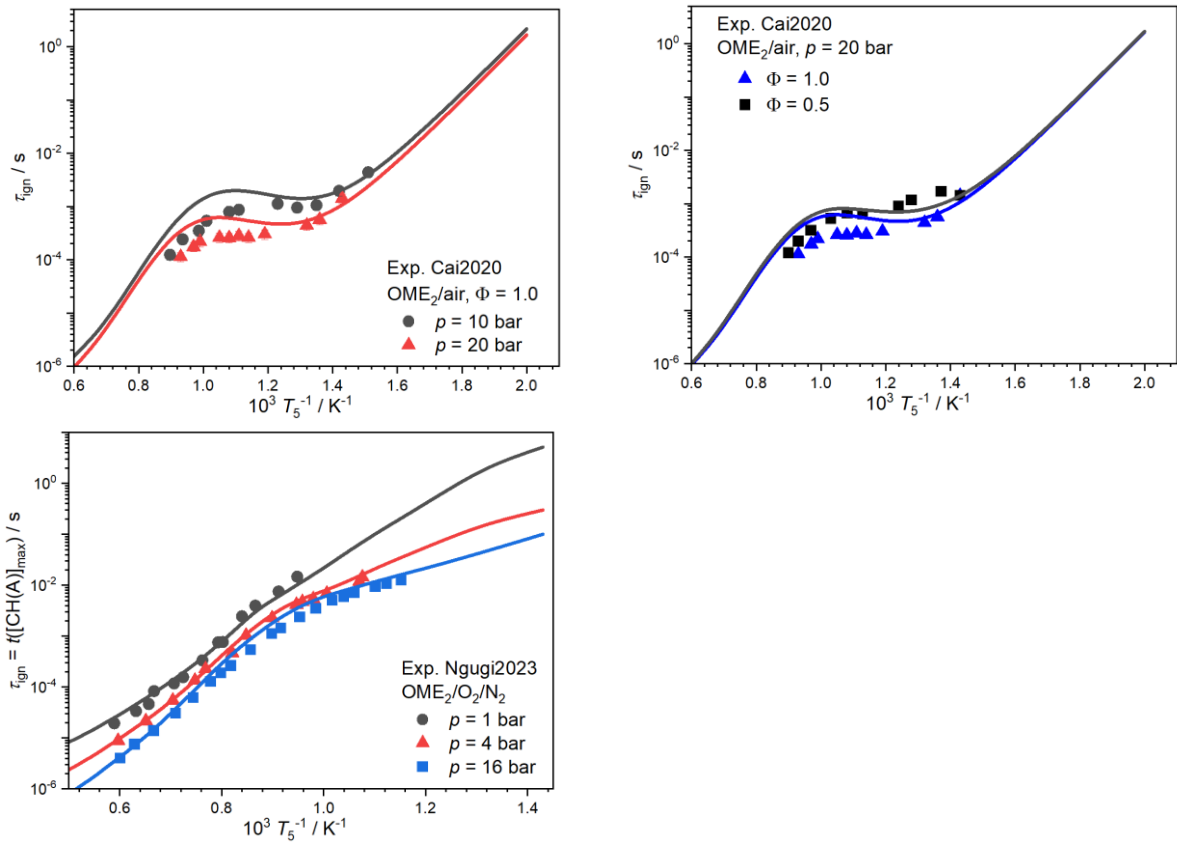


Fig. S8: DLR Concise model predictions of ignition delay times of OME2 [Cai2020, Ngugi2023].

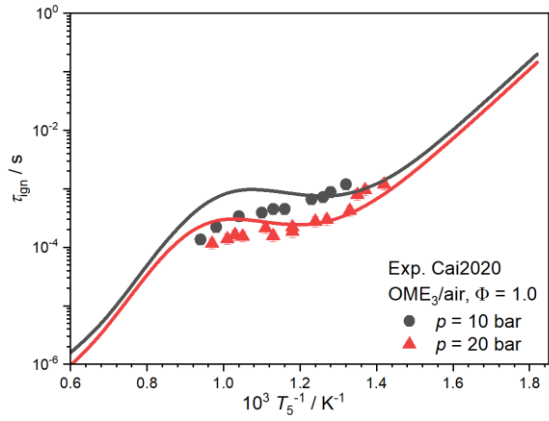


Fig. S9: DLR Concise model predictions of ignition delay times of OME3 [Cai2020].

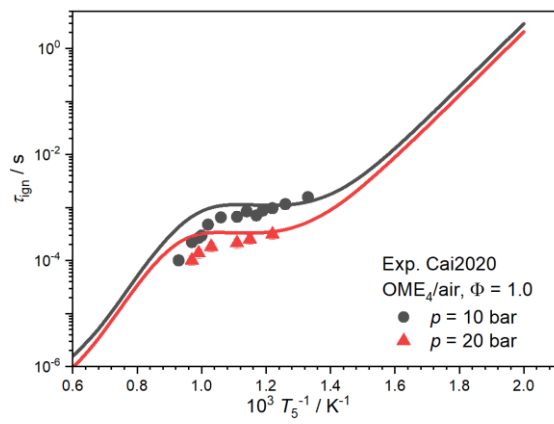
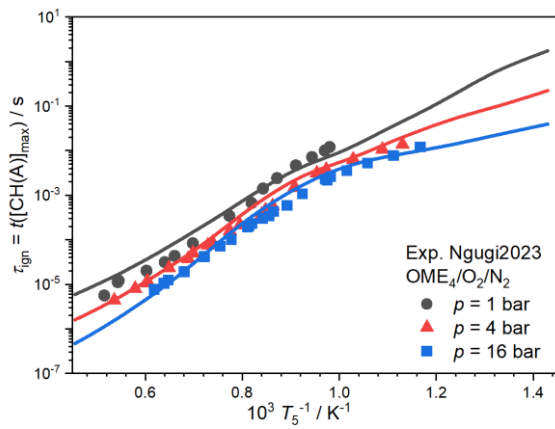


Fig. S10: DLR Concise model predictions of ignition delay times of OME4 [Ngugi2023, Cai2020].

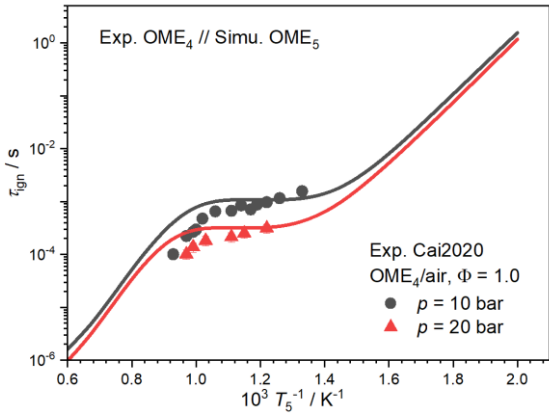


Fig. S11: DLR Concise model predictions of ignition delay times of OME5. Due to absence of any measurements of OME5, the OME5 model data are compared with measurements of OME4 [Cai2020].

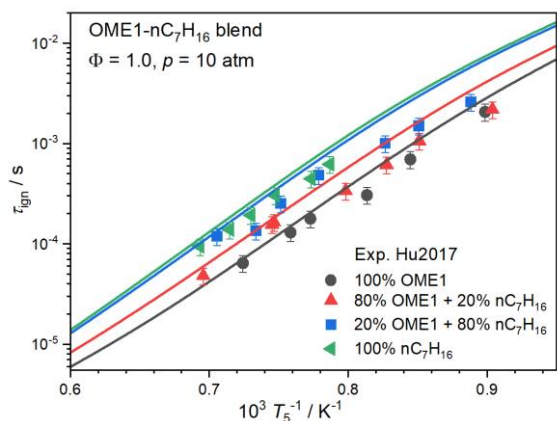


Fig. S12: DLR Concise model predictions of ignition delay times of OME1-nheptane blends [Hu2017].

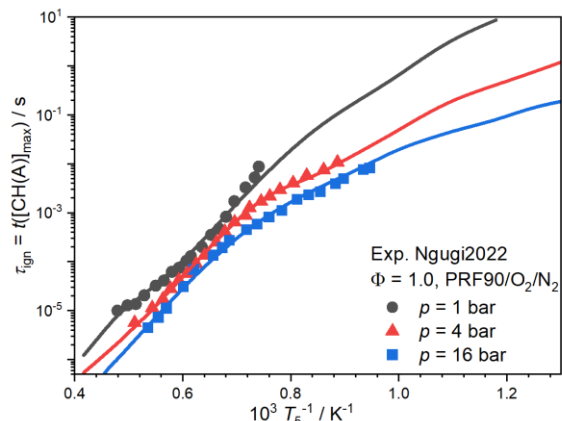


Fig. S13: DLR Concise model predictions of ignition delay times of PRF90 in air [Ngugi2022].

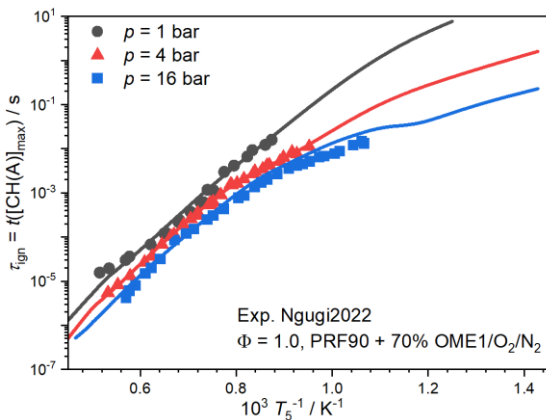
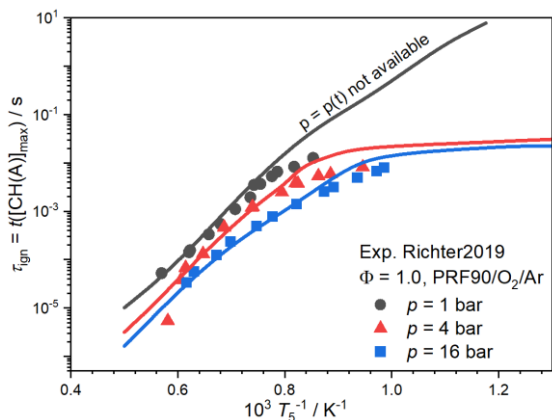


Fig. S14: DLR Concise model predictions of ignition delay times of PRF90 and its blend with 70% OME1 in air [Ngugi2022]. Measured pressure profiles used as input to model.

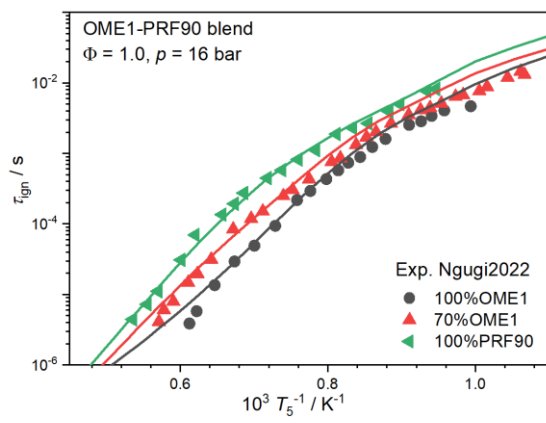
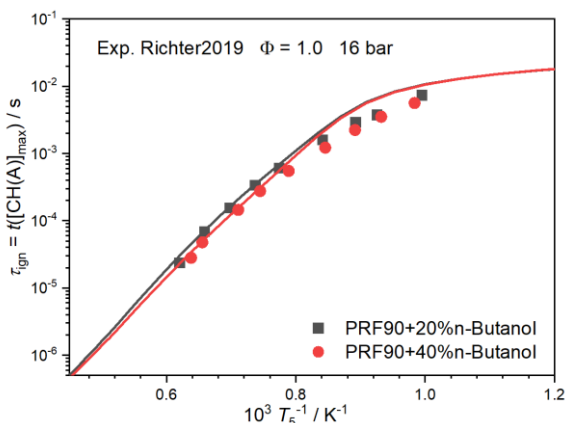


Fig. S15: DLR Concise model predictions of ignition delay times of PRF90 blended with n-butanol [Richter2019] and OME1 [Ngugi2022].

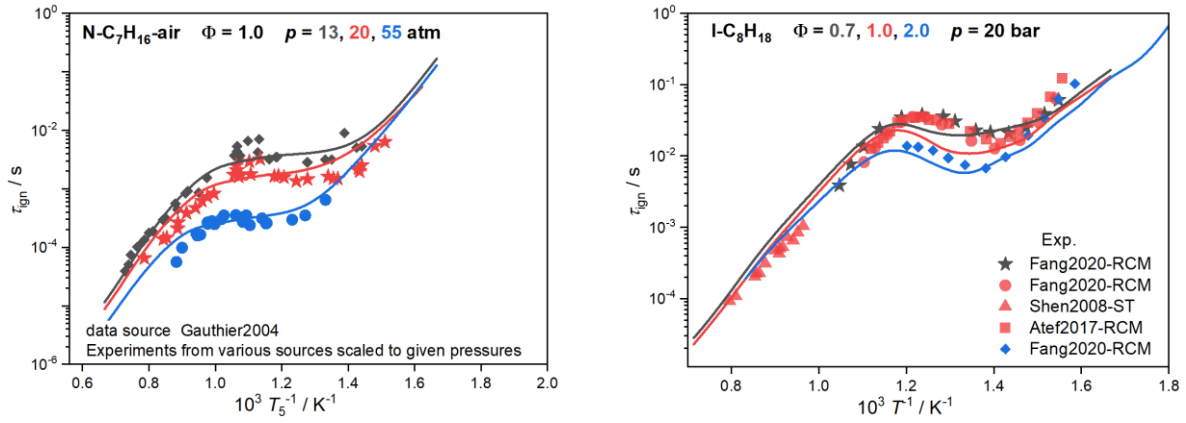


Fig. S16: DLR Concise model predictions of ignition delay times of n-heptane [Gauthier2004] and iso-octane [Fang2020, Shen2008, Atef2017]. ST: shock-tube, RCM- Rapid Compression Machine.

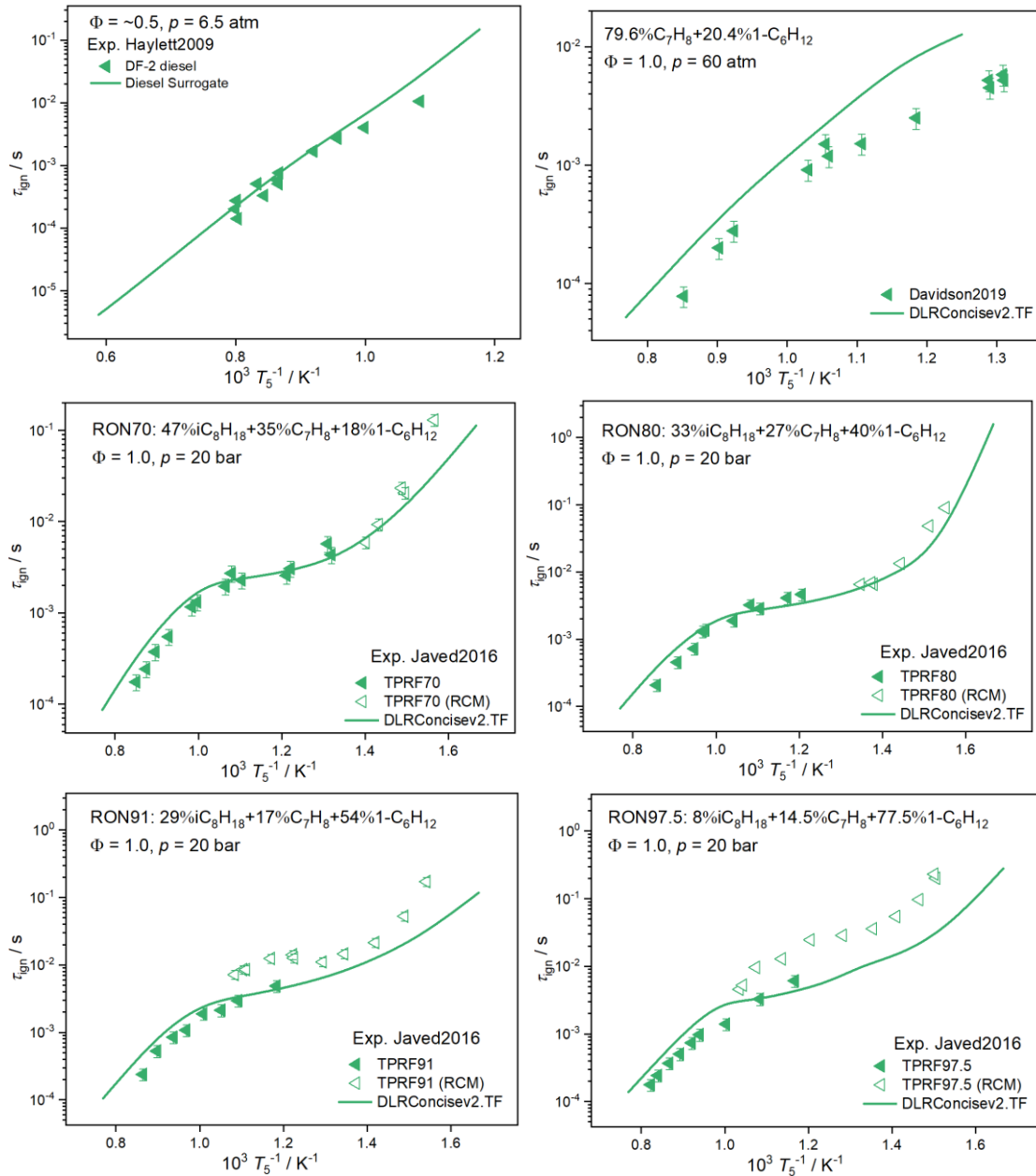


Fig. S17: DLR Concise model predictions of ignition delay times of gasoline surrogate [Davidson2019, Javed2016] and diesel surrogate [Haylett2009].

(1.3) Laminar flame speeds

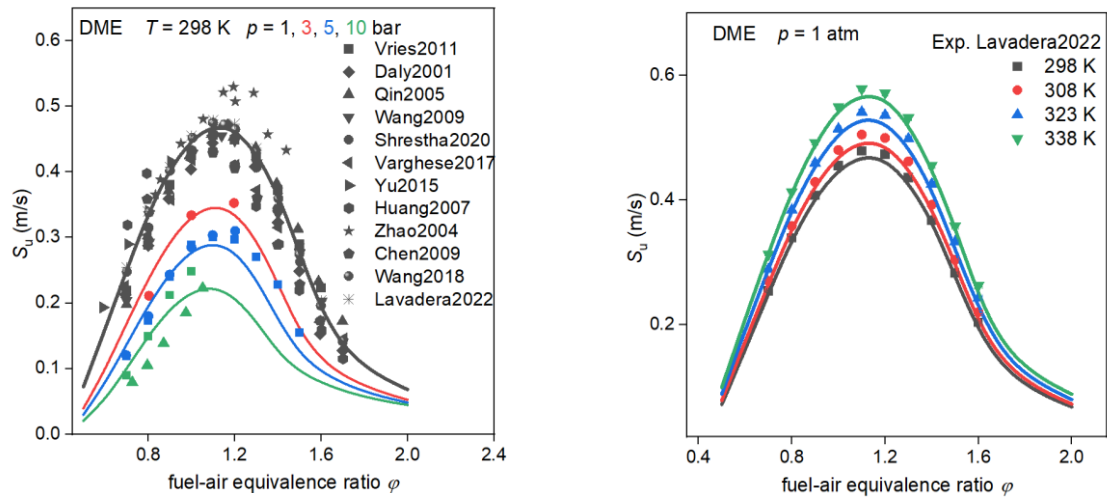


Fig. S18: DLR Concise model predictions of laminar flame speed of DME at various preheat temperatures and pressures [Vries2011, Daly2001, Qin2005, Wang2009, Shrestha2020, Varghese2017, Yu2015, Huang2007, Zhao2004, Chen2009, Wang2018, Lavadera2022].

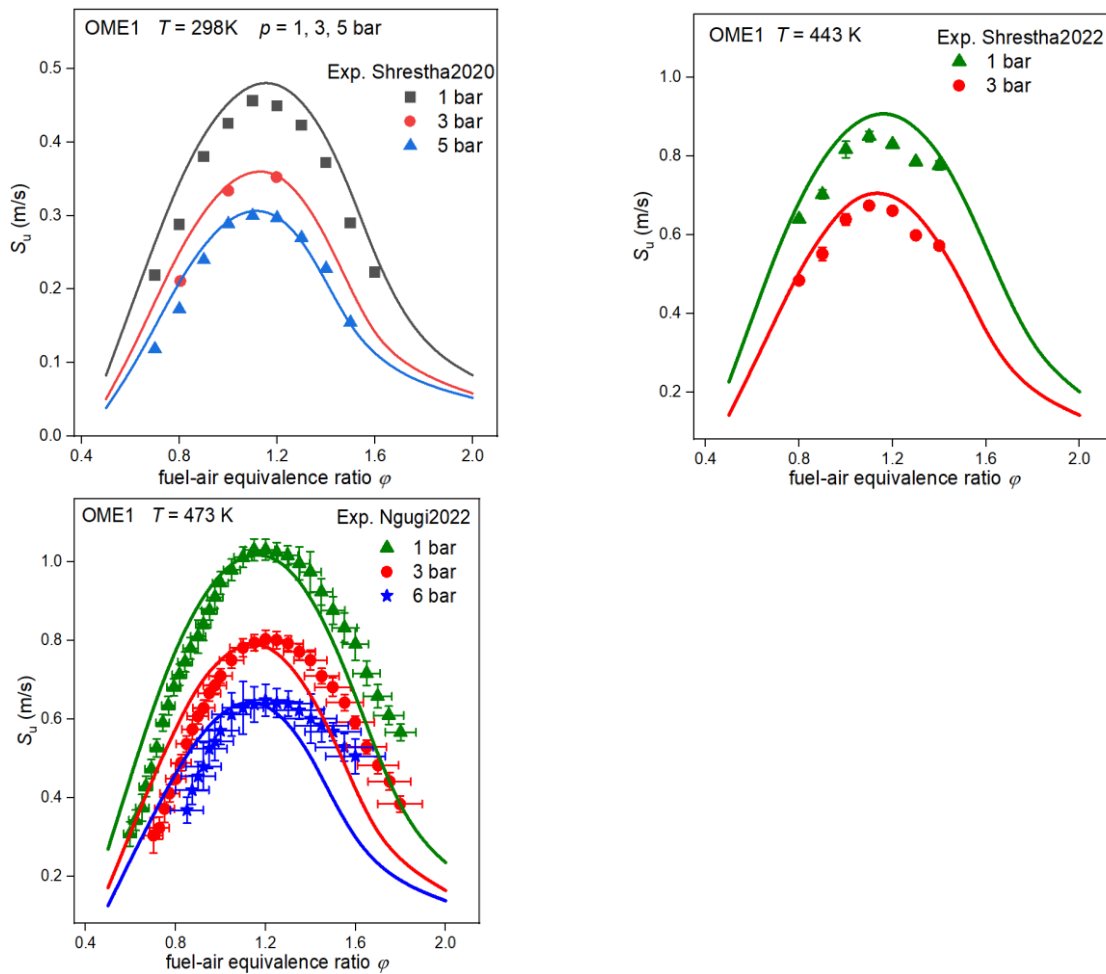


Fig. S19: DLR Concise model predictions of laminar flame speed of OME1 at different preheat temperatures and pressures [Shrestha2020, Shrestha2022, Ngugi2022].

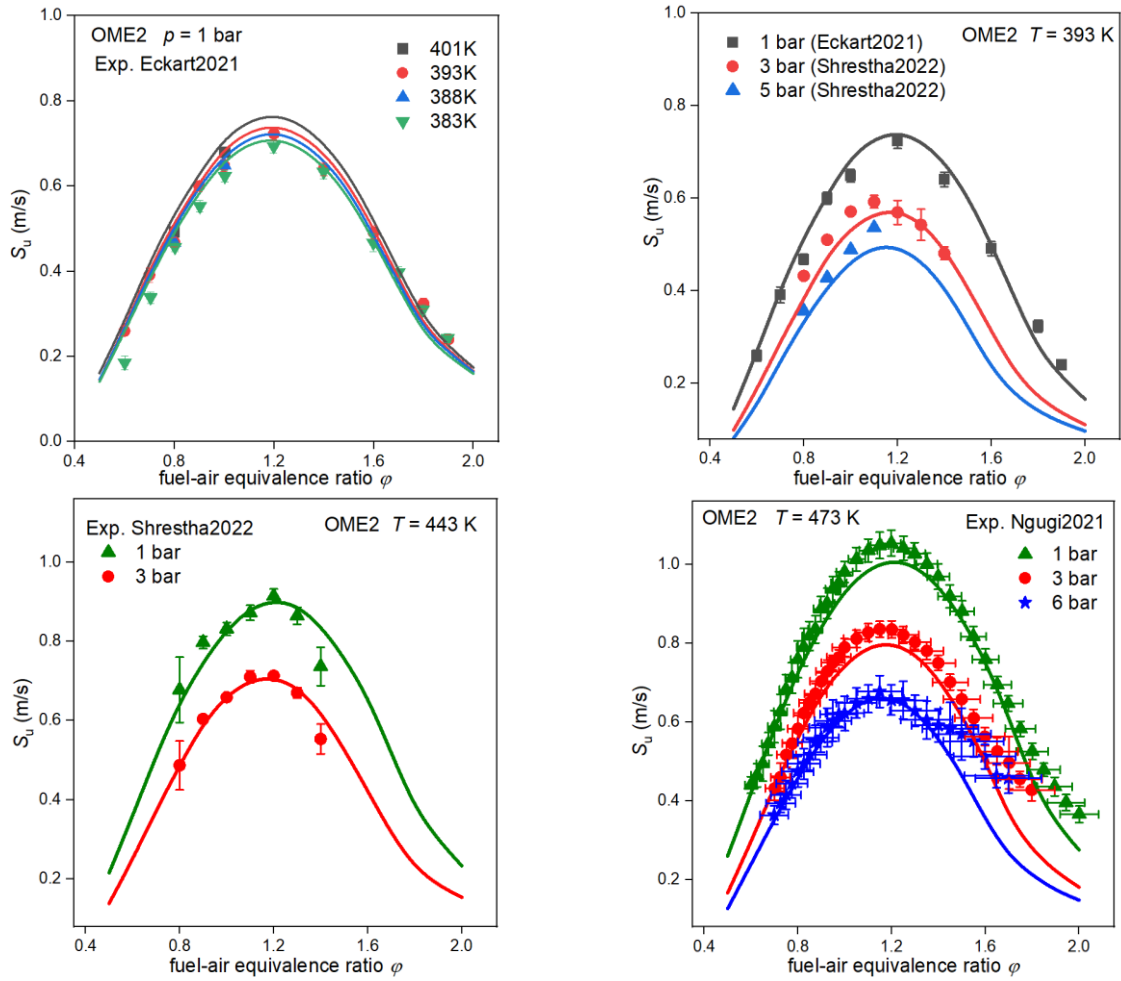


Fig. S20: DLR Concise model predictions of laminar flame speed of OME2 at various preheat temperatures and pressures [Eckart2021, Shrestha2022, Ngugi2021].

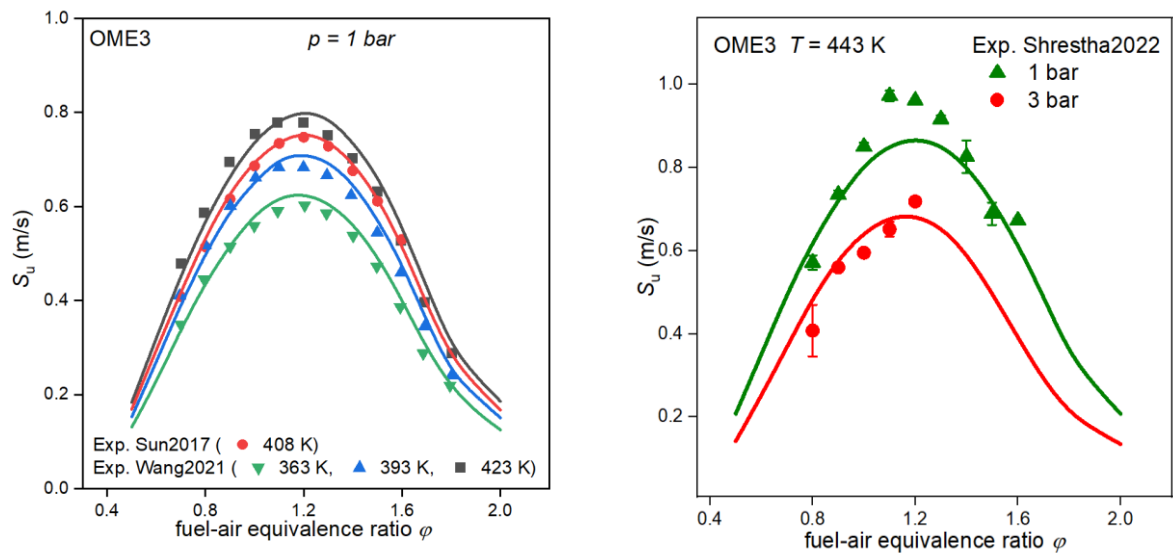


Fig. S21: DLR Concise model predictions of laminar flame speed of OME3 at various preheat temperatures and pressures [Sun2017-OME3, Wang2021, Shrestha2022].

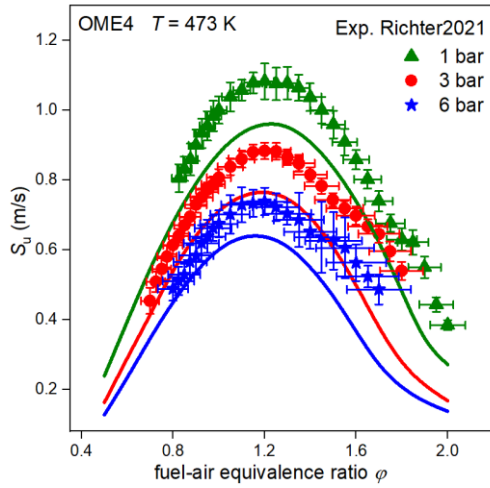


Fig. S22: DLR Concise model predictions of laminar flame speed of OME4 at different pressures [Richter2021].

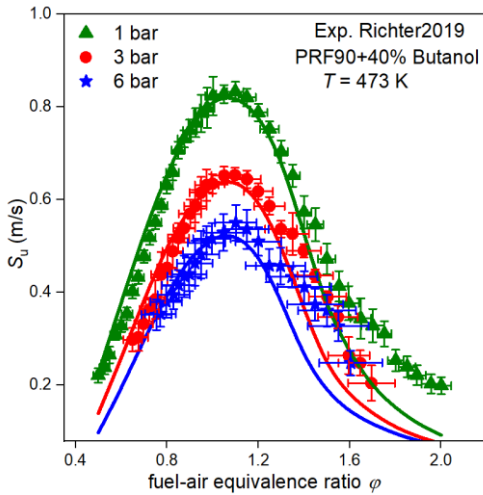
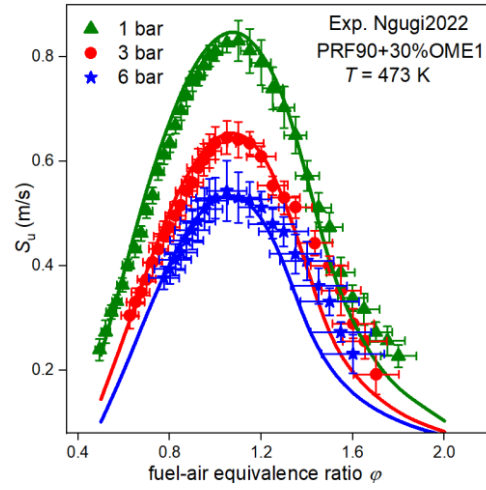
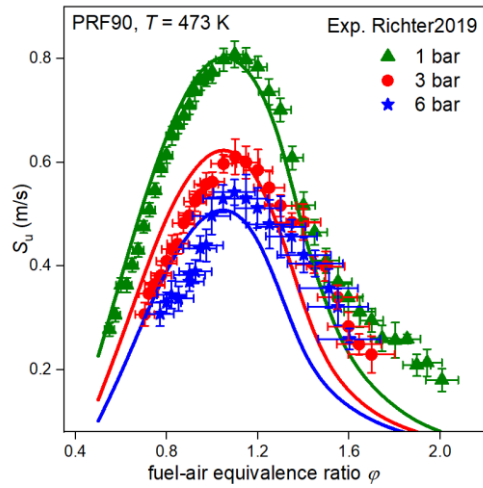


Fig. S23: DLR Concise model predictions of laminar flame speed of PRF90 and its blend with OME1 and n-butanol [Richter2019, Ngugi2022].

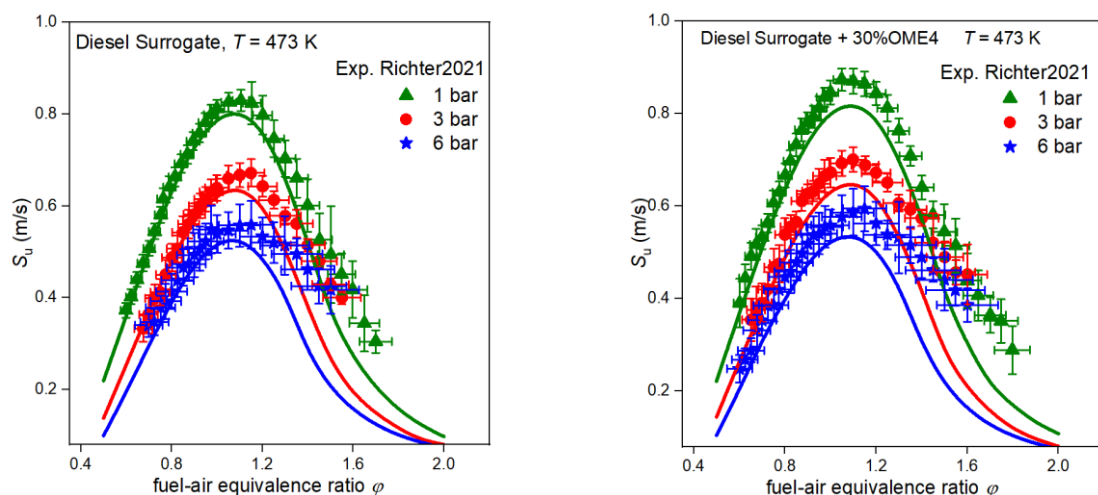


Fig. S24: DLR Concise model predictions of laminar flame speed of diesel surrogate and OME4-diesel surrogate blend [Richter2021].

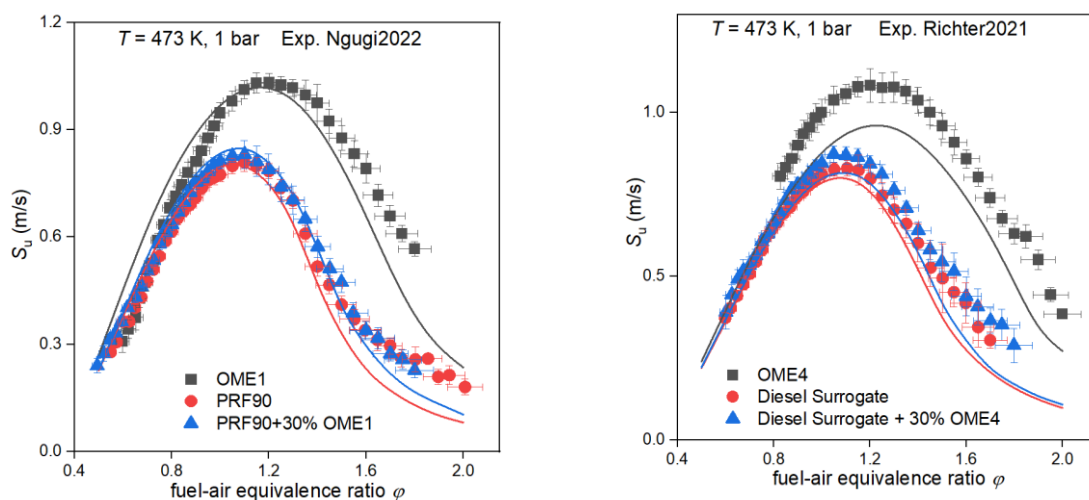
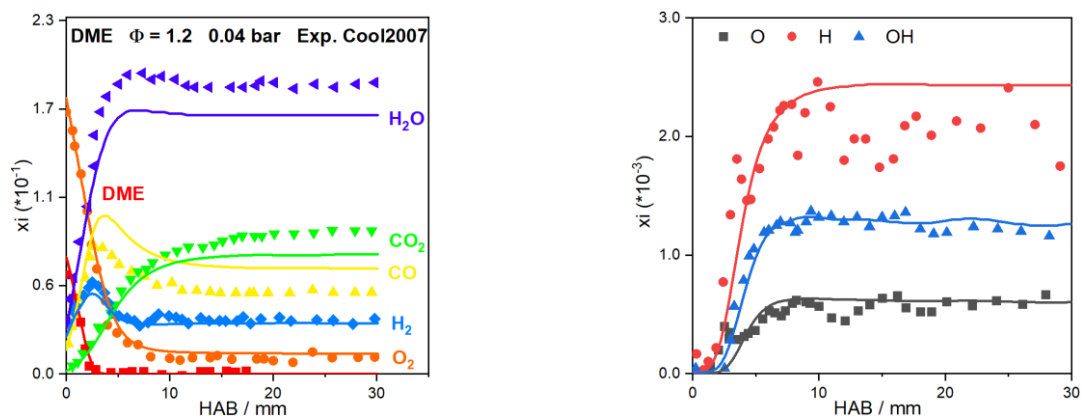


Fig. S25: Relative comparison of laminar flame speed of OME1-PRF90 [Ngugi2022] and OME4-diesel surrogate [Richter2021] blends and pure components with DLR Concise model predictions.

(1.4) Laminar burner-stabilized flames

This section presents model prediction of measured fuel and oxidizer conversion as well as important intermediates species and product formation. In some cases, radicals are also measured which are compared with model.



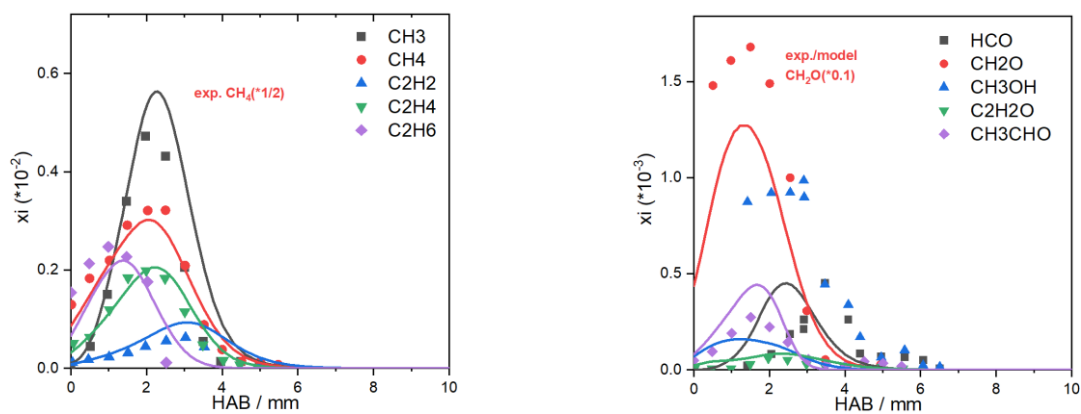


Fig. S26: Speciation in burner-stabilized DME flame [Cool2007].

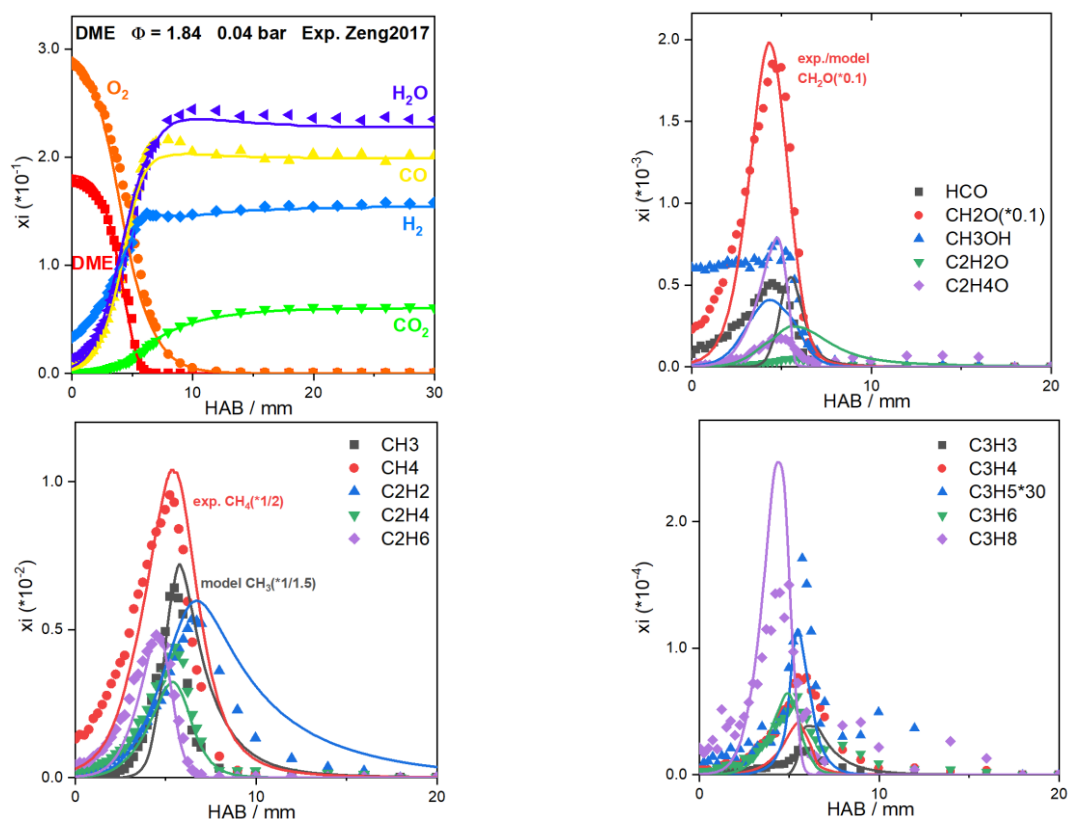
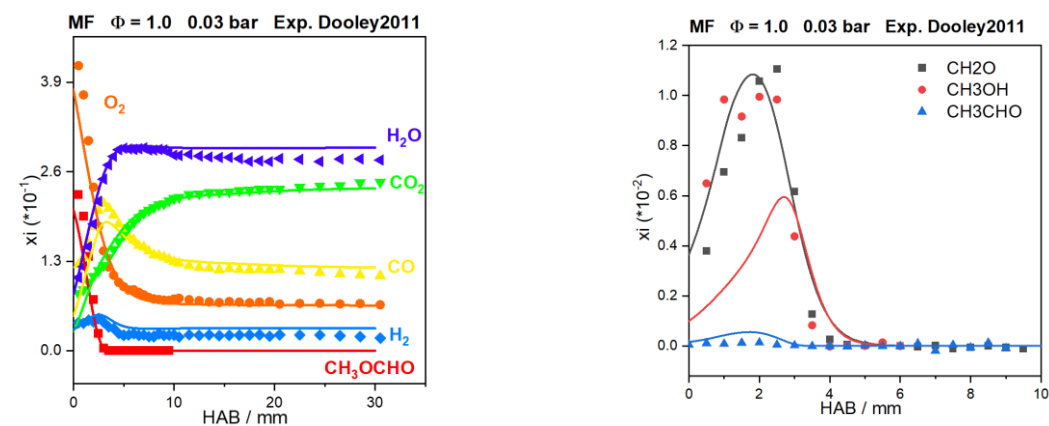


Fig. S27: Speciation in burner-stabilized DME flame [Zeng2017].



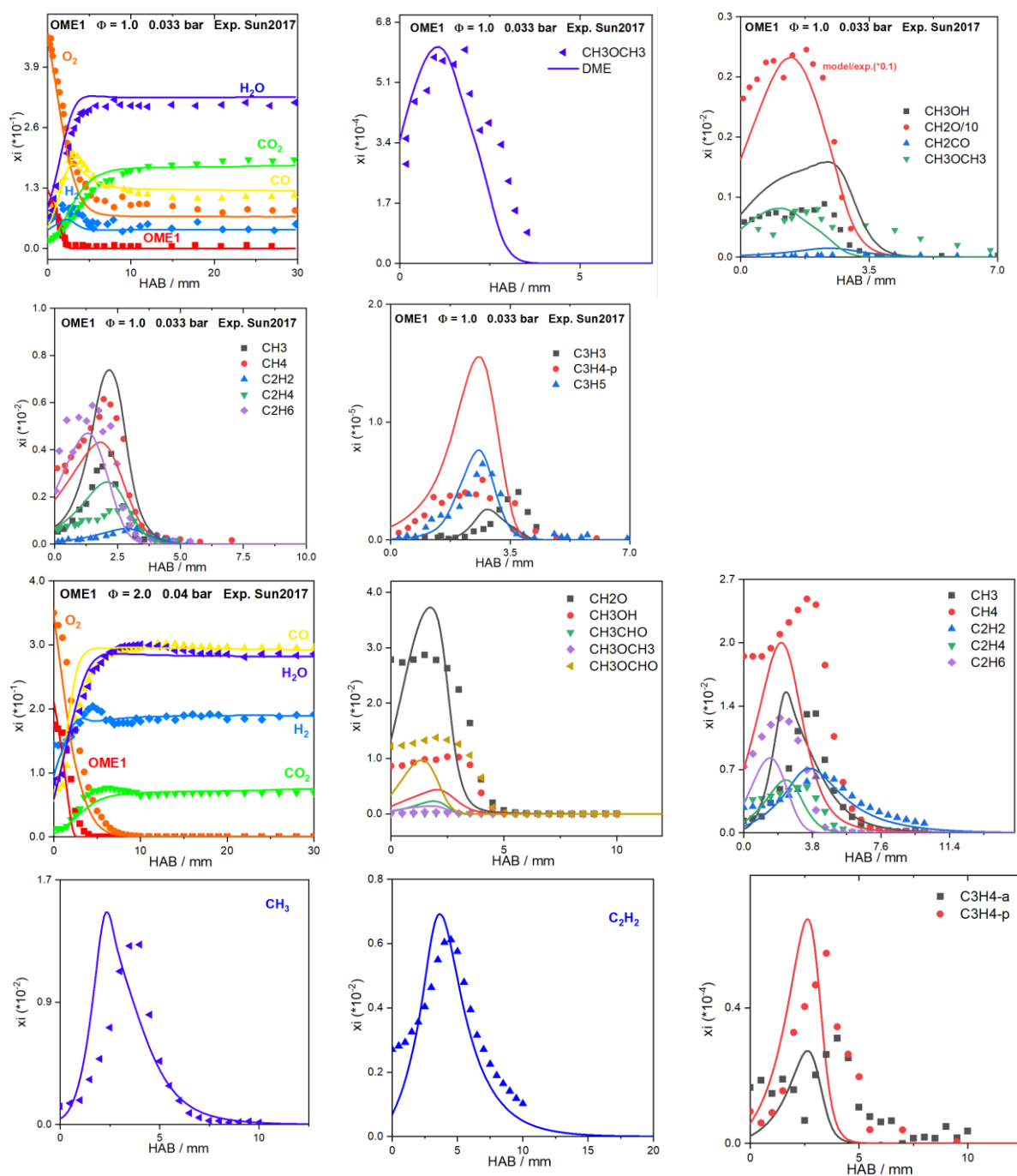
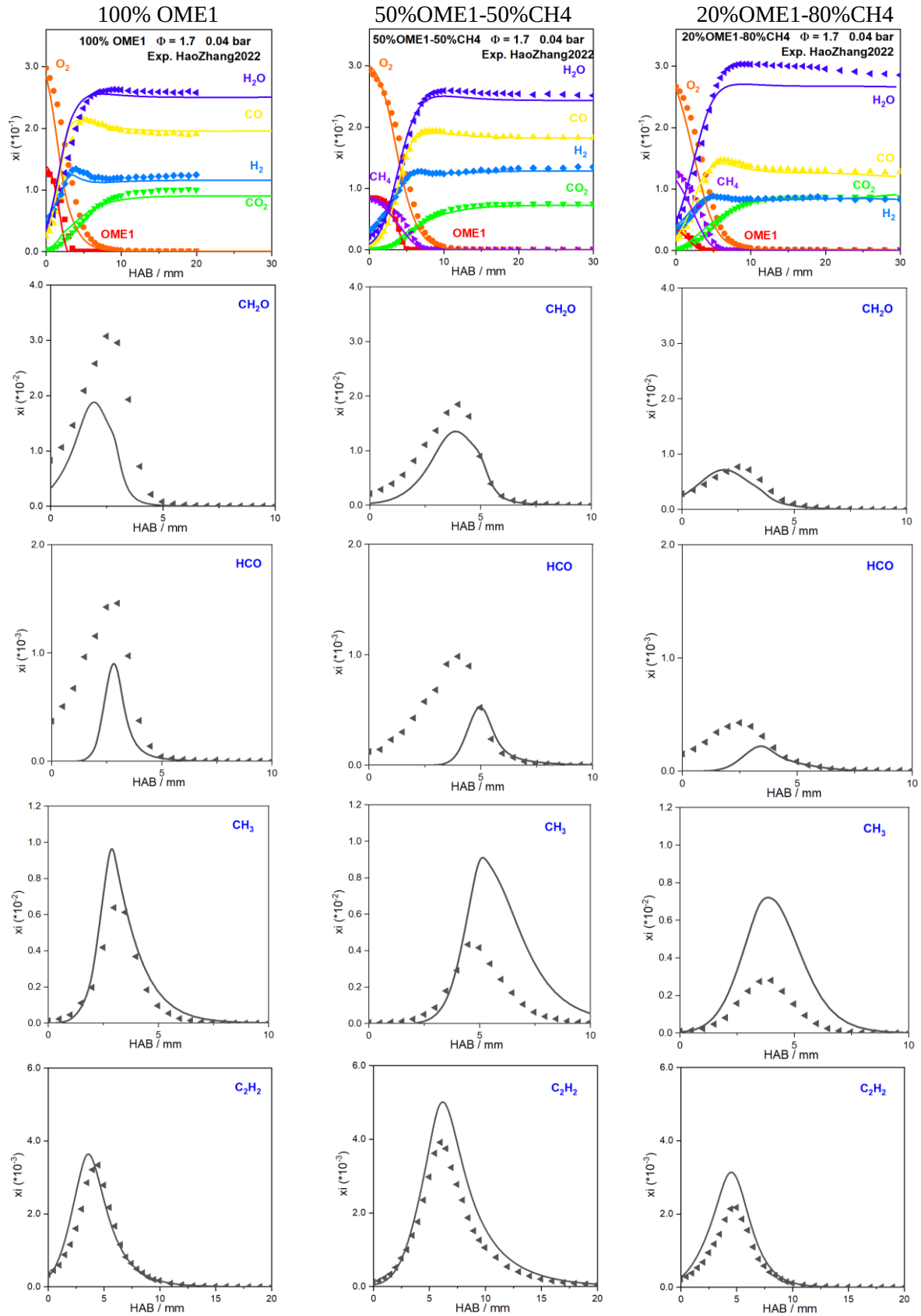


Fig. S29: Speciation in burner-stabilized OME1 flame; $\Phi = 1.0$, 0.033 bar [Sun2017-OME3], $\Phi = 2.0$, 0.04 bar [Sun2017-OME1].



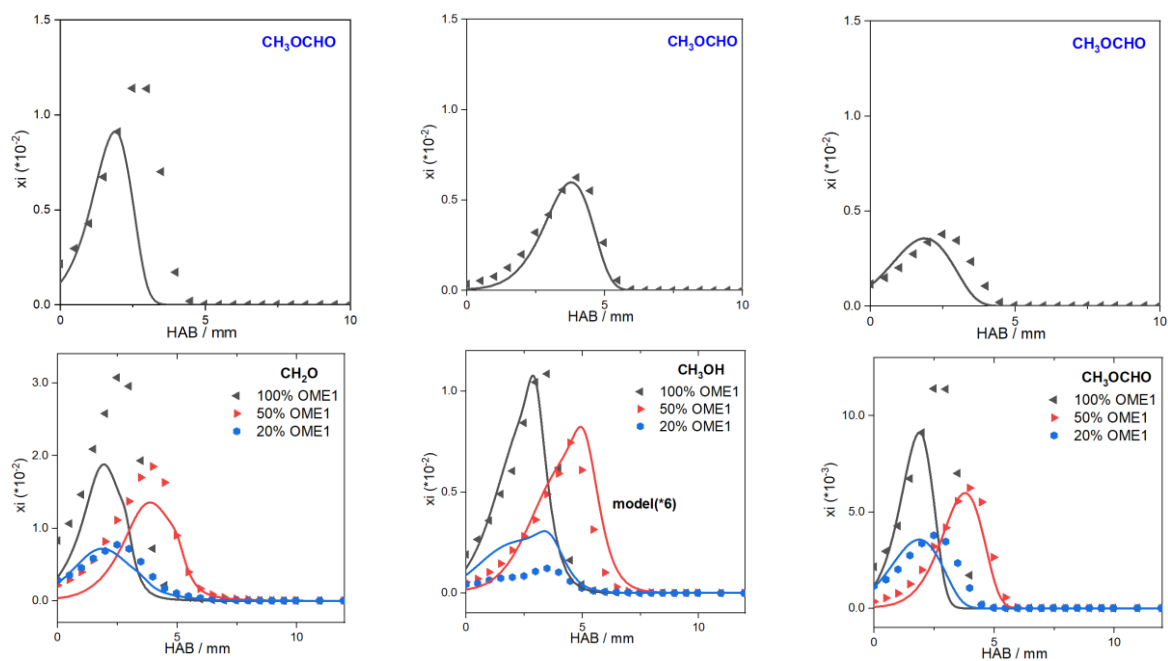


Fig. S30: Speciation in burner-stabilized OME1-CH₄ flames [Hao-Zhang2022].

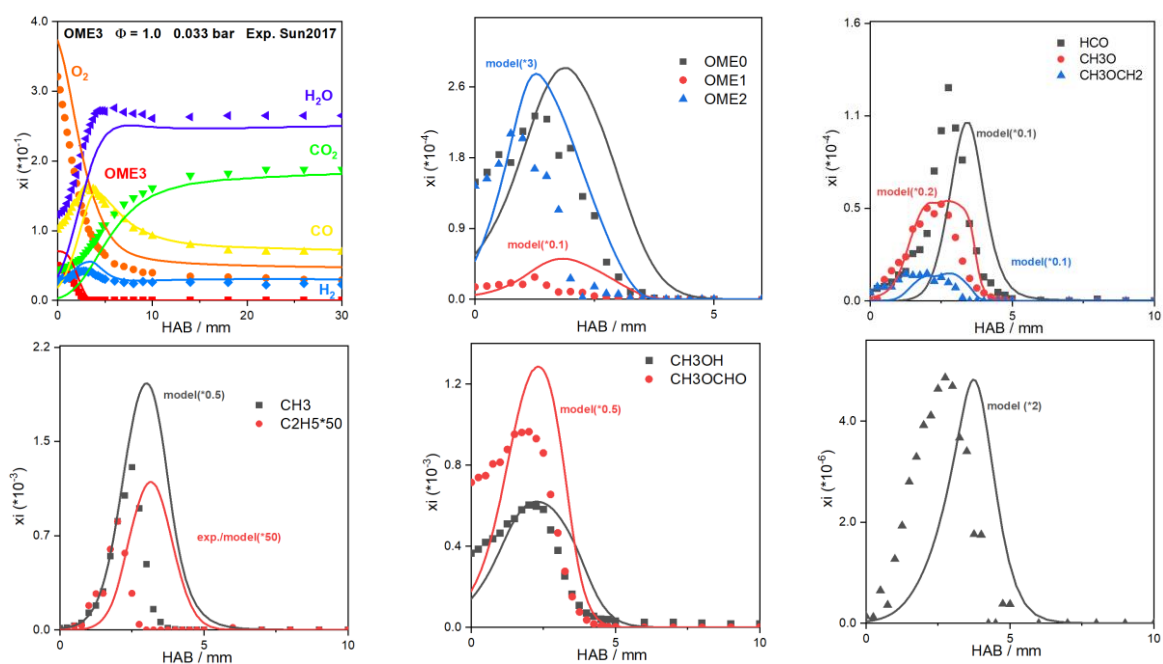
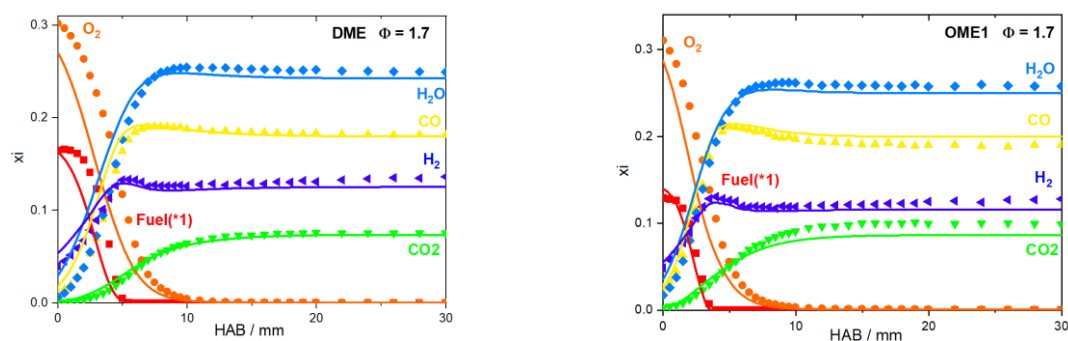
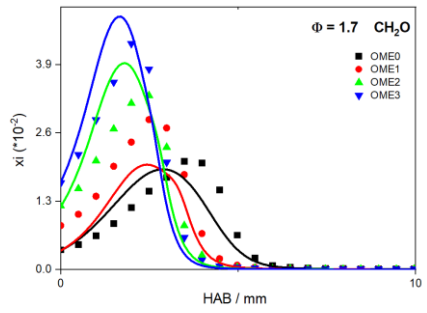
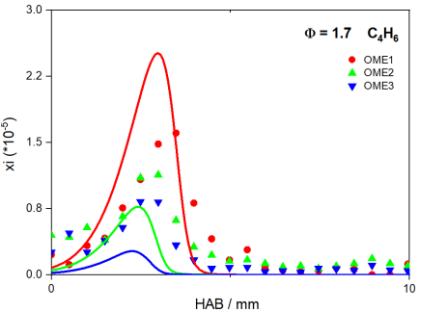
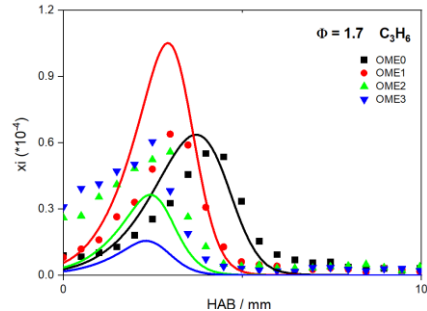
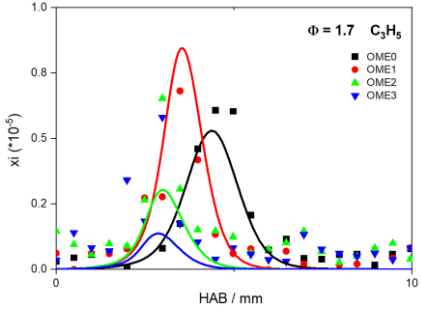
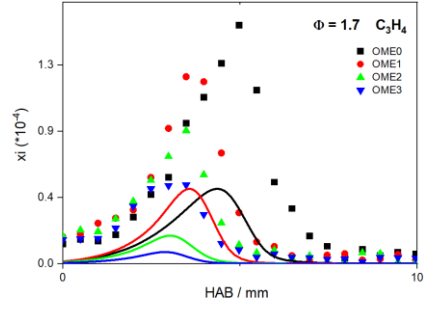
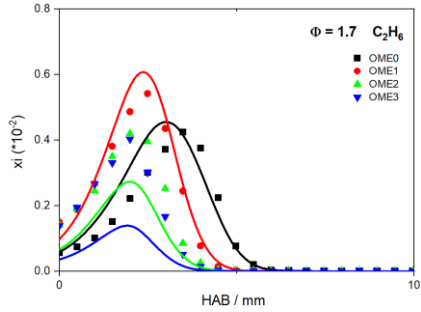
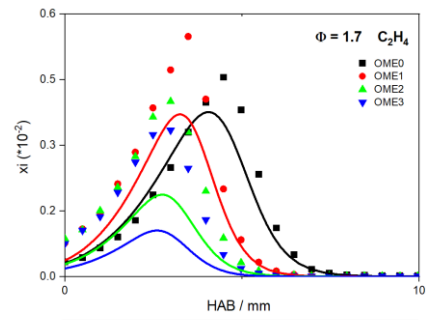
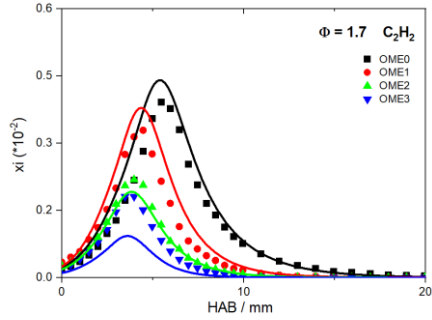
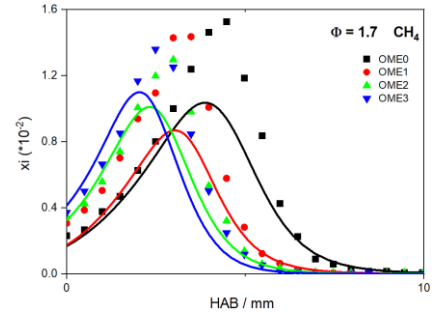
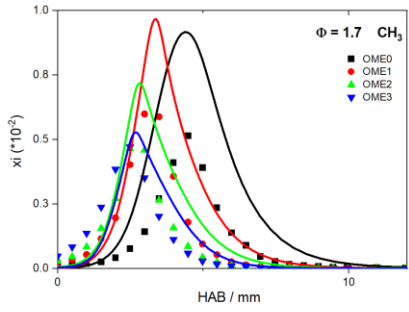
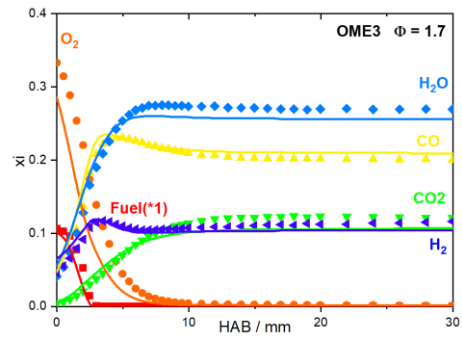
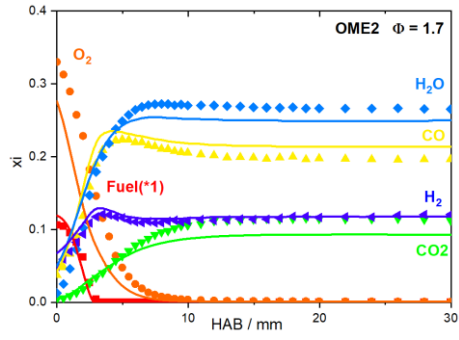


Fig. S31: Speciation in burner-stabilized OME3 flame [Sun207-OME3].





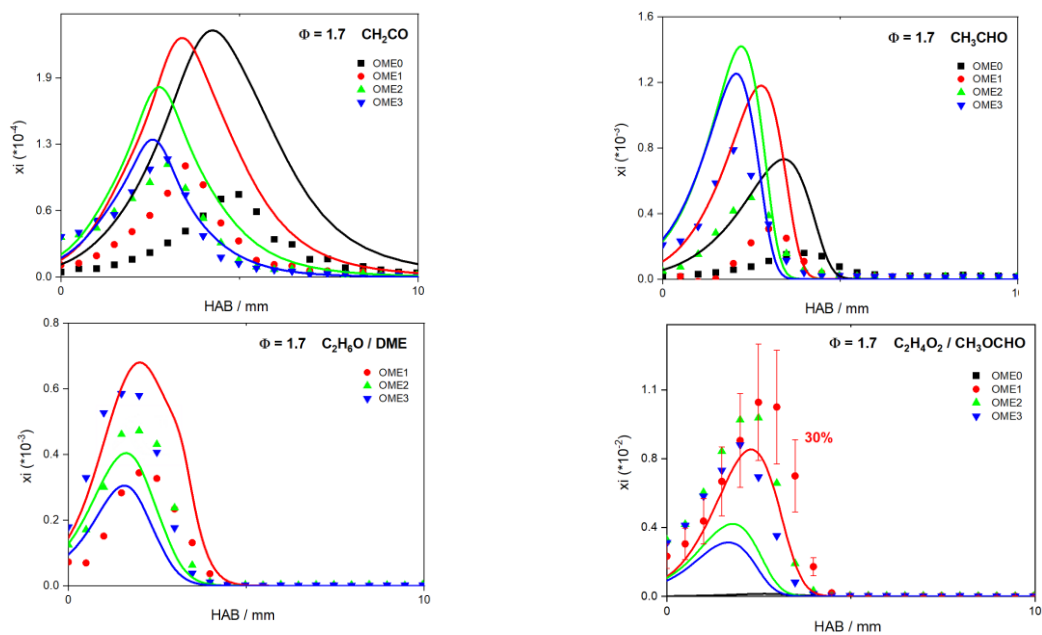
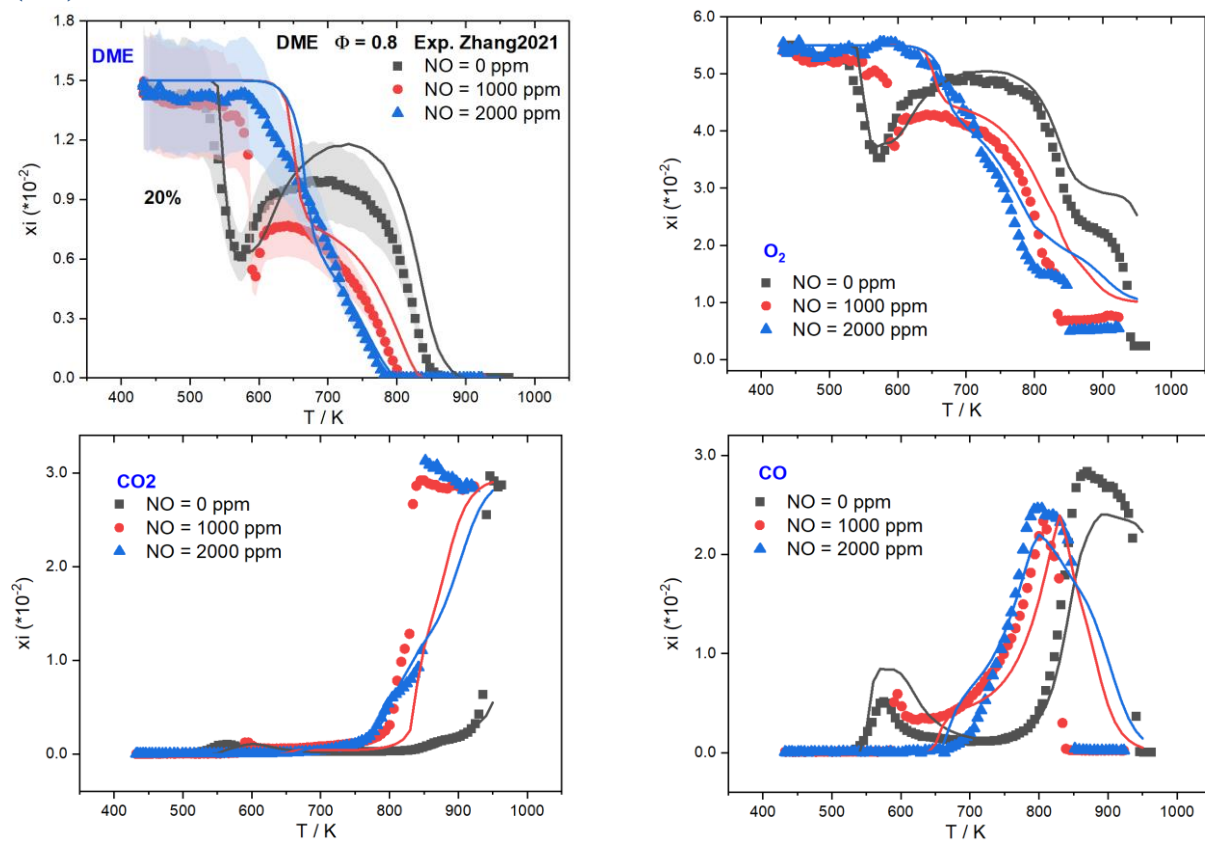
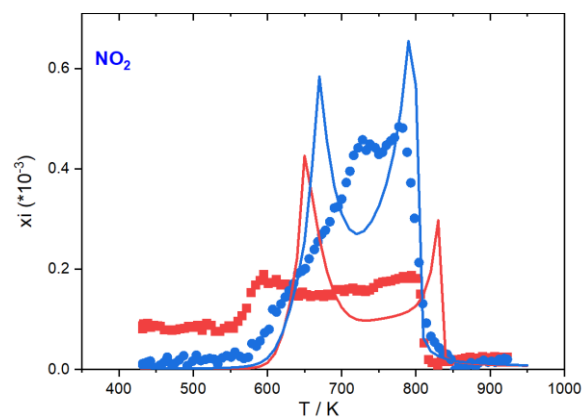
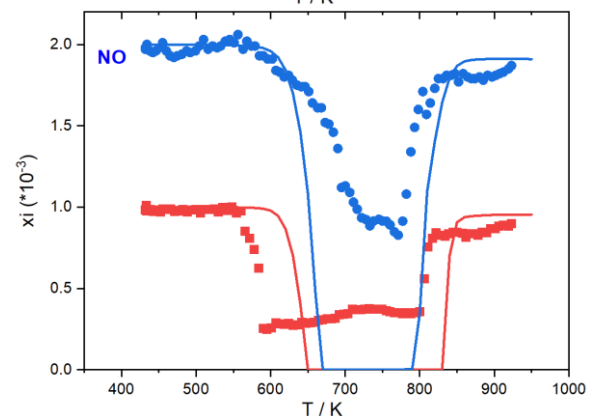
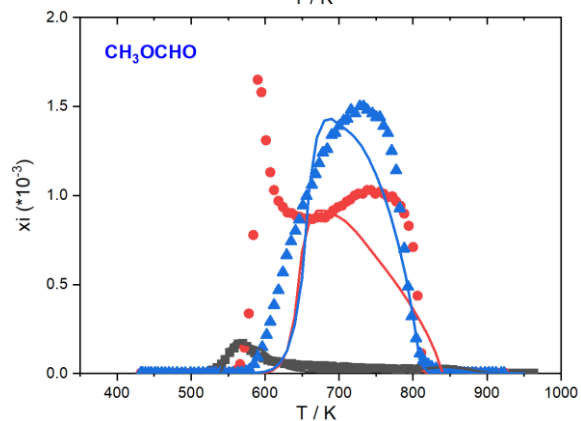
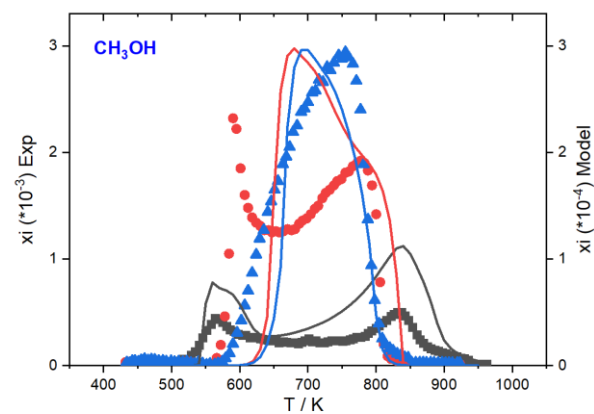
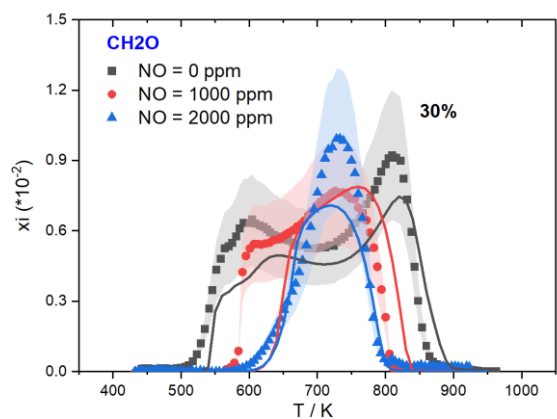
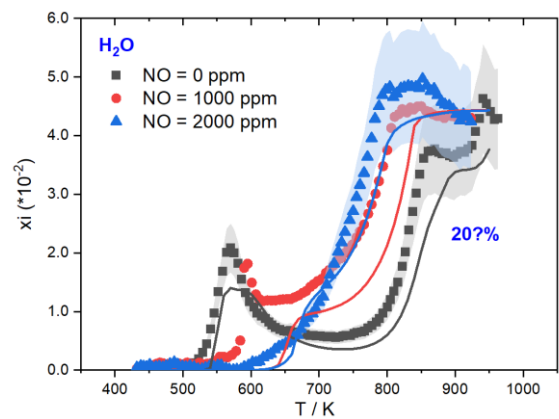
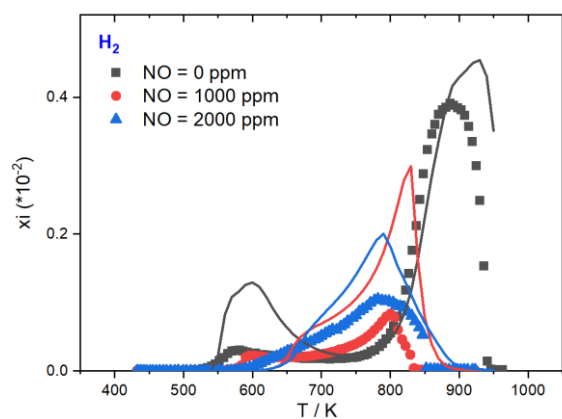


Fig. S32: Speciation in burner-stabilized OME0-OME3 flames [Gaiser2022C].

(1.5) Flow reactor





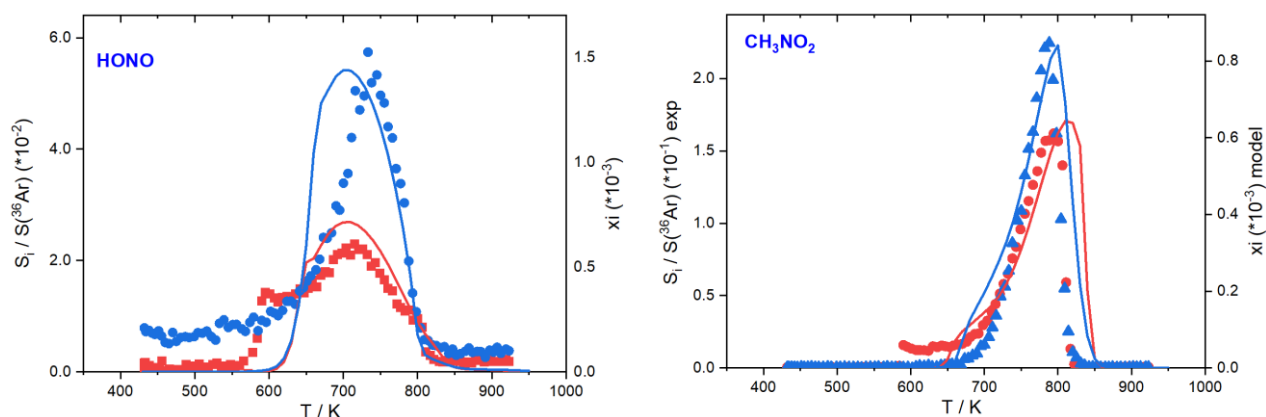
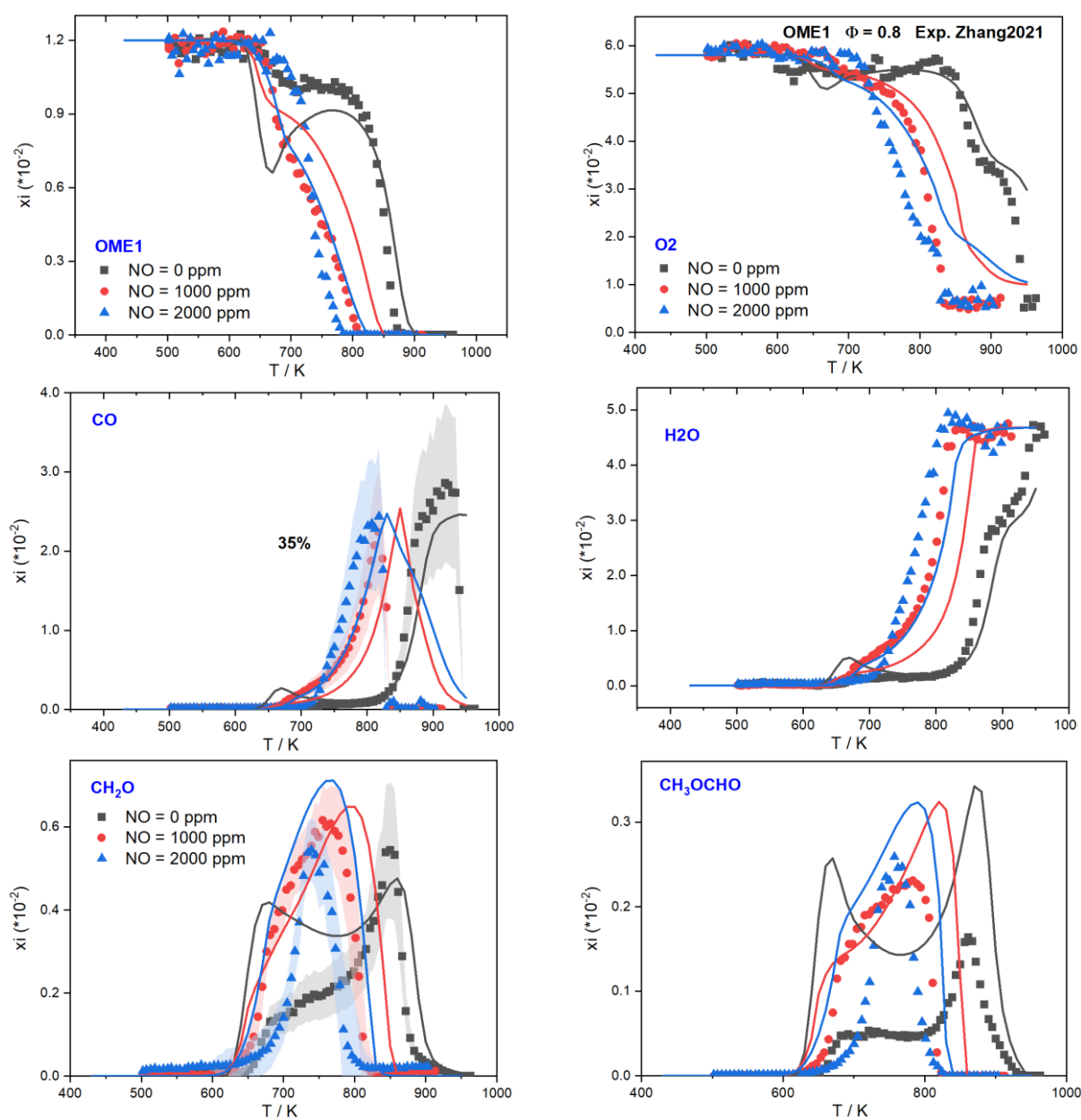


Fig. S33: Speciation in flow reactor [Zhang2021] DME/NO mixtures.



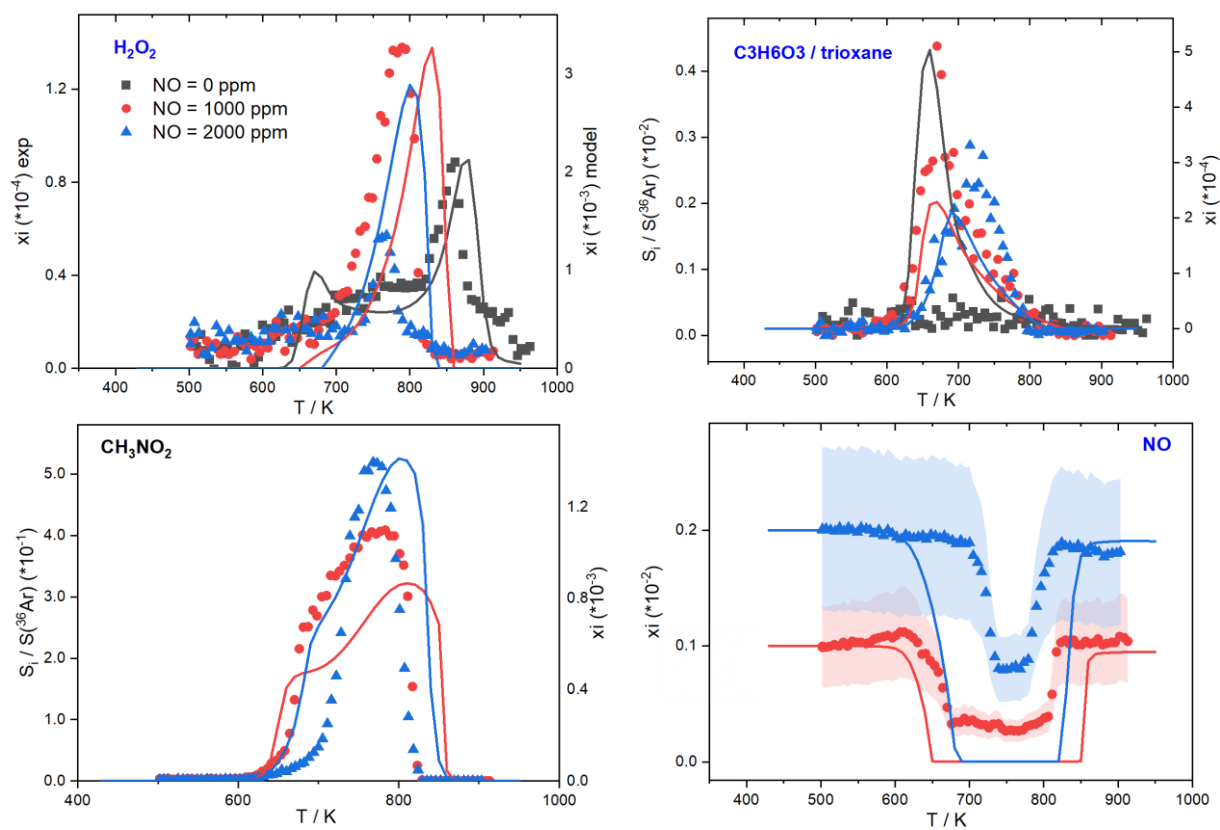
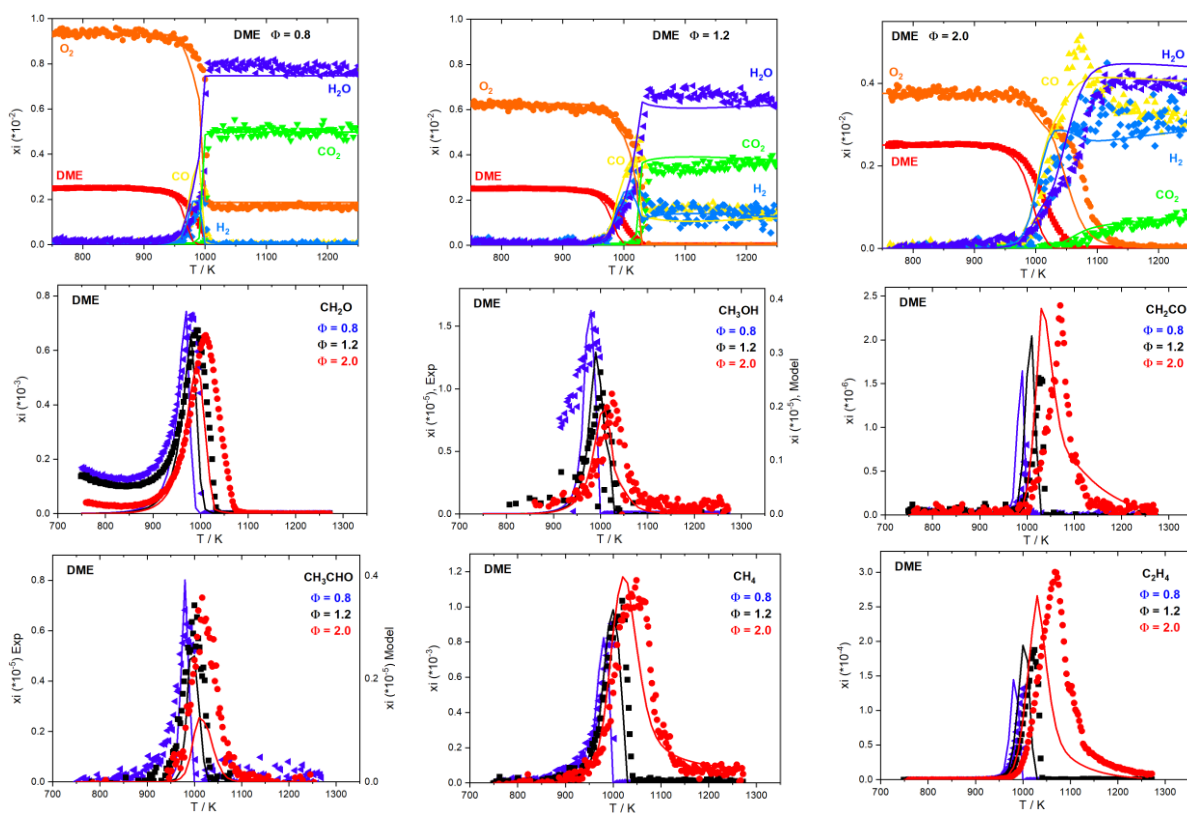


Fig. S34: Speciation in flow reactor [Zhang2021] OME1 / NO mixtures.



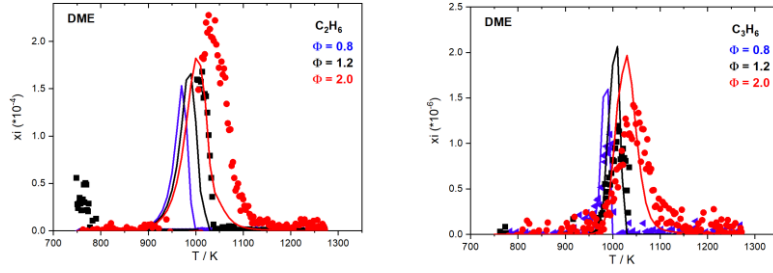


Fig. S35: Speciation in high-temperature DLR flow reactor, DME measurements at three fuel stoichiometries [Gaiser2022F].

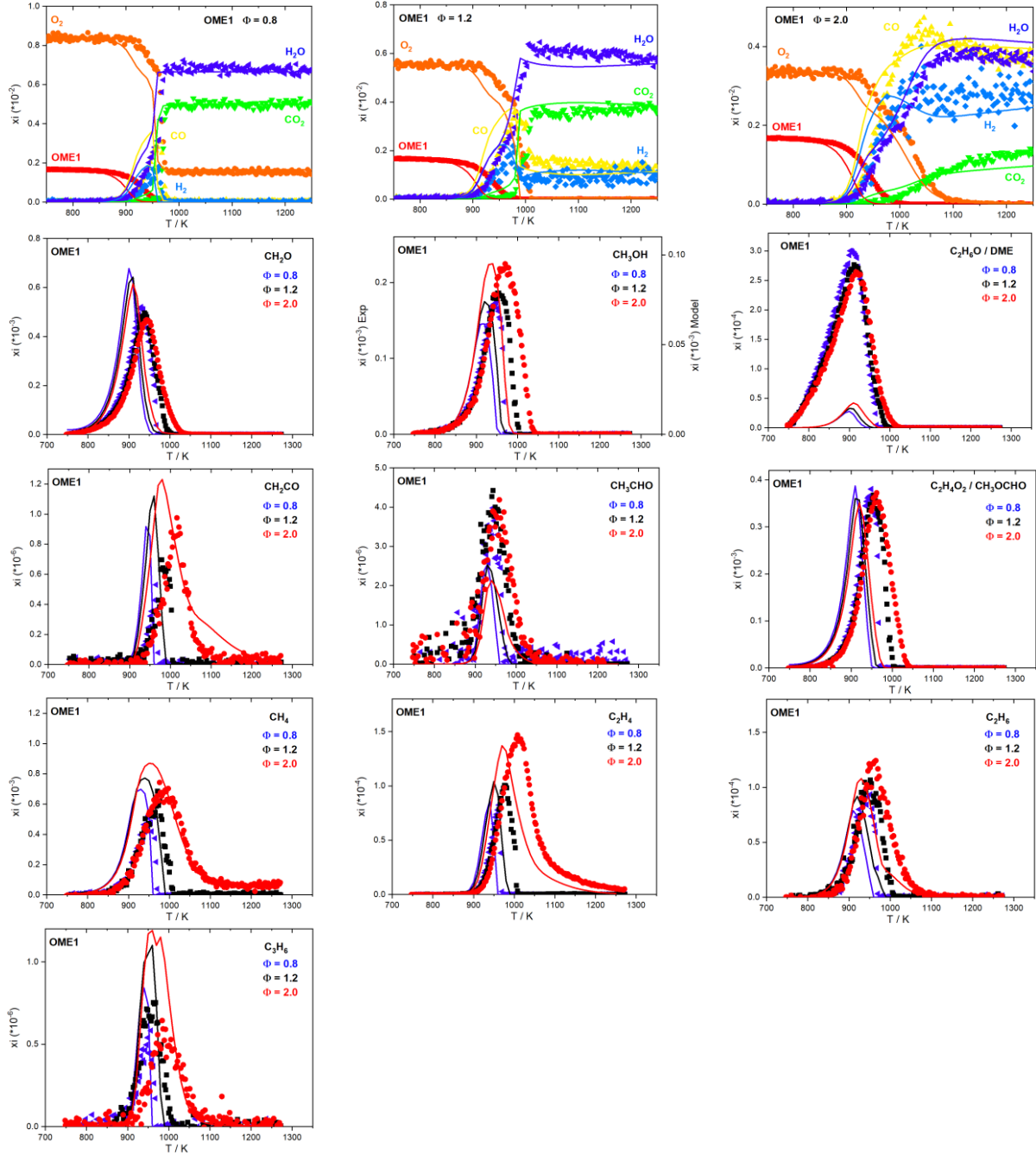


Fig. S36: Speciation in high-temperature DLR flow reactor, OME1 measurements at three fuel stoichiometries [Gaiser2022F].

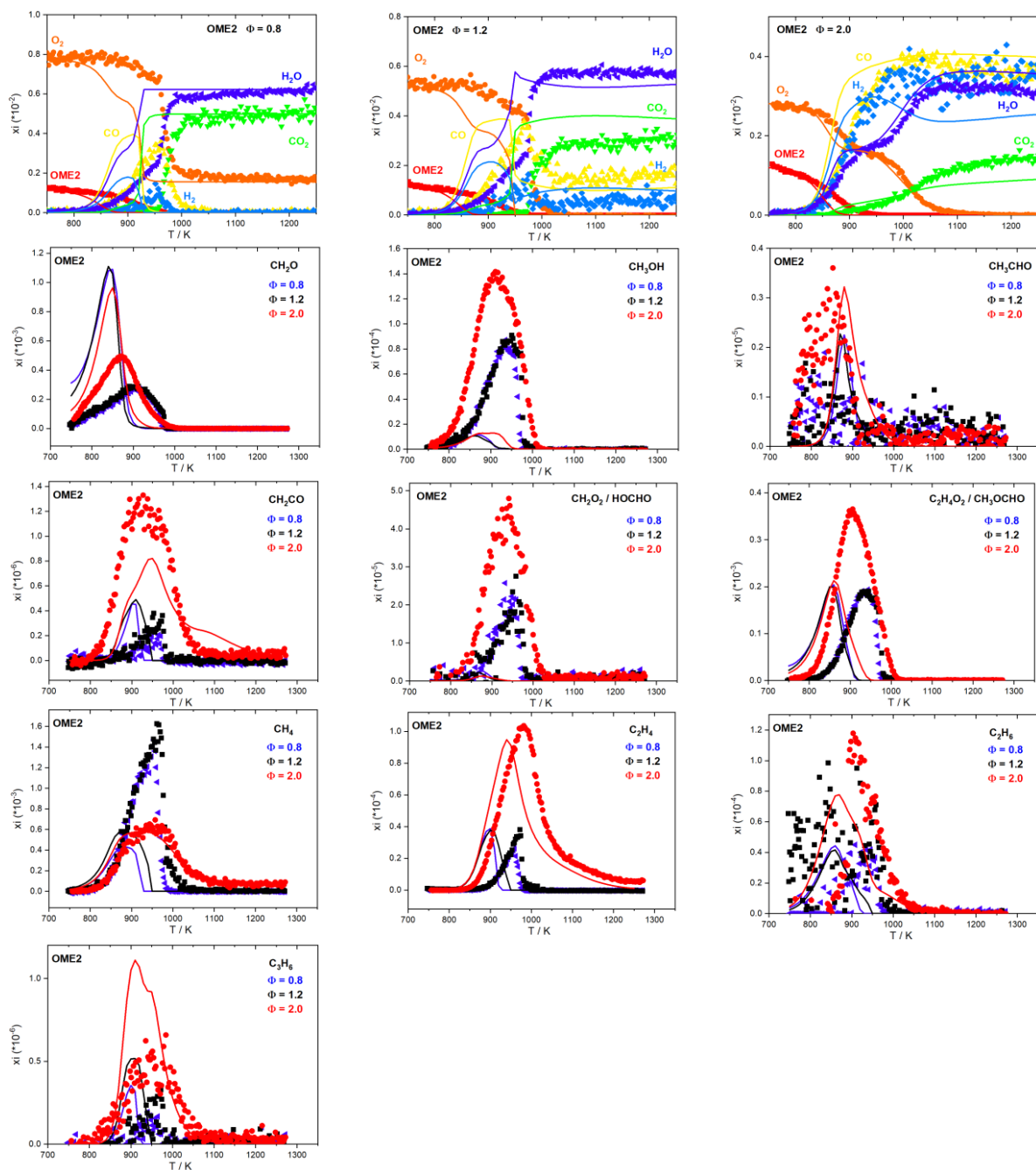
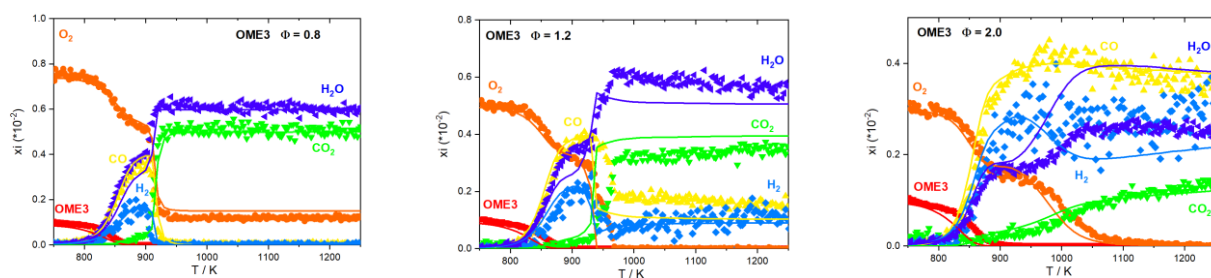


Fig. S37: Speciation in high-temperature DLR flow reactor, OME2 measurements at three fuel stoichiometries [Gaiser2022F].



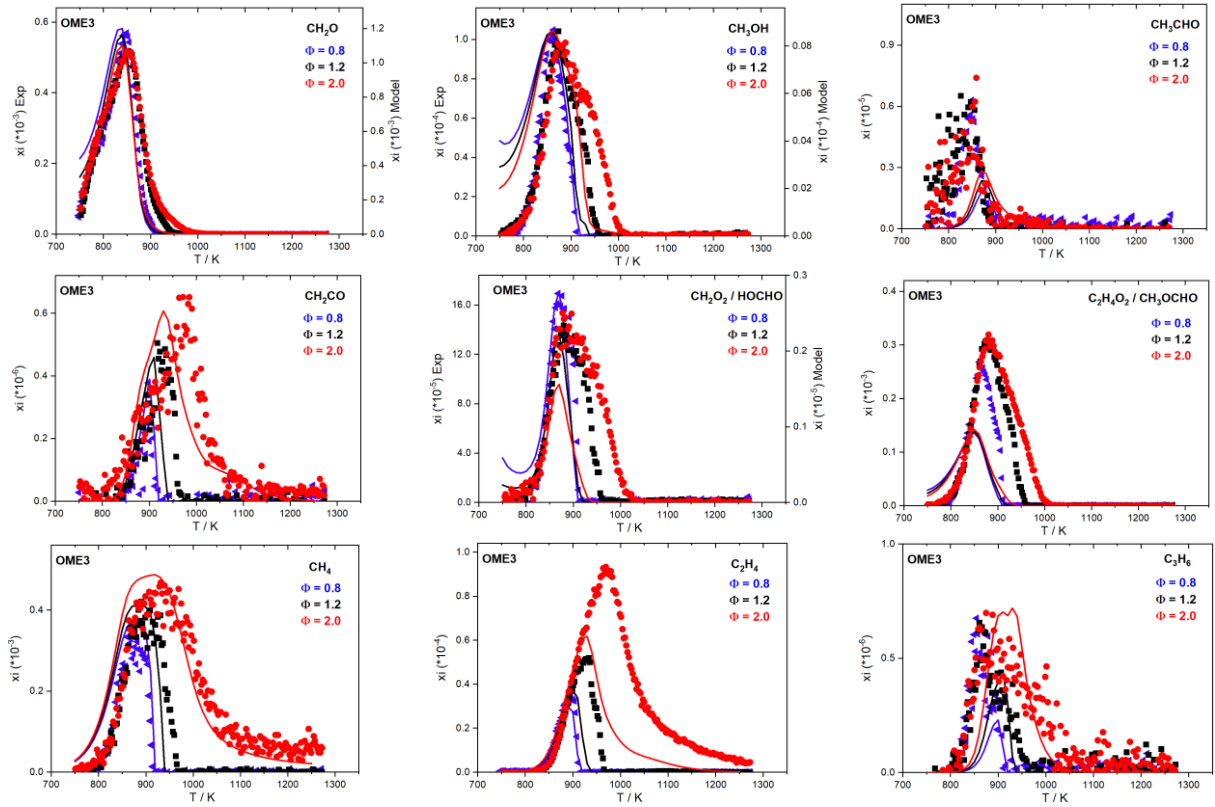
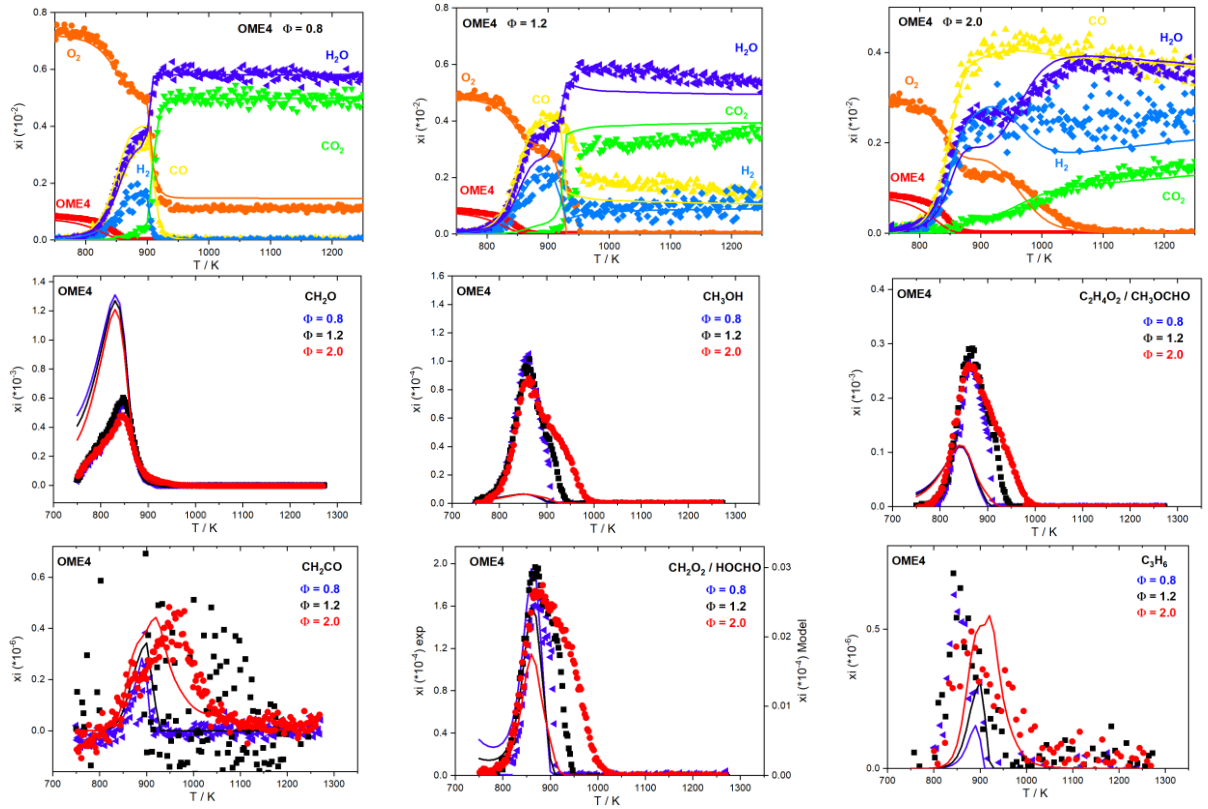


Fig. S38: Speciation in high-temperature DLR flow reactor, OME3 measurements at three fuel stoichiometries [Gaiser2022F].



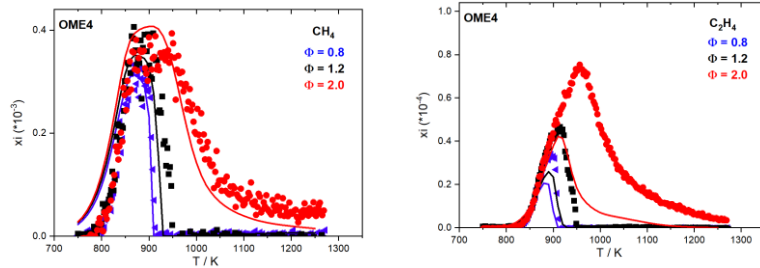


Fig. S39: Speciation in high-temperature DLR flow reactor, OME4 measurements at three fuel stoichiometries [Gaiser2022F].

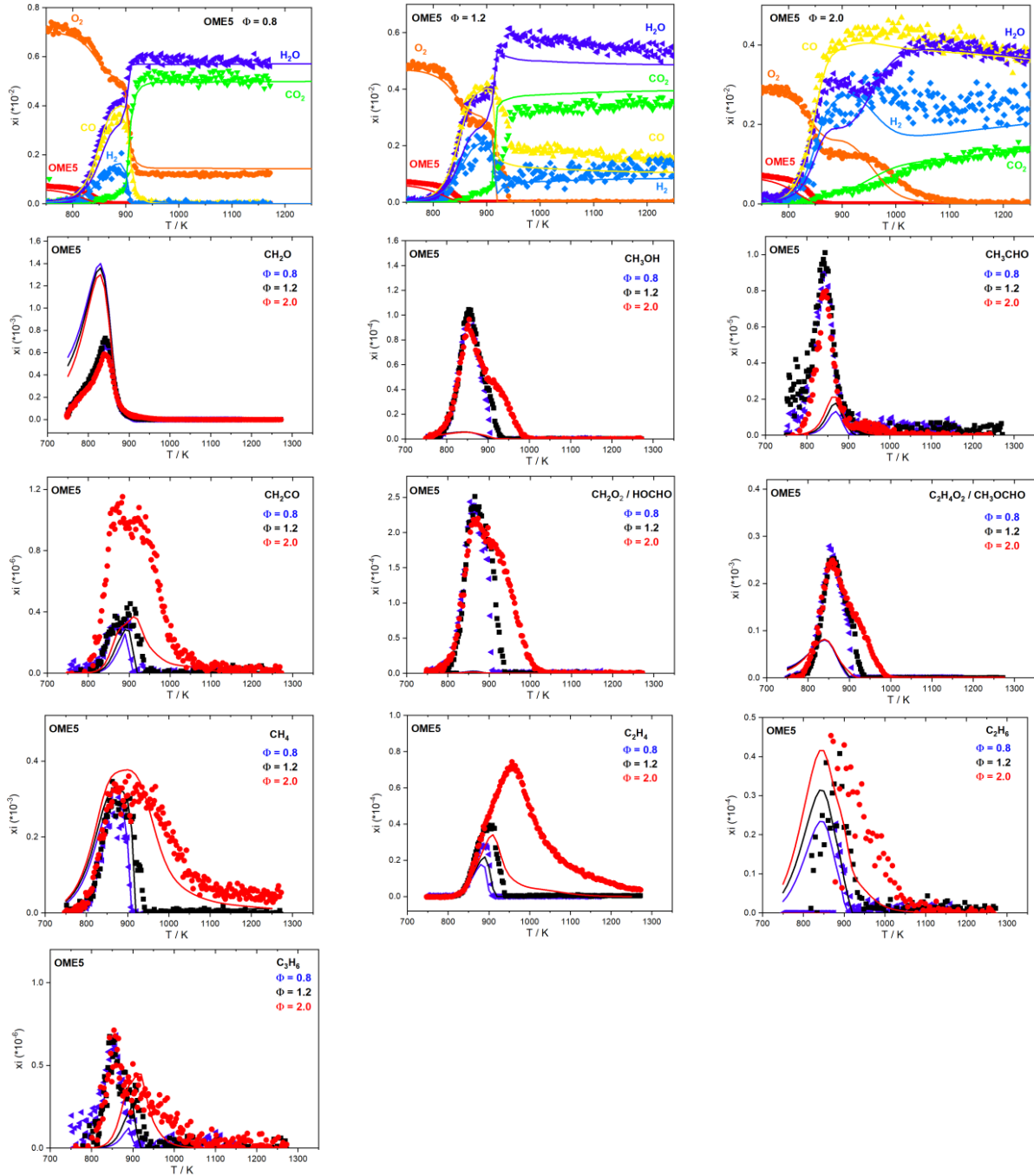


Fig. S40: Speciation in high-temperature DLR flow reactor, OME5 measurements at three fuel stoichiometries [Gaiser2022F].

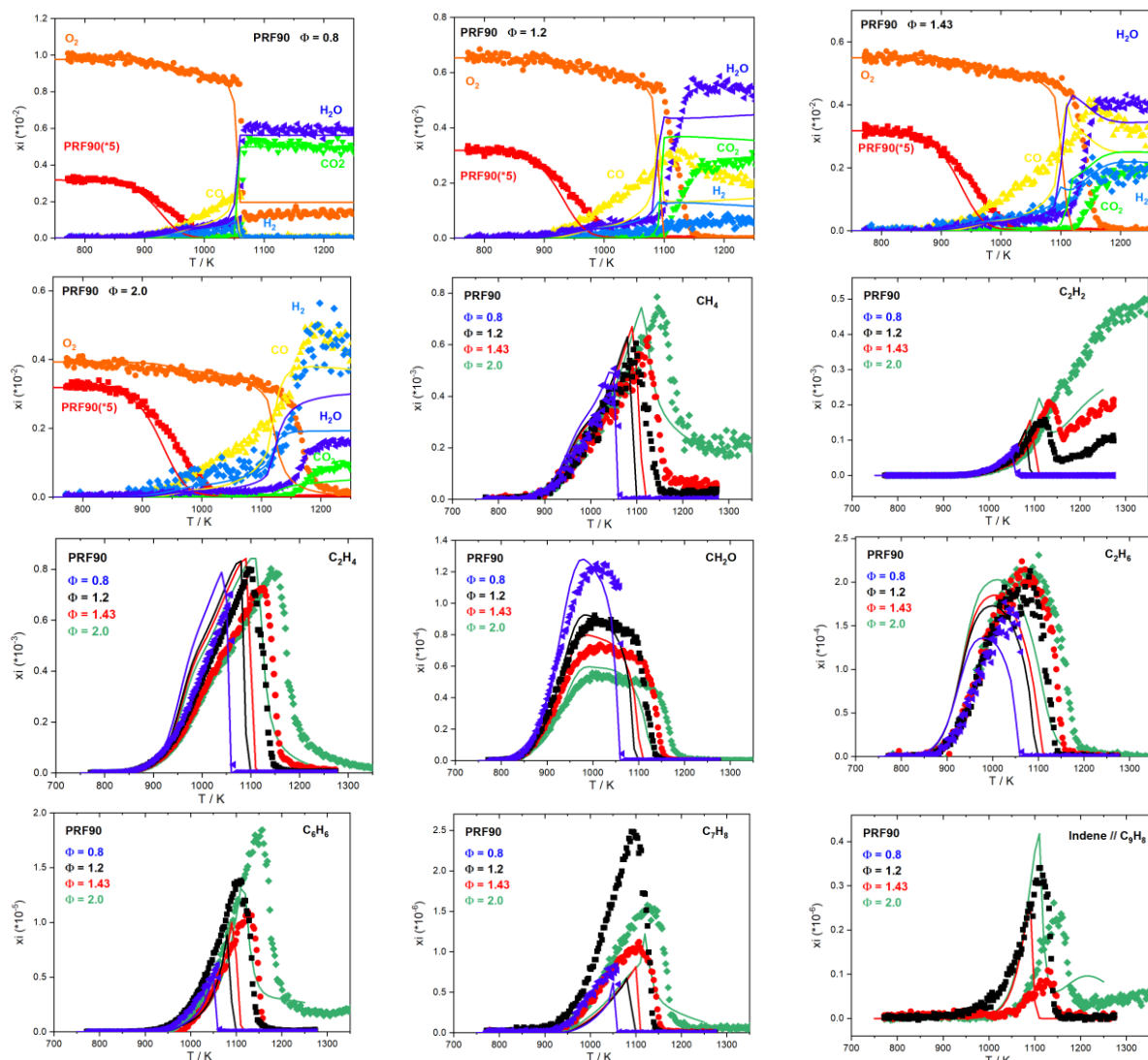


Fig. S41: Speciation in high-temperature DLR flow reactor, PRF90 measurements at three fuel stoichiometries [present work].

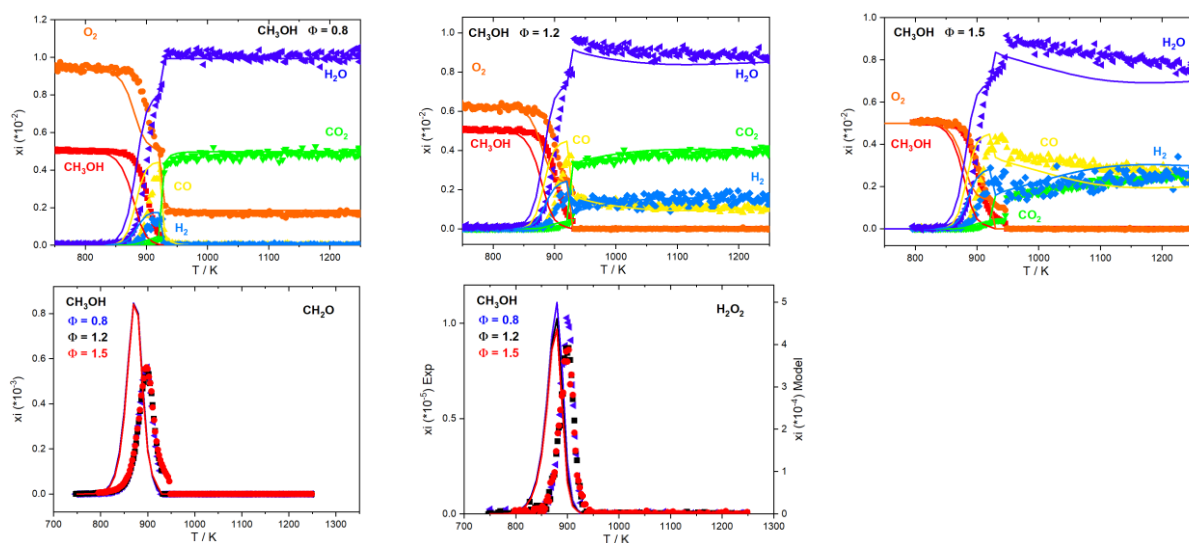


Fig. S42: Speciation in high-temperature DLR flow reactor, Methanol measurements at three fuel stoichiometries [present work].

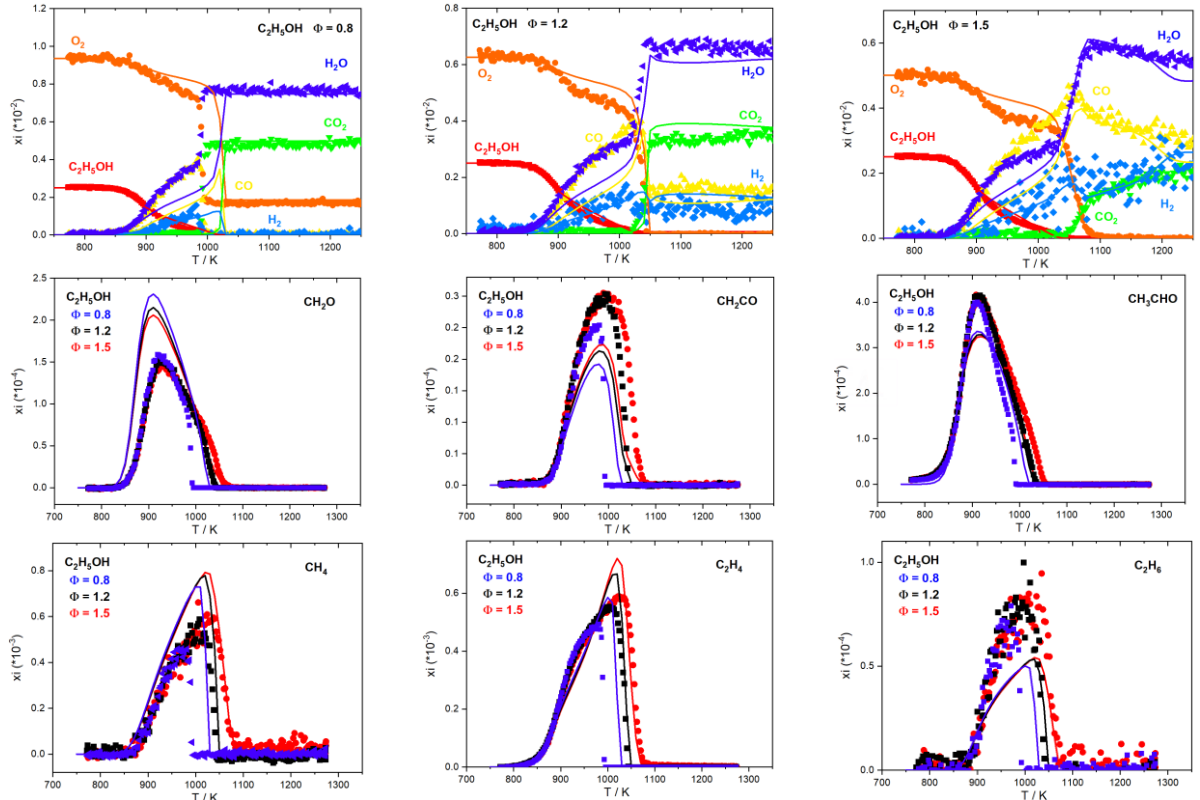


Fig. S43: Speciation in high-temperature DLR flow reactor, Ethanol measurements at three fuel stoichiometries [present work].

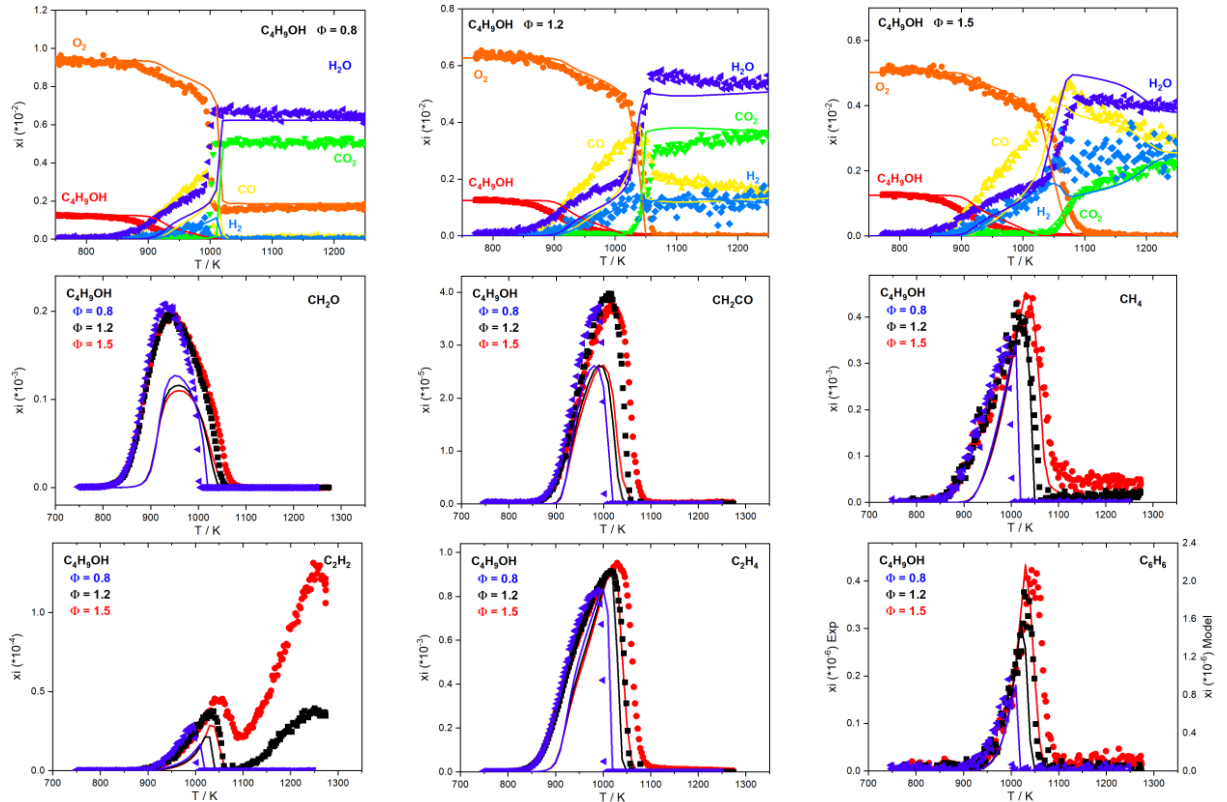


Fig. S44: Speciation in high-temperature DLR flow reactor, n-Butanol measurements at three fuel stoichiometries [present work].

(1.6) Jet-stirred reactor (JSR)

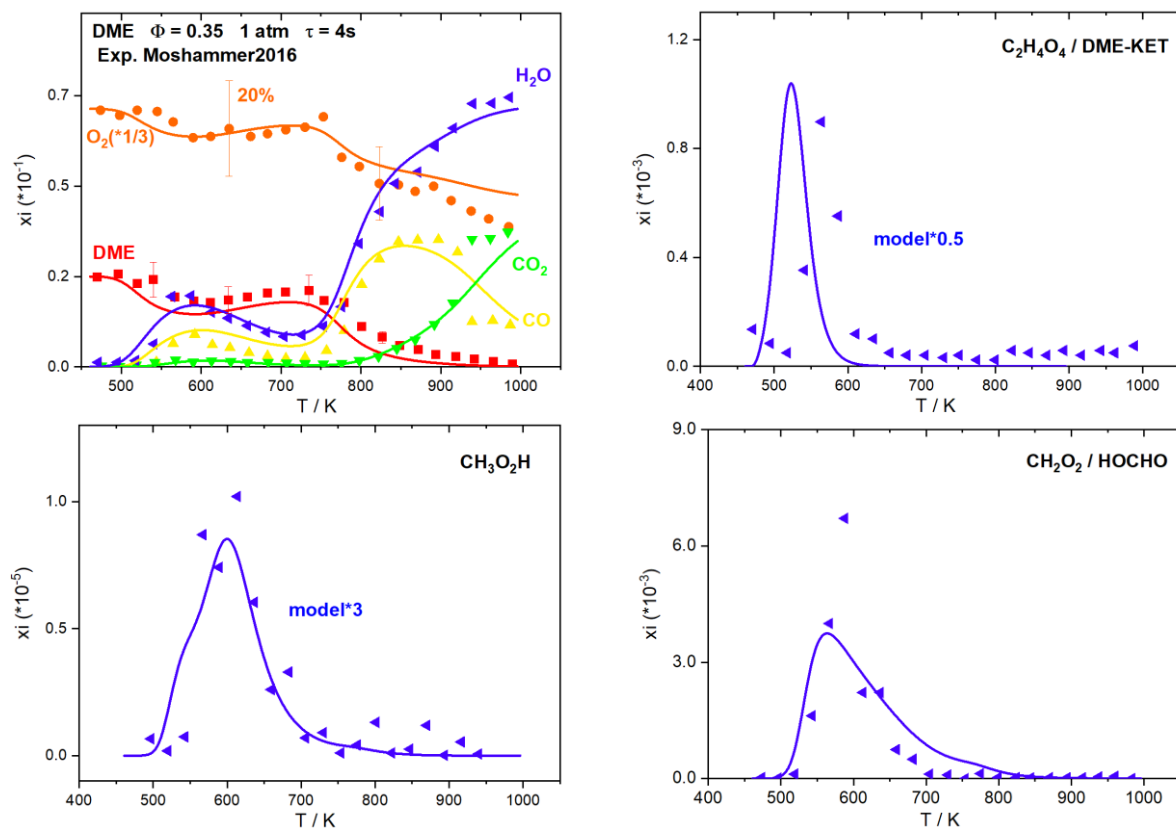
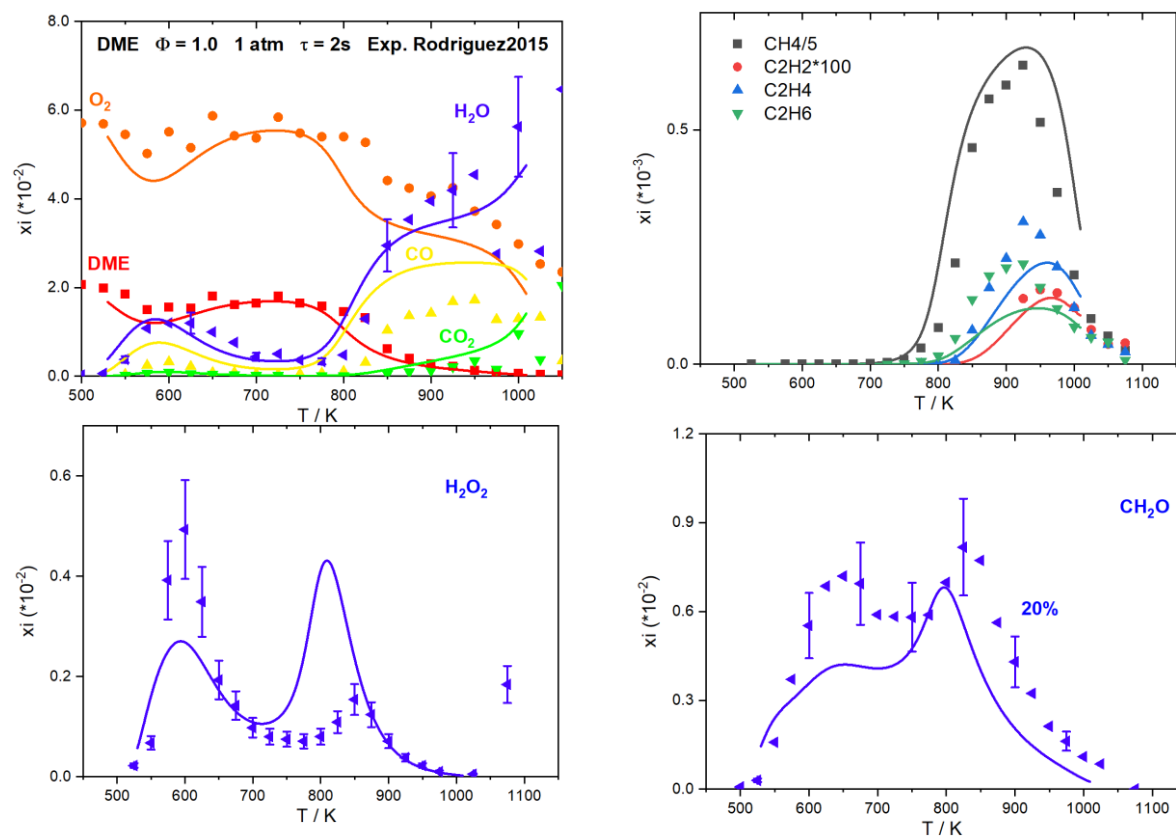


Fig. S45: Speciation in JSR, DME measurements [Moshammer2016].



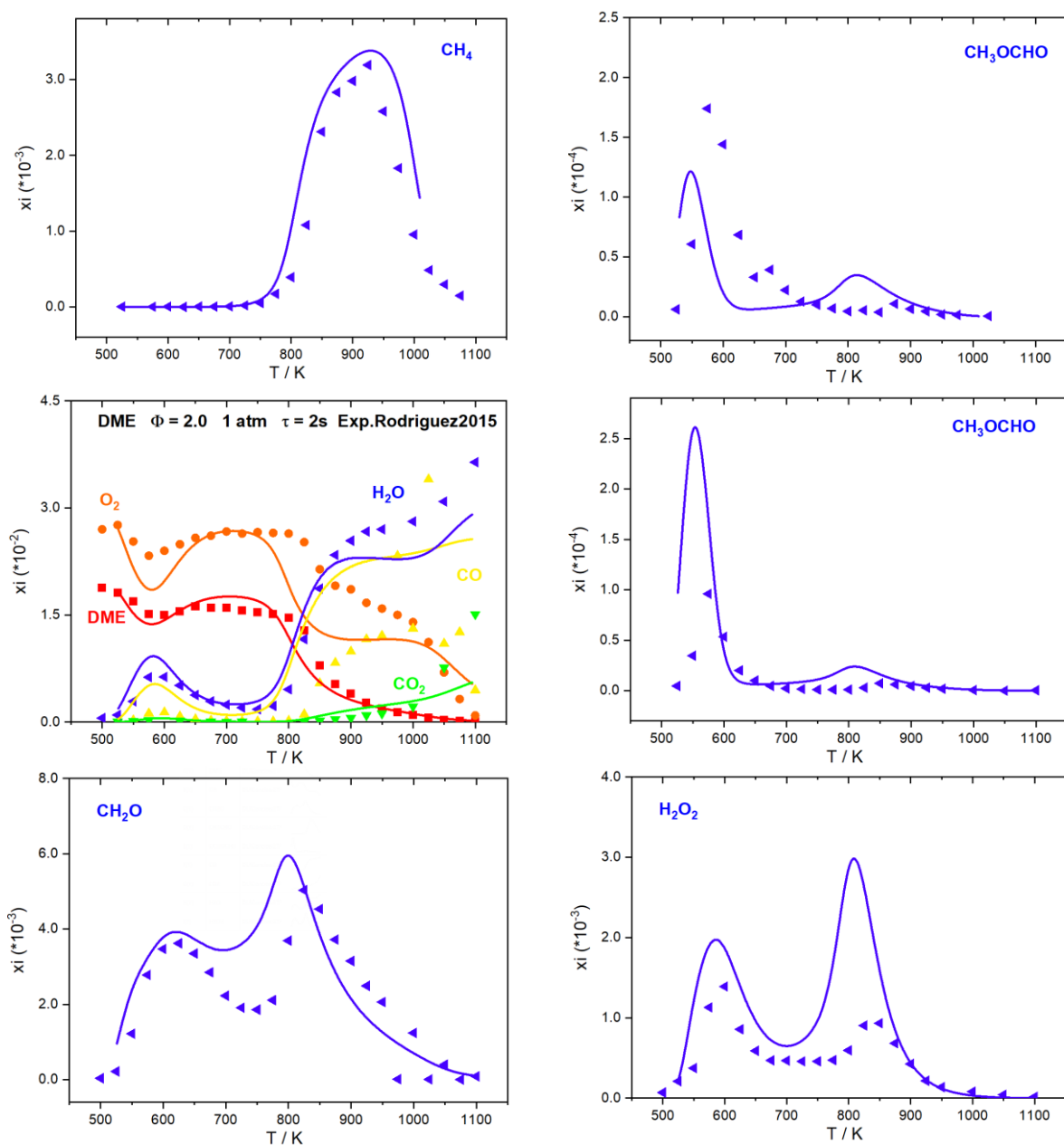
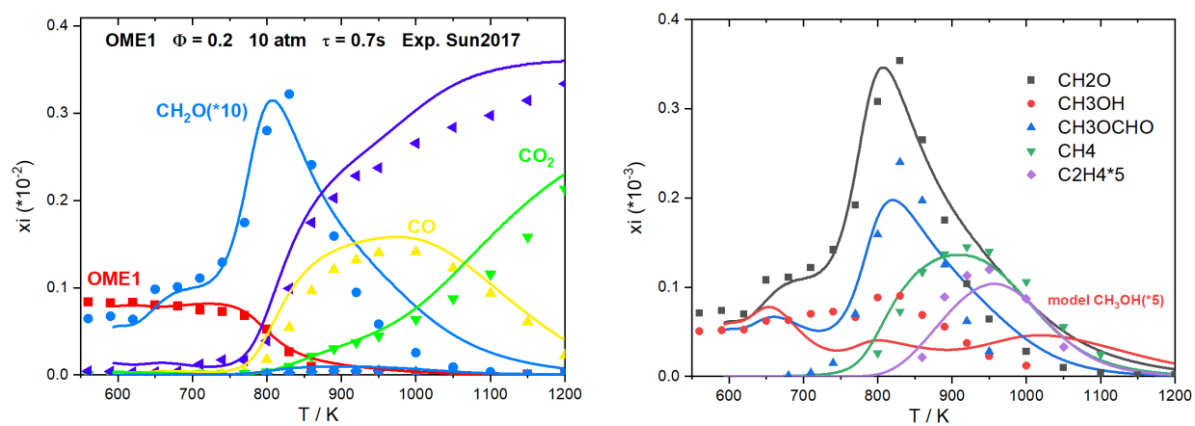


Fig. S46: Speciation in JSR, DME measurements for $\Phi = 1.0$ and 2.0 [Rodriguez2015].



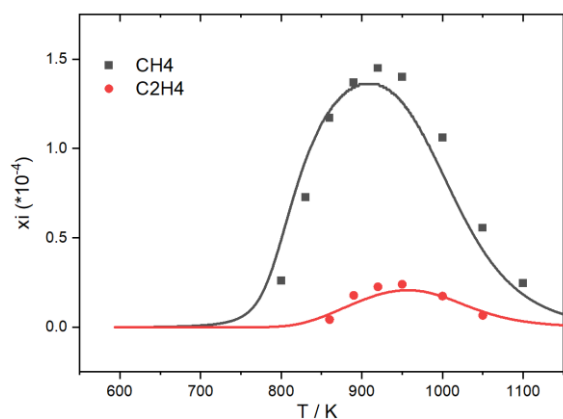


Fig. S47: Speciation in JSR, OME1 measurements [Sun2017-OME1].

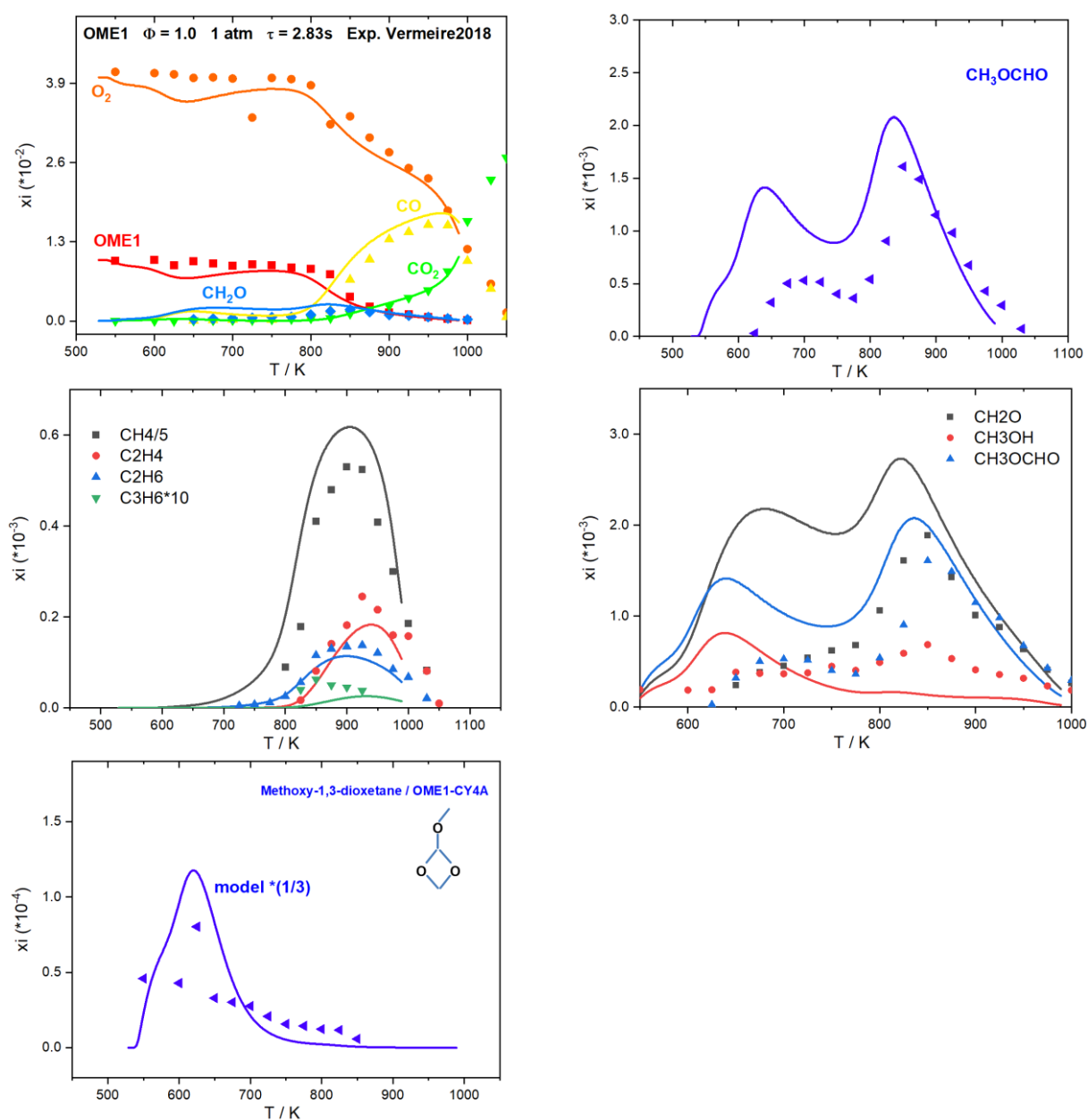


Fig. S48: Speciation in JSR, OME1 oxidation measurements [Vermeire2018].

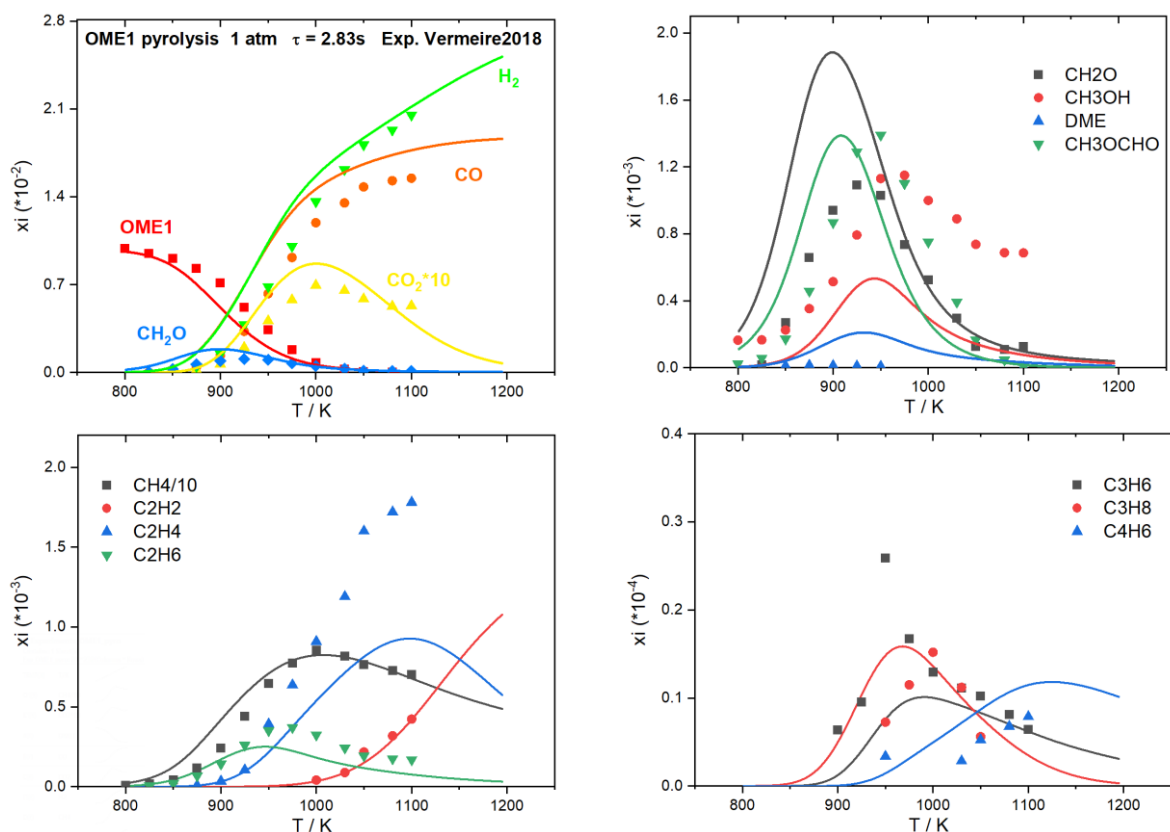
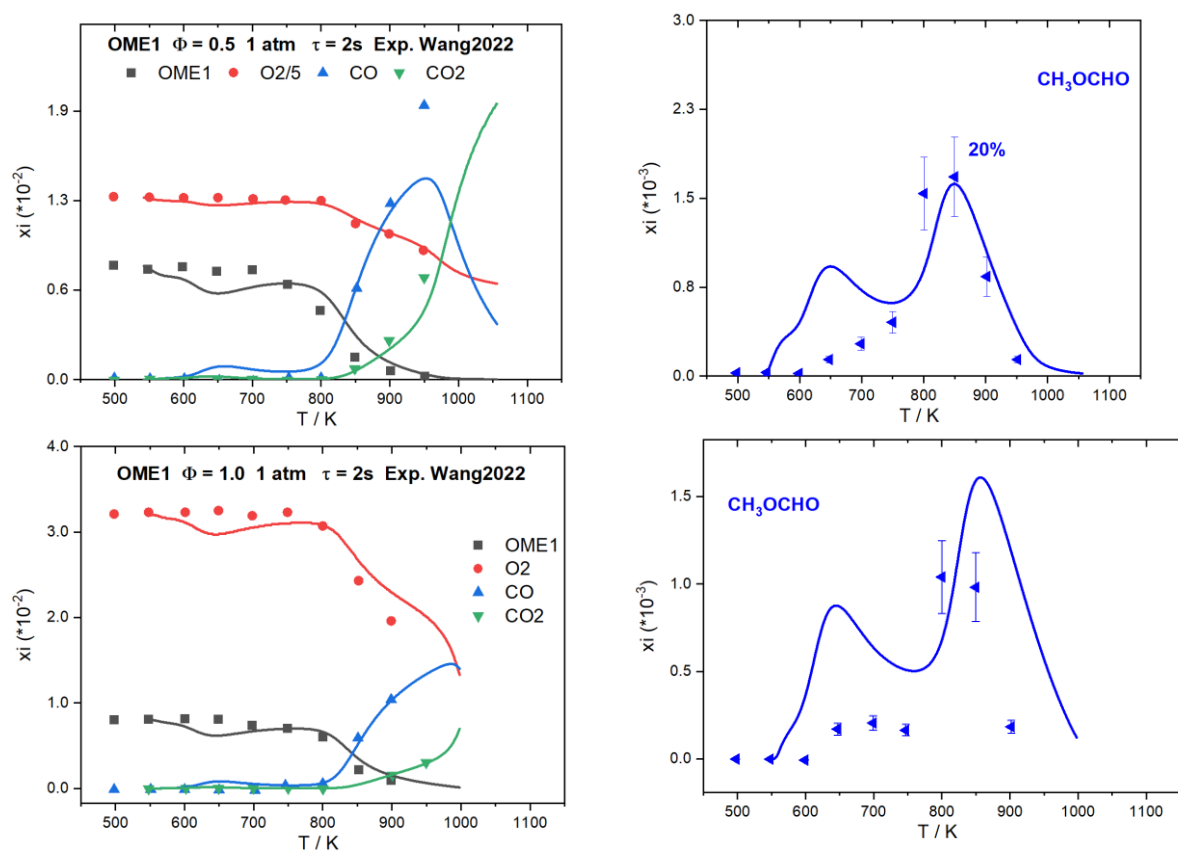


Fig. S49: Speciation in JSR, OME1 pyrolysis measurements [Vermeire2018].



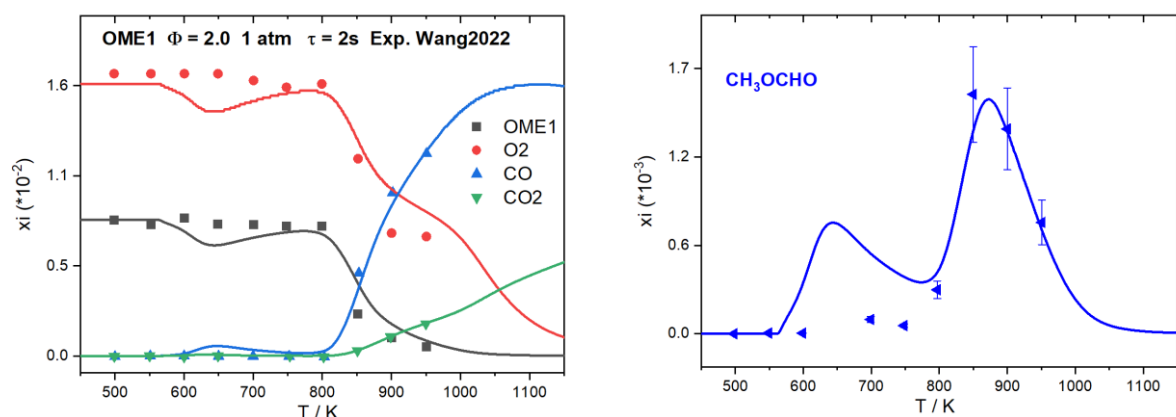


Fig. S50: Speciation in JSR, OME1 measurements at three fuel stoichiometries [Wang2022].

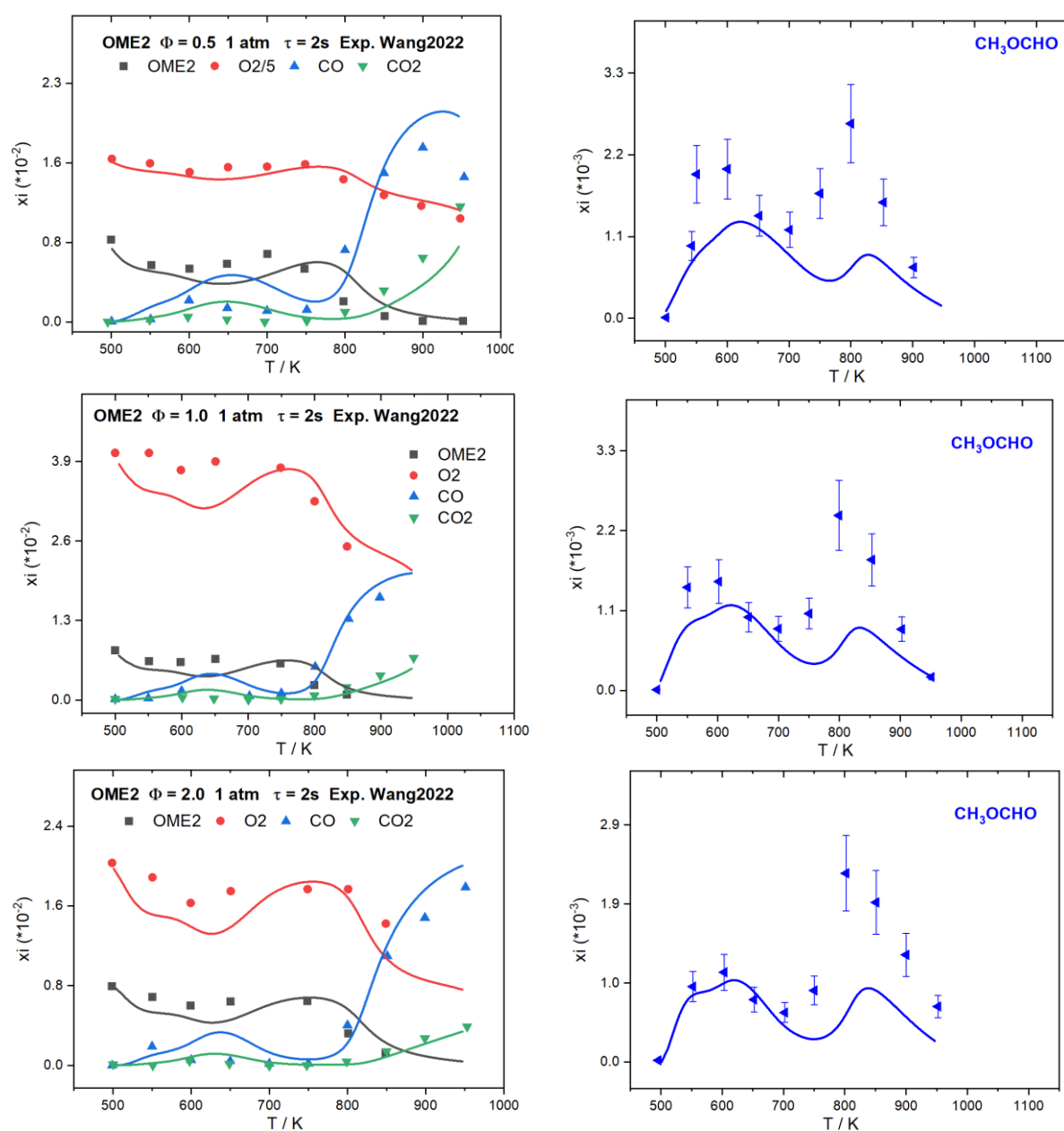


Fig. S51: Speciation in JSR, OME2 measurements at three fuel stoichiometries [Wang2022].

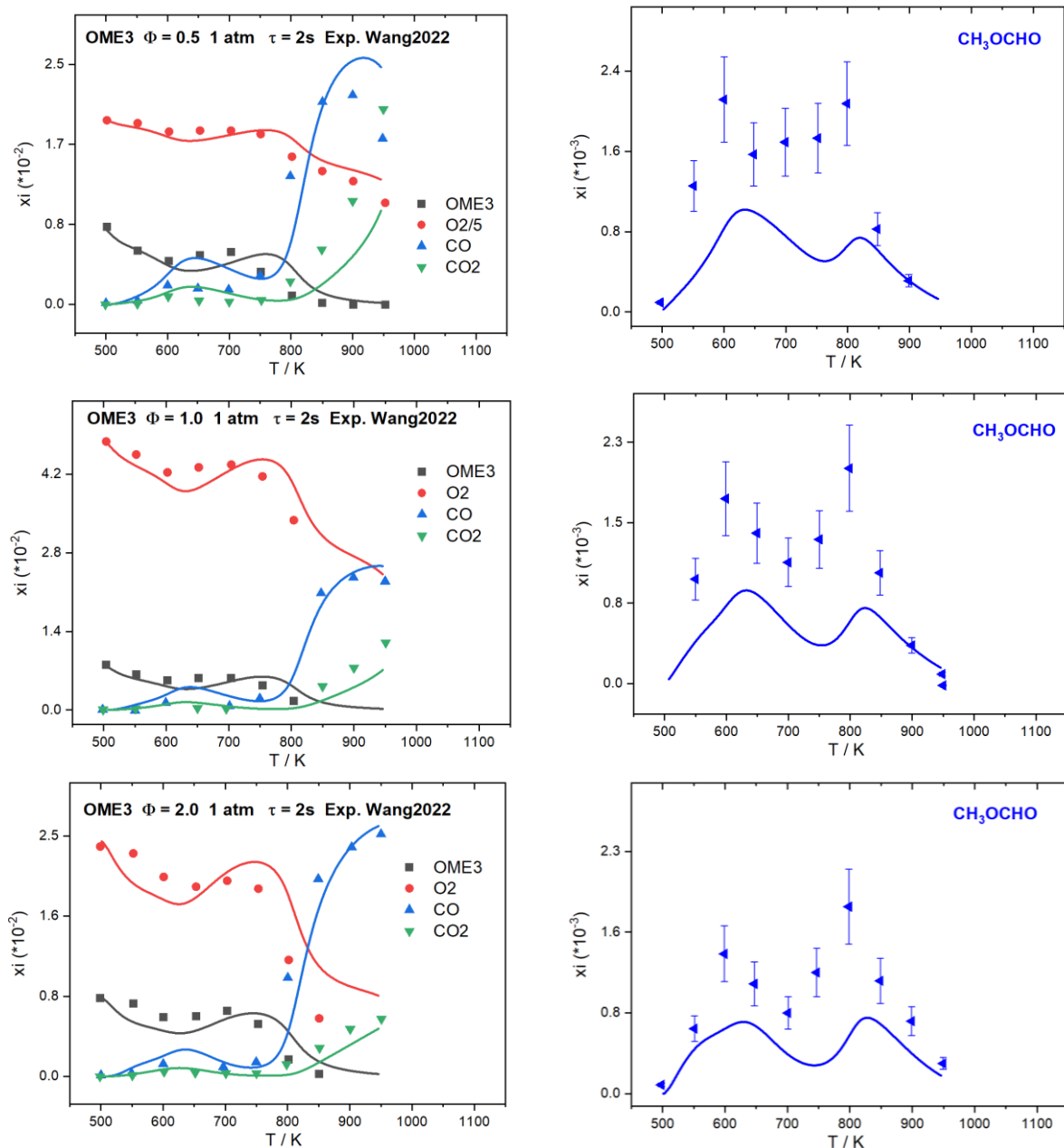


Fig. S52: Speciation in JSR, OME3 measurements at three fuel stoichiometries [Wang2022].

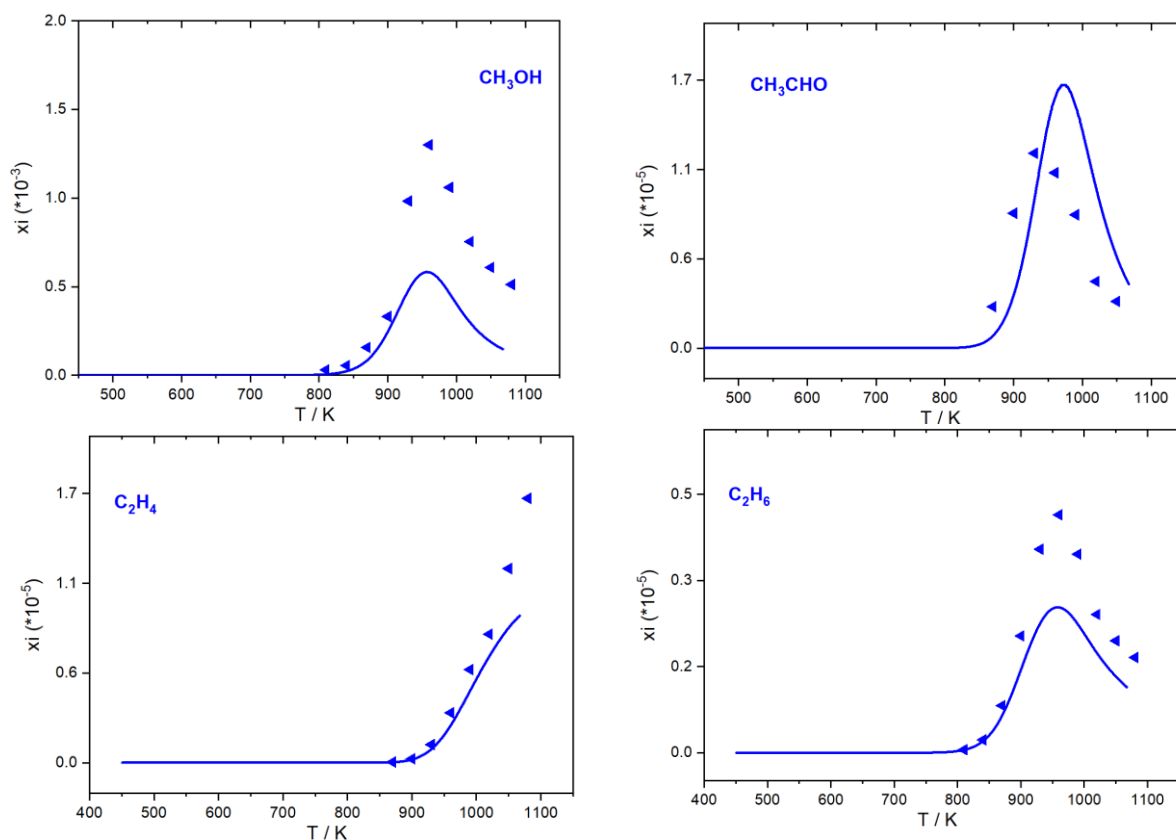
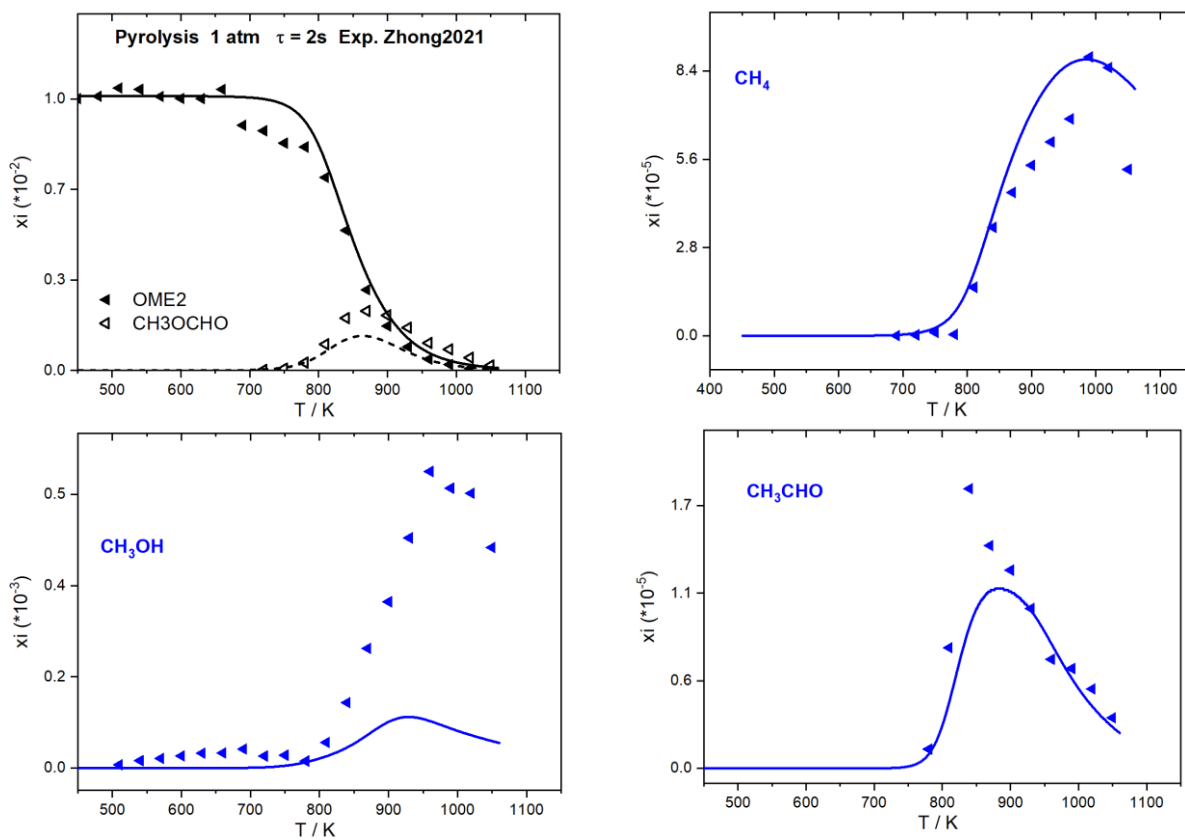


Fig. S53: Speciation in JSR, OME1 pyrolysis measurements [Zhong2021].



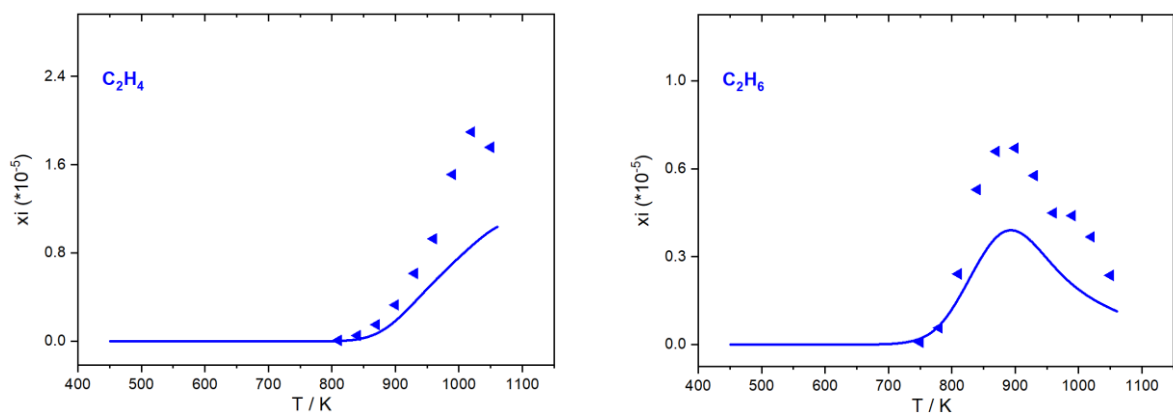


Fig. S54: Speciation in JSR, OME2 pyrolysis measurements [Zhong2021].

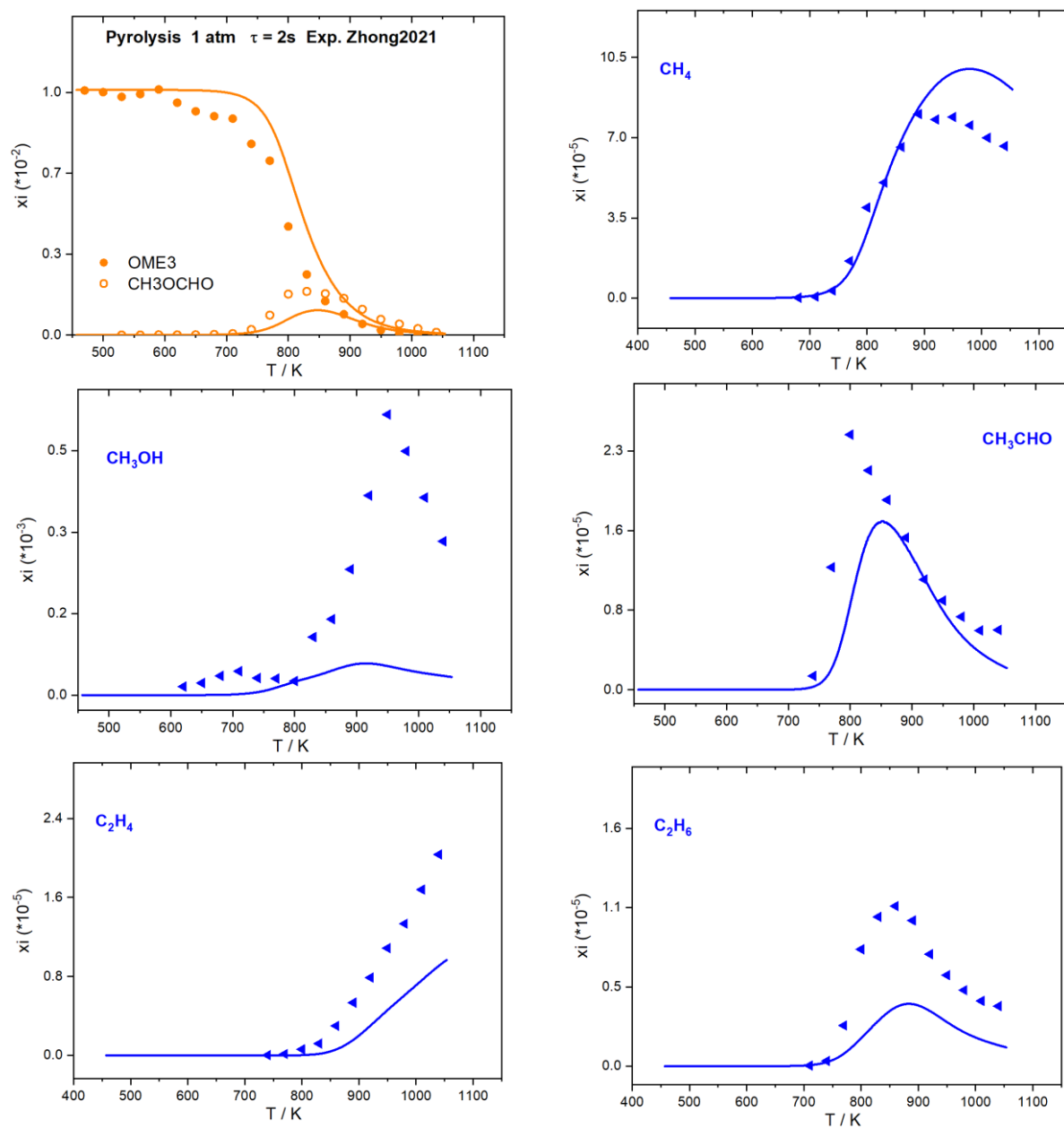


Fig. S55: Speciation in JSR, OME3 pyrolysis measurements [Zhong2021].

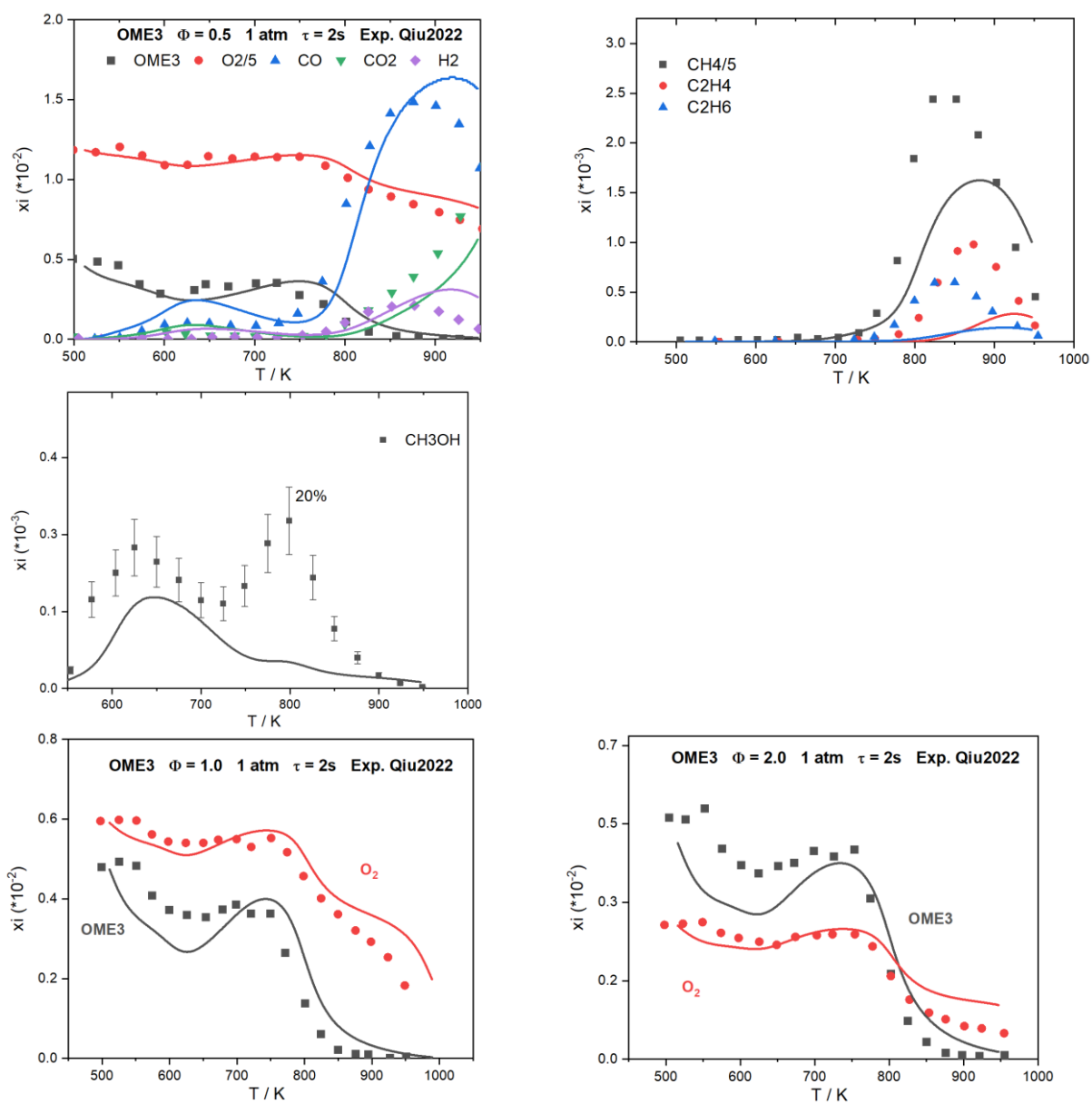
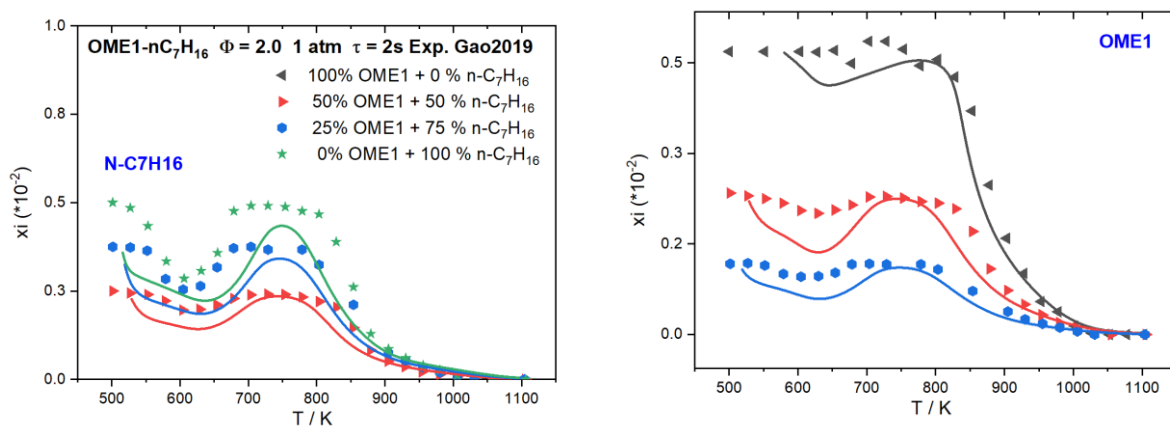
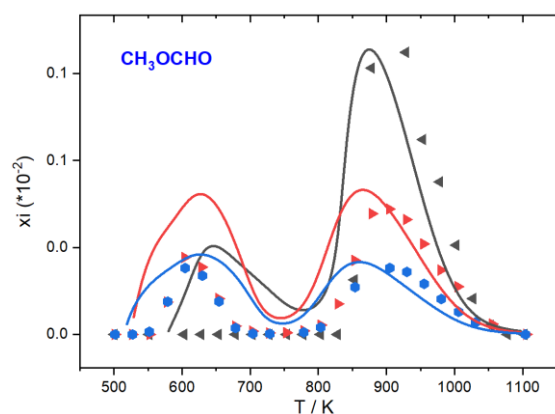
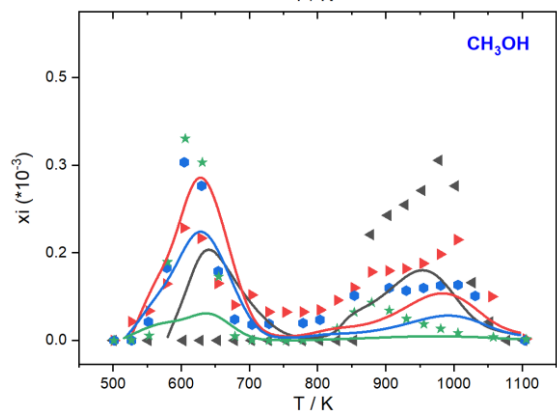
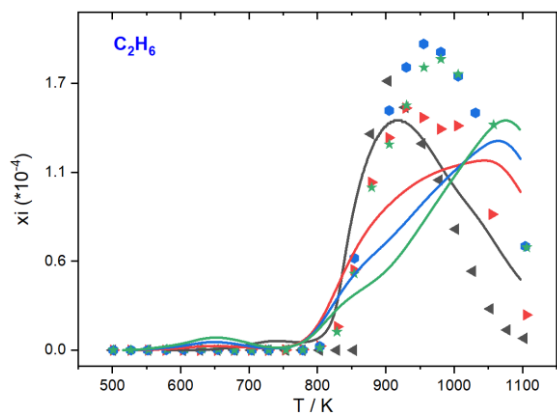
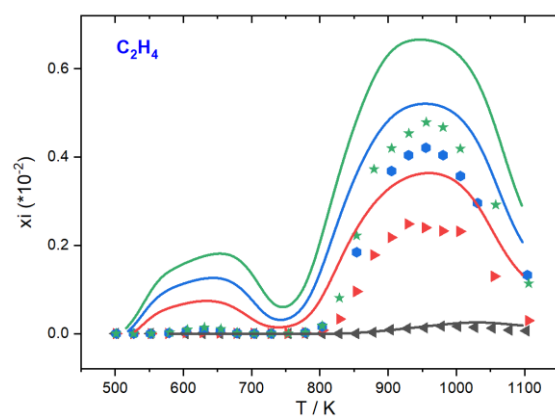
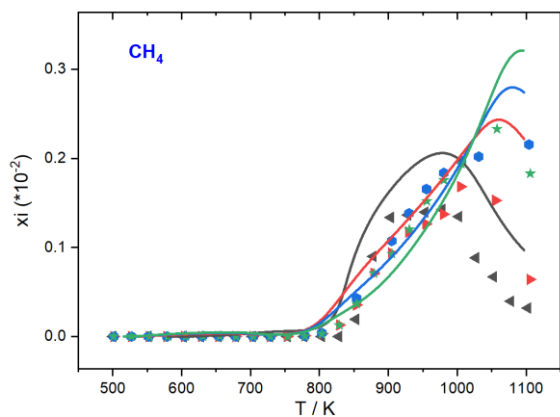
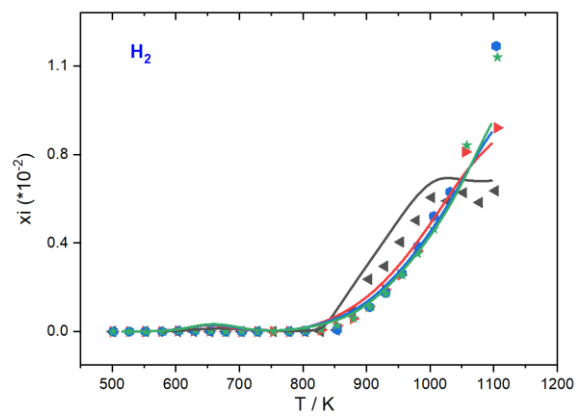
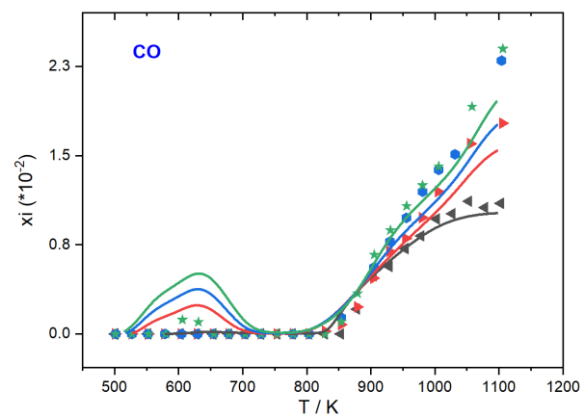


Fig. S56: Speciation in JSR, OME3 oxidation measurements [Qiu2022].





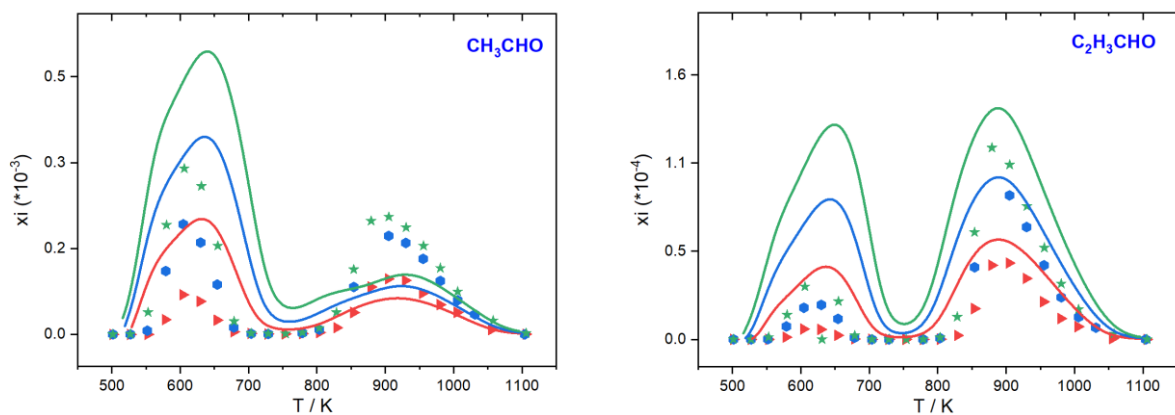


Fig. S57: Speciation in JSR, OME1-n-heptane mixtures [Gao2019].

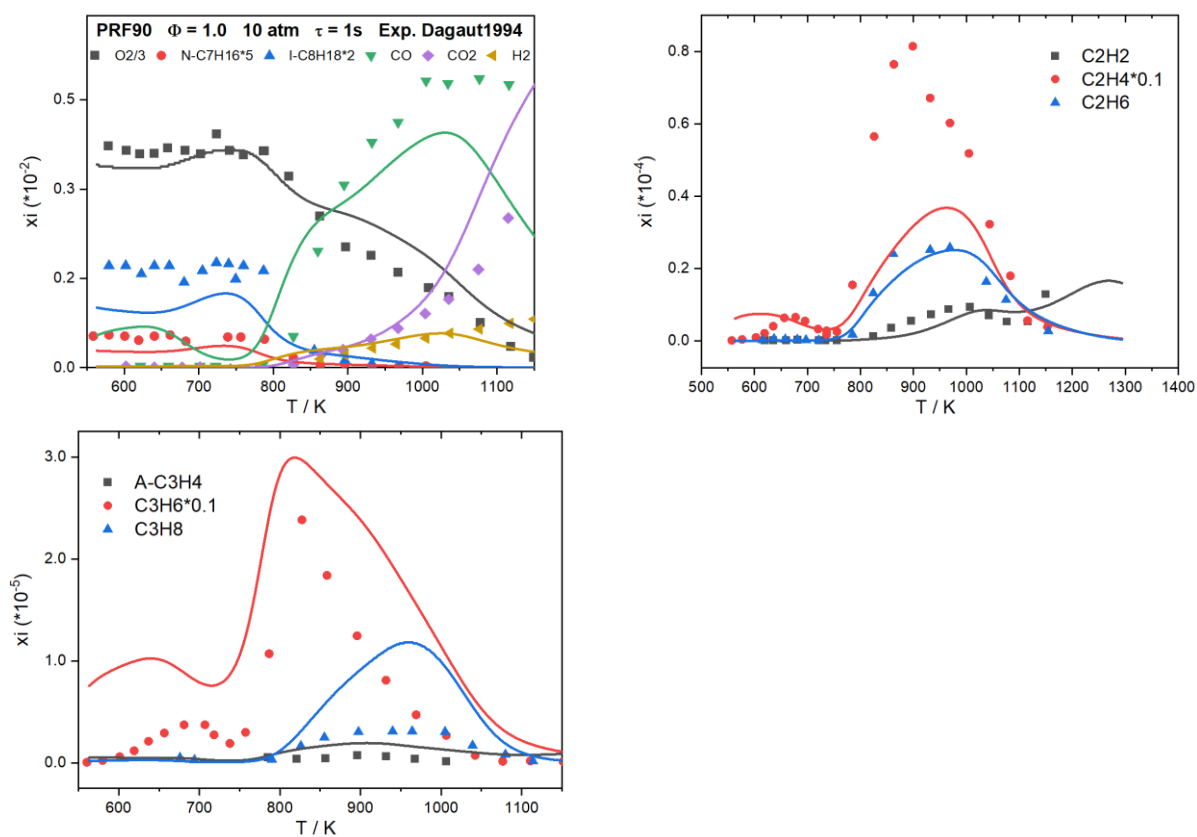


Fig. S58: Speciation in JSR, PRF90 oxidation measurements [Dagaut1994].

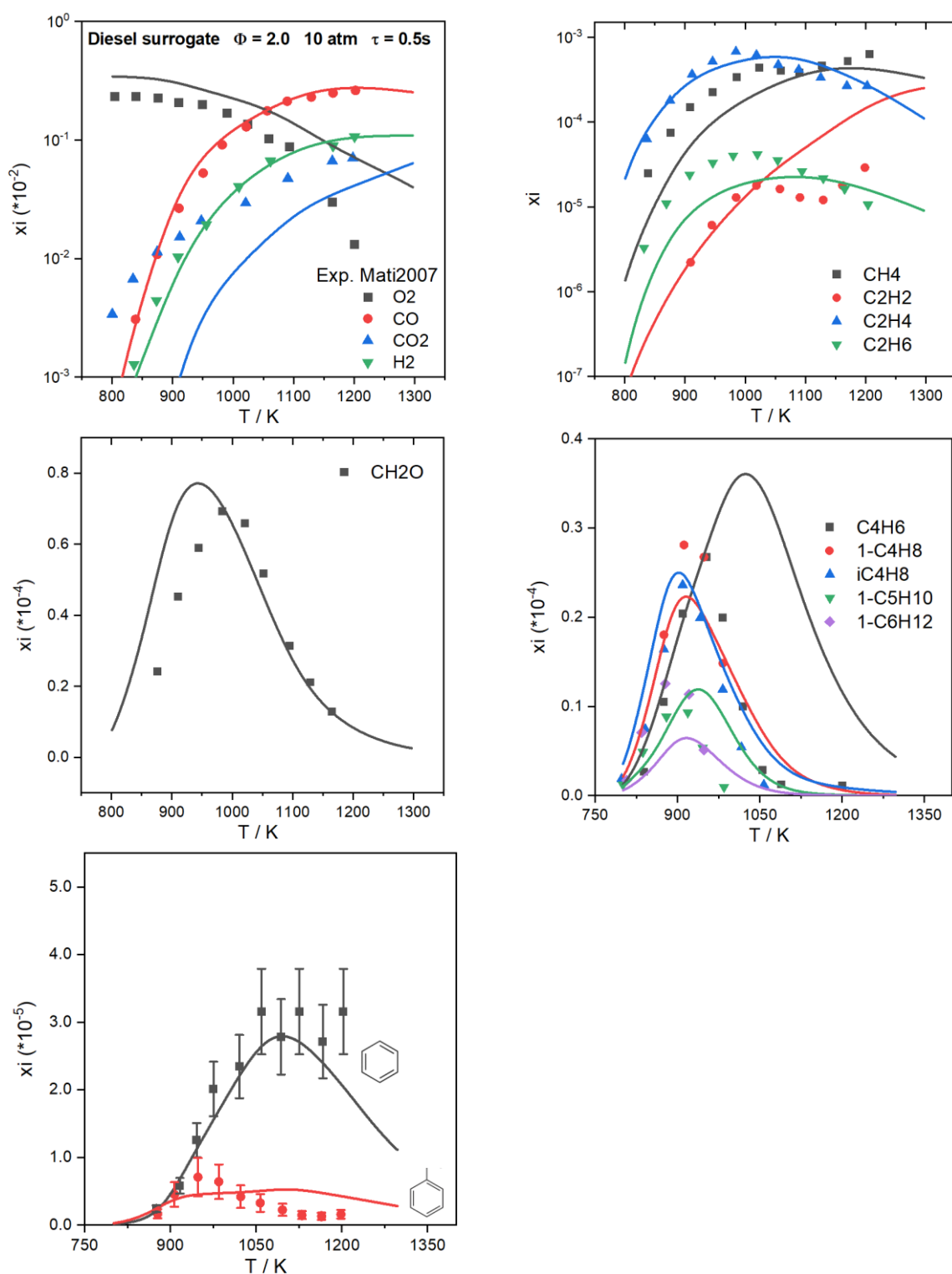


Fig. S59: Speciation in JSR, Diesel fuel surrogate measurements [Mati2007].

(S2) Comparison of DLR Concise with literature models

In this section we compare major reaction models with the experiments. The aim of this comparison is two-fold: (1) it presents collective picture of models in comparison with the measurements and (2) it shows the predictability of DLR Concise in comparison with other models. The first point also helps to showcase that experiments can also be prone to uncertainties and error and in some cases, at no fault of model, not all experiments are well reproduced.

Due to availability of many reaction models and large amount of data, individual model predictions may not always be distinguishable in the plots.

A list of reaction mechanisms available in the literature is presented in the Table below. There are few mechanisms available for DME or for OME0-3 whereas only 3 mechanisms including present work are available for OME ≥ 4 . Furthermore, most of the mechanisms include up to C4 as base chemistry whereas only two reduced mechanisms provide PRF components. Inclusion of PAH or NO_x are even less present in these models. The list shows also models which are not tested for flame chemistry interpreted from the lack of transport properties data. Among them, DLR Concise provides variety of hydrocarbons for modeling OME mixtures with alternative fuel components including NO_x and PAH soot precursors' chemistry.

Table S6: List of reaction mechanisms of OMEs available in literature.

OME	Mech/Group	Base mech	Ref	Low T OME _x	Transport properties	Mech type
DME	LLNL	C2	Kaiser2000	✓		
DME		C2	Cool2007	✗		
DME	NUI Galway	C3	Burke2015	✓		
DME		C2	Wang2015	✓		
DME	W. Green, MIT	C3	Dames2016	✓		
DME	Aramco 3.0	C4 + PAH	Zhou2018	✓		
DME	Glarborg	C2	Hashemi2019	✓		
DME	POLIMI	C4+PAH	Stagni2022	✓		S
OME0-1	Ghent	C3	Vermeire2018	✓	✗	D
OME0-1	Aachen	C4	Jacobs2019	✓		D
OME0-2	Ghent/CNRS	C5	Ras2022	✓	✗	
OME0-3		C4	Sun2017-OME3	✗		
OME0-3		C3	He2018	✓	✗	
OME0-3		C4+PRF+PAH	Ren2019	✓		R
OME0-3		C2+NO _x	Shrestha2022	✓		
OME0-3		C4+PAH	Zhong2021	✓	✗	
OME3		C3+PRF	Lin2019	✓		R
OME0-4	Aachen	C4+PAH	Cai2020	✓		
OME1-6		C3	Niu2022	✓	✗	R
OME0-5	DLR Concise	C16+PAH+NO _x	Present work	✓		S
*PRF includes iC ₈ H ₁₈ , NC ₇ H ₁₆ , Detail (D) / semi-detail (S) / reduced (R)						

Each mechanism present strengths and weaknesses of their own and the purpose of this work is to show the comparison of predictions of DLR Concise with other mechanisms.

(2.1) Ignition delay times

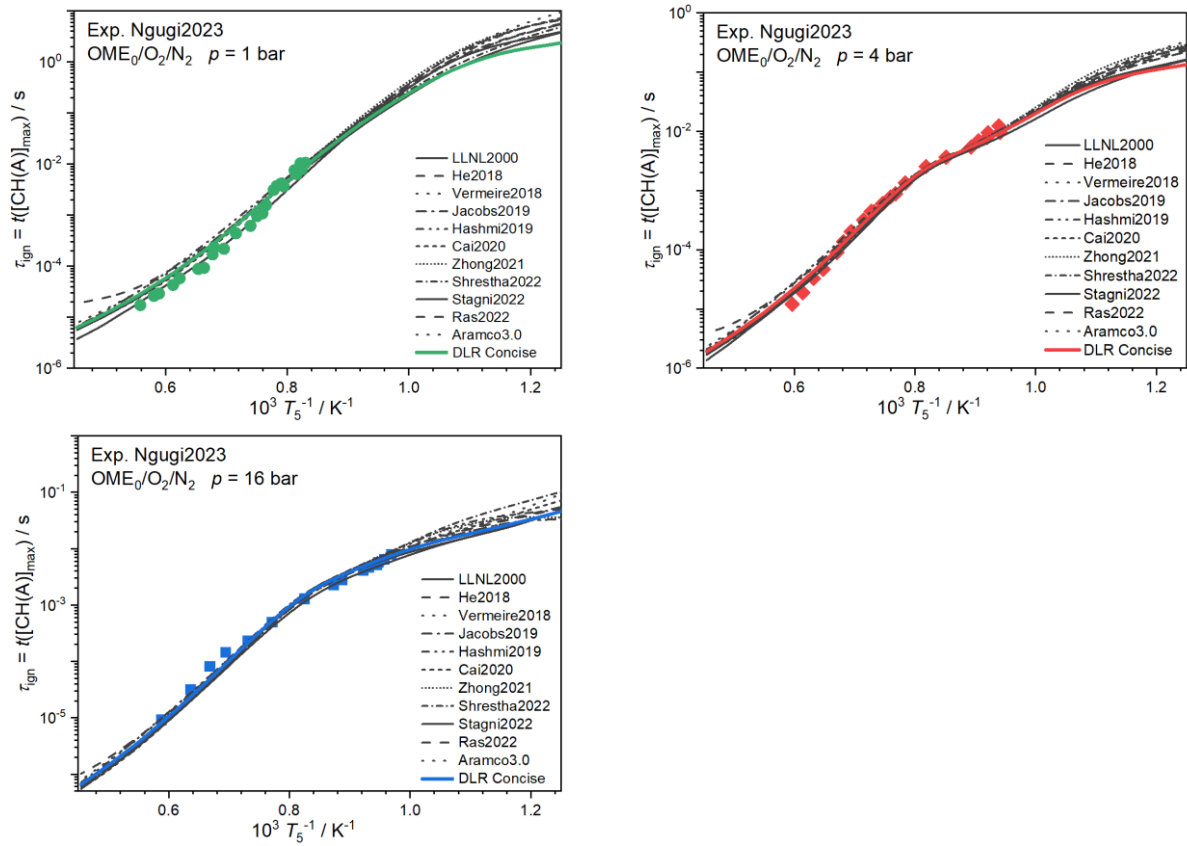


Fig. S60: Predictions of ignition delay times of DME compared with literature models [Ngugi2023].

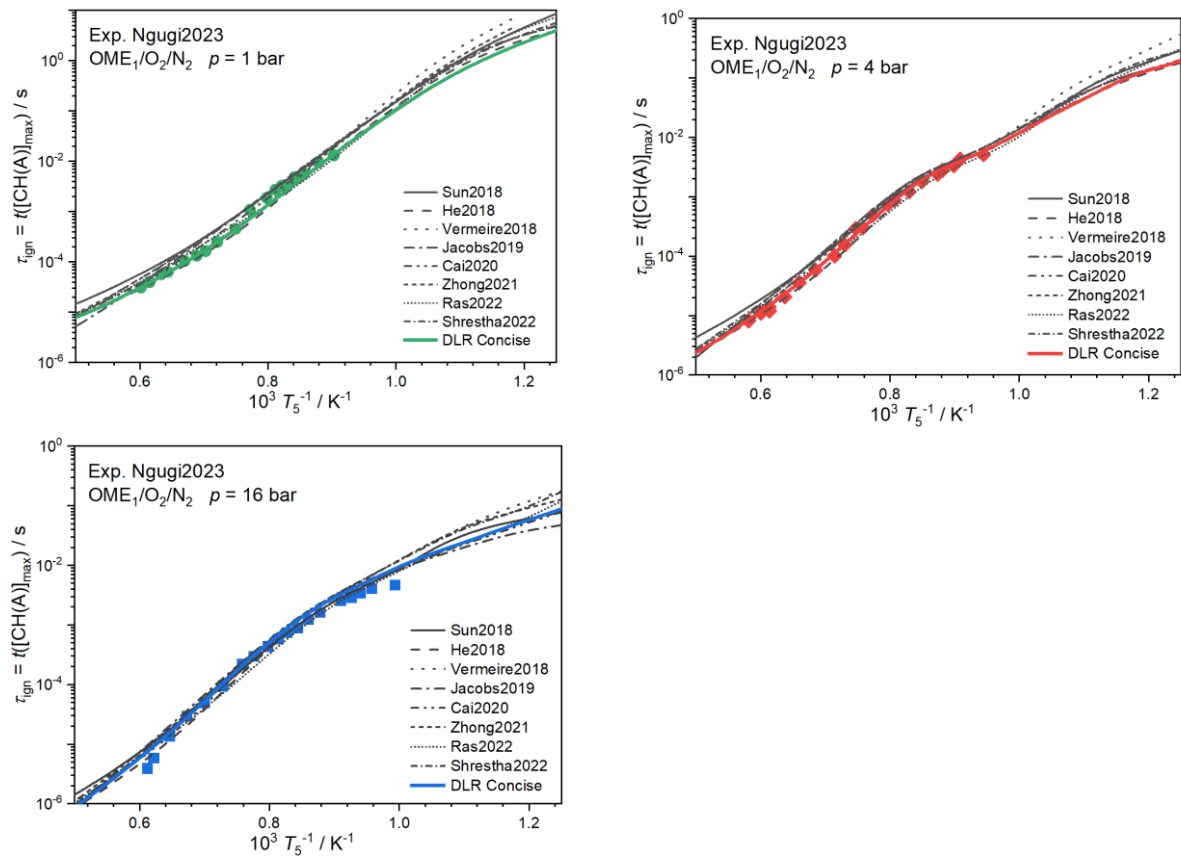


Fig. S61: Predictions of ignition delay times of OME1 compared with literature models [Ngugi2023].

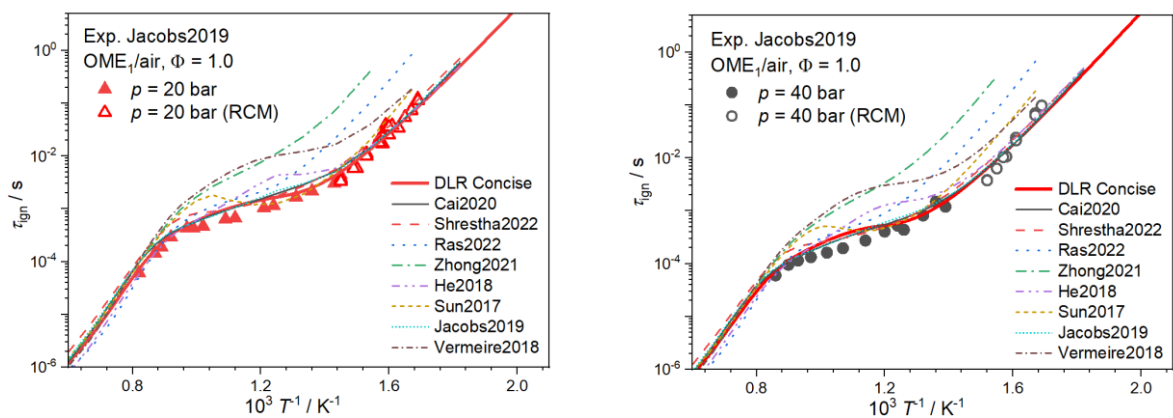


Fig. S62: Predictions of ignition delay times of OME1 compared with literature models [Jacobs2019].

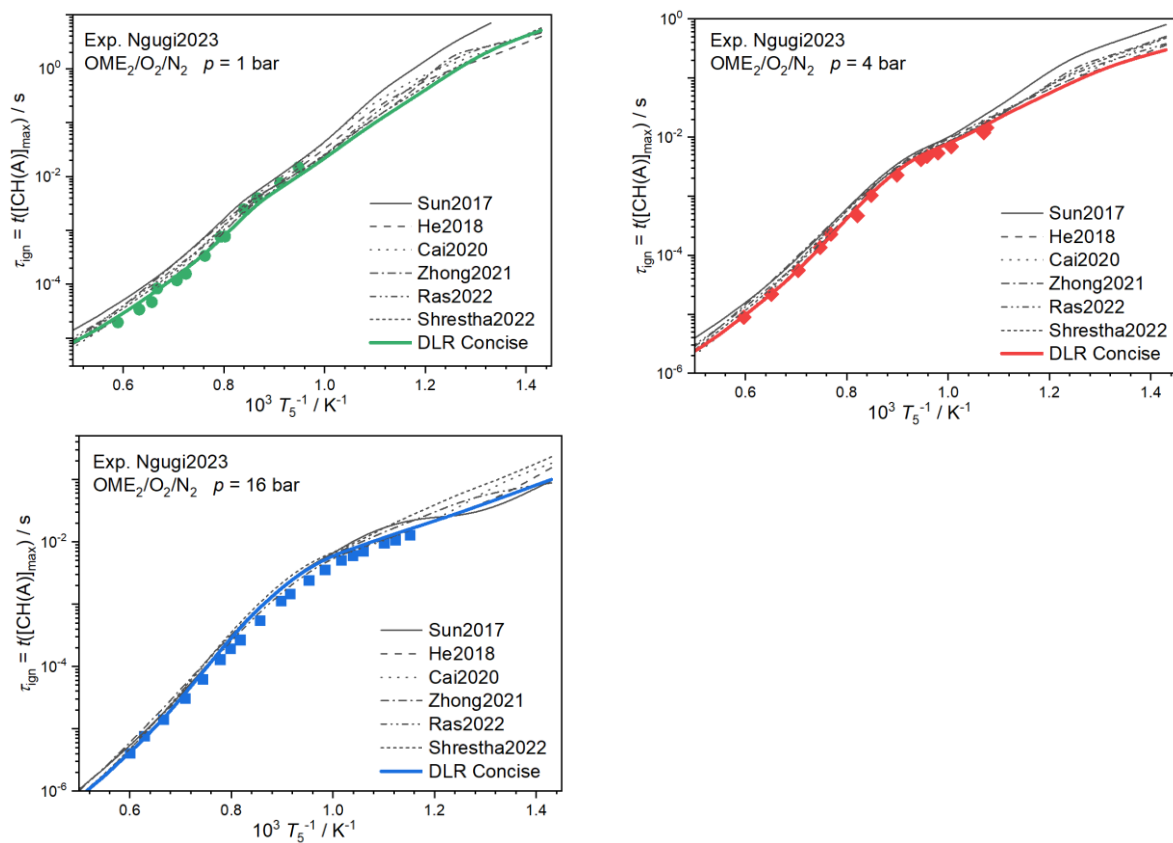


Fig. S63: Predictions of ignition delay times of OME2 compared with literature models [Ngugi2023].

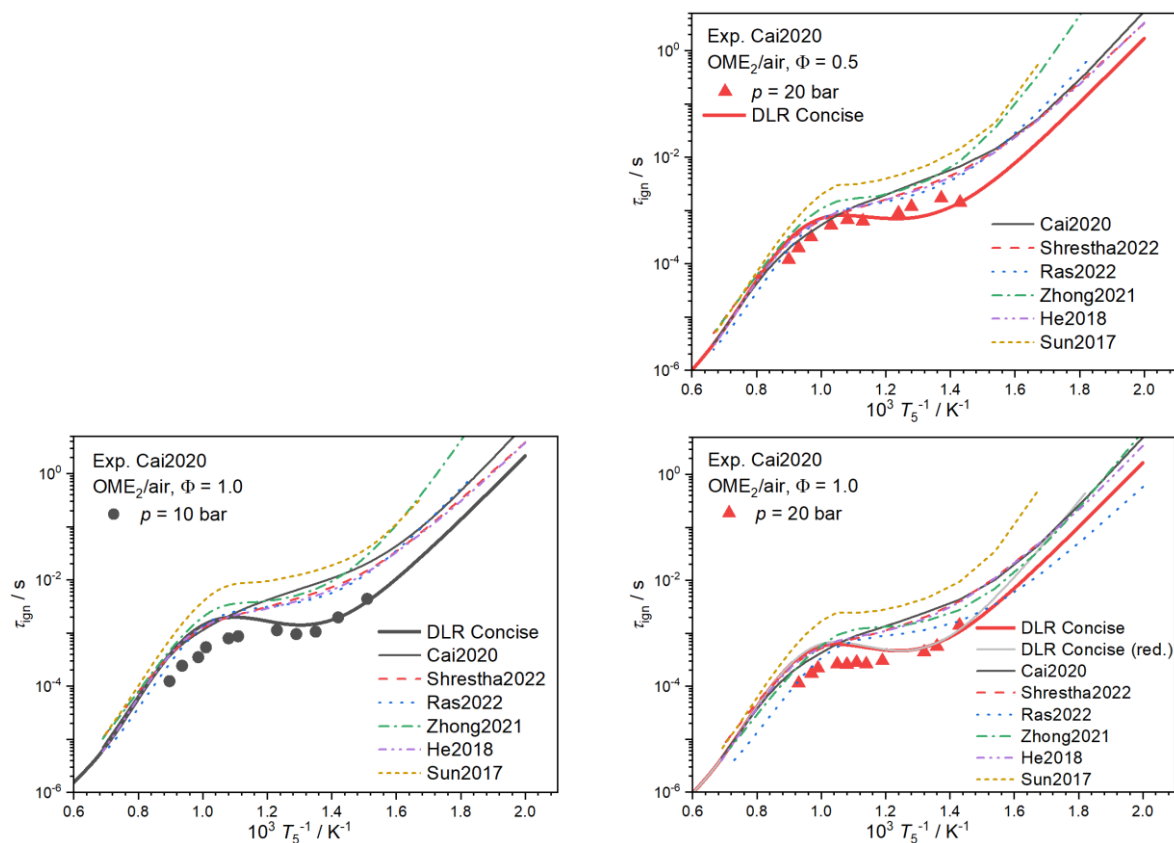


Fig. S64: Predictions of ignition delay times of OME2 compared with literature models [Cai2020]. Symbol: experiments, lines: models. DLR Concise (red.) is reduced model based on insignificance of peroxy chemistry at secondary radical positions (See 4.1 in main manuscript).

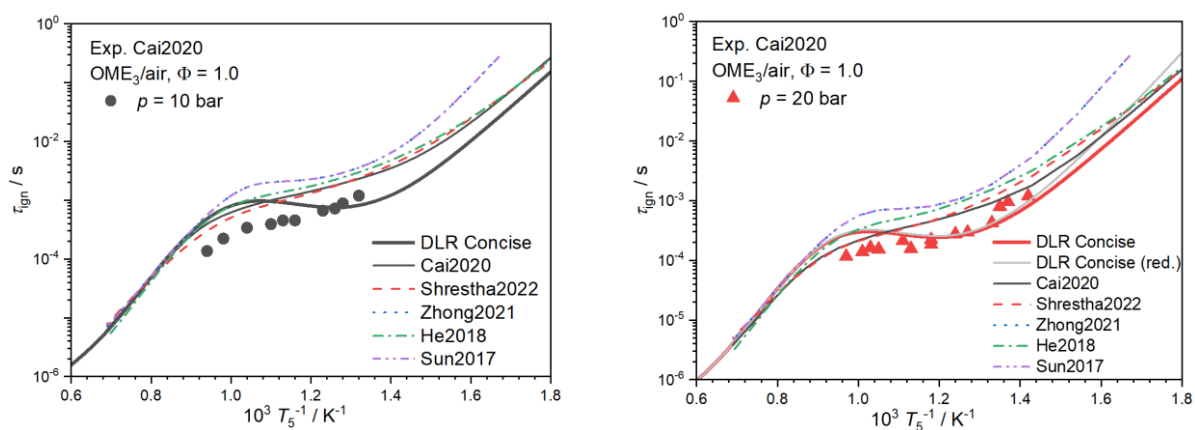


Fig. S65: Predictions of ignition delay times of OME3 compared with literature models [Cai2020]. DLR Concise (red.) is reduced model based on insignificance of peroxy chemistry at secondary radical positions (See 4.1 in main manuscript).

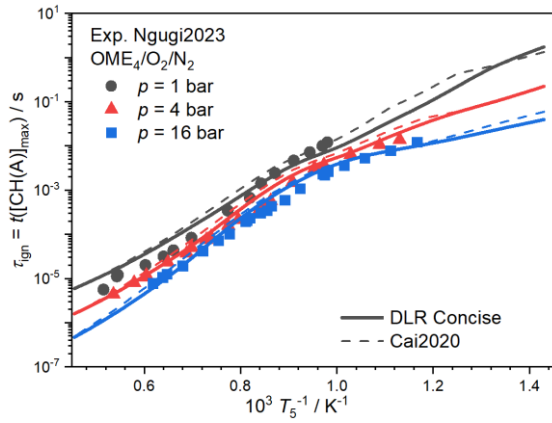


Fig. S66: Predictions of ignition delay times of OME4 compared with available literature model.

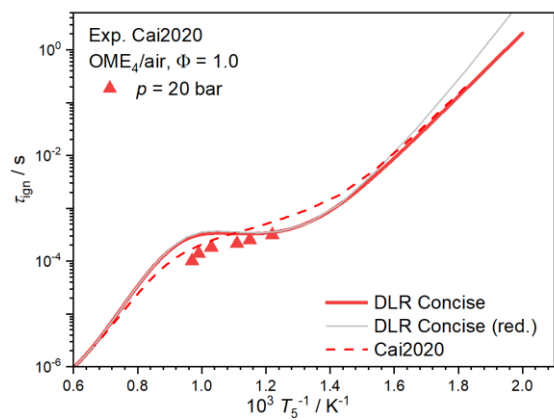
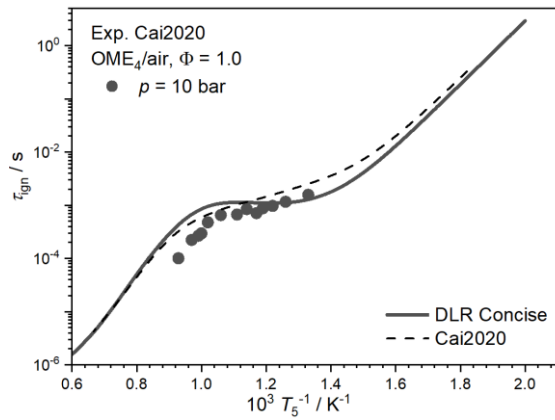
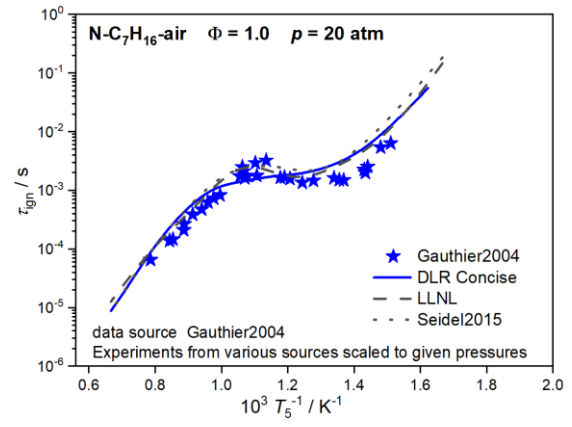
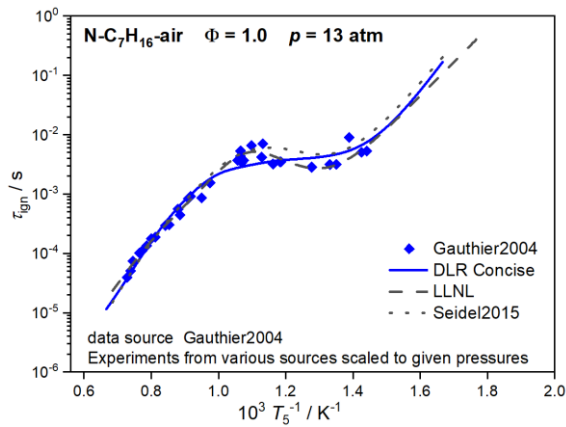


Fig. S67: Predictions of ignition delay times of OME4 compared with literature models [Cai2020]. DLR Concise (red.) is reduced model based on insignificance of peroxy chemistry at secondary radical positions (See 4.1 in main manuscript).



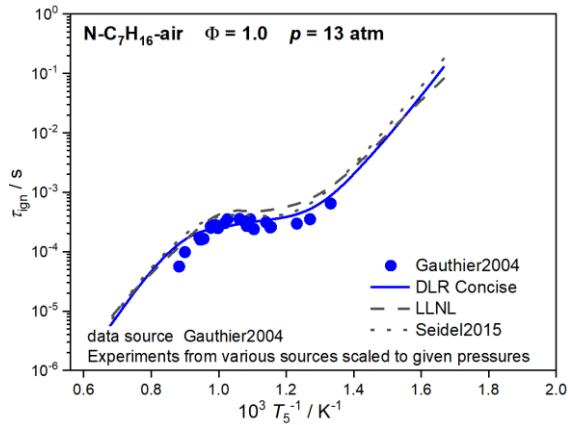


Fig. S68: Predictions of ignition delay times of n-heptane compared with literature models [Gauthier2004, Seidel2015, LLNL].

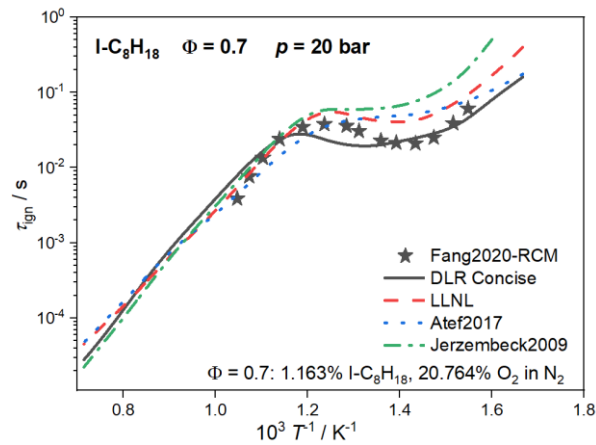


Fig. S69: Predictions of ignition delay times of I-C₈H₁₈ [Fang2020] compared with literature models [LLNL, Atef2017, Jerzembeck2009].

(2.2) Laminar flame speeds

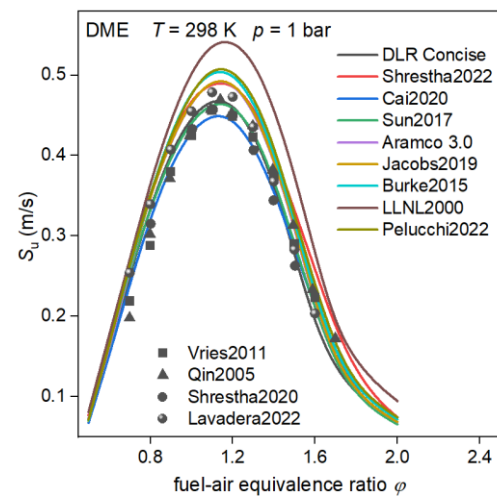


Fig. S70: Predictions of laminar flame speeds of DME [Vries2011, Qin2005, Shrestha2020, Lavadera2022] compared with literature models.

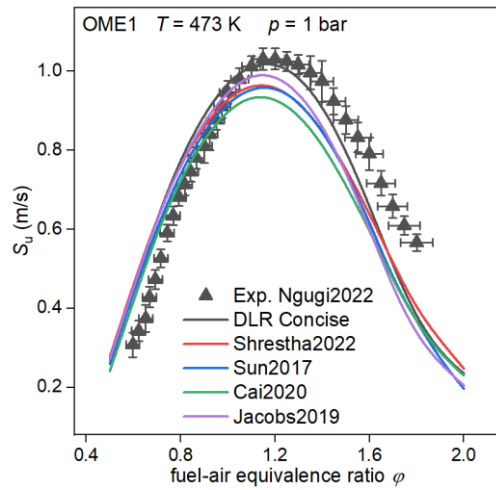


Fig. S71: Prediction of laminar flame speeds of OME1 [Ngugi2022] compared with literature models.

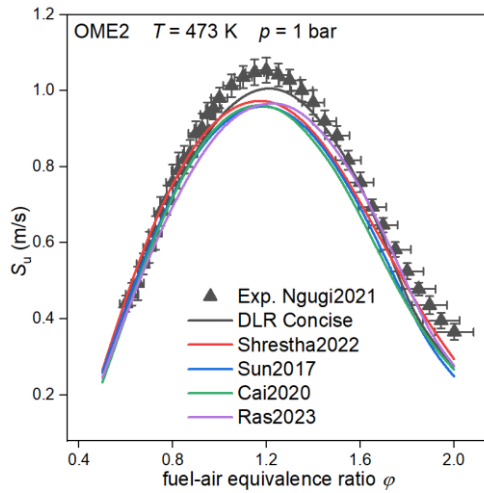


Fig. S72: Prediction of laminar flame speeds of OME2 [Ngugi2021] compared with literature models.

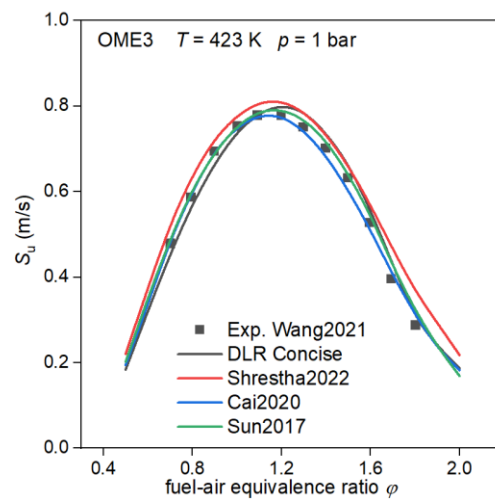
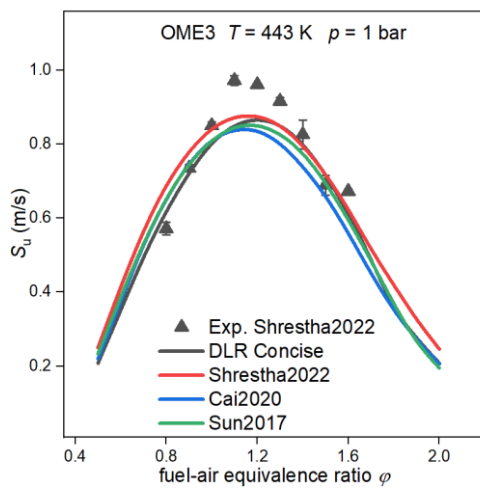


Fig. S73: Predictions of laminar flame speeds of OME3 [Shrestha2022, Wang2021] compared with literature models.

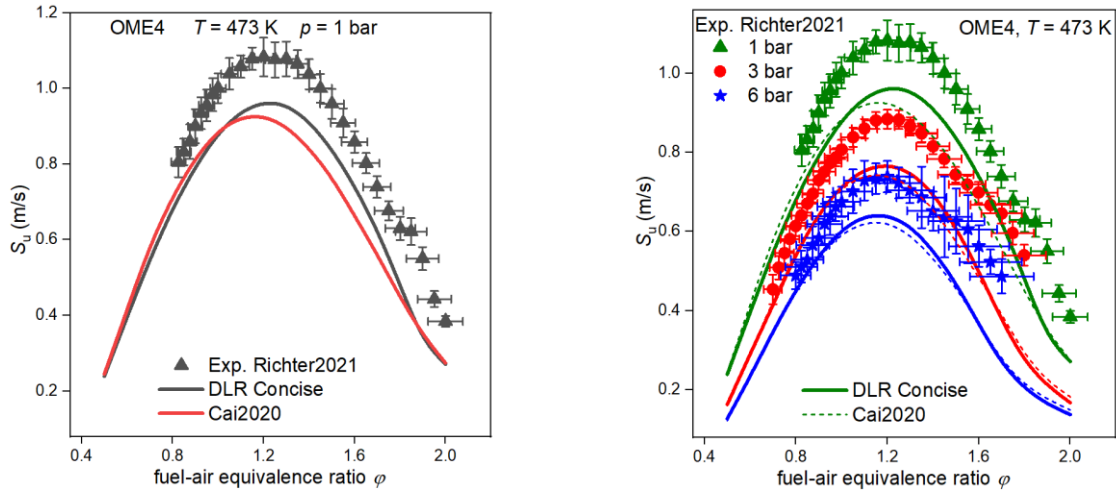
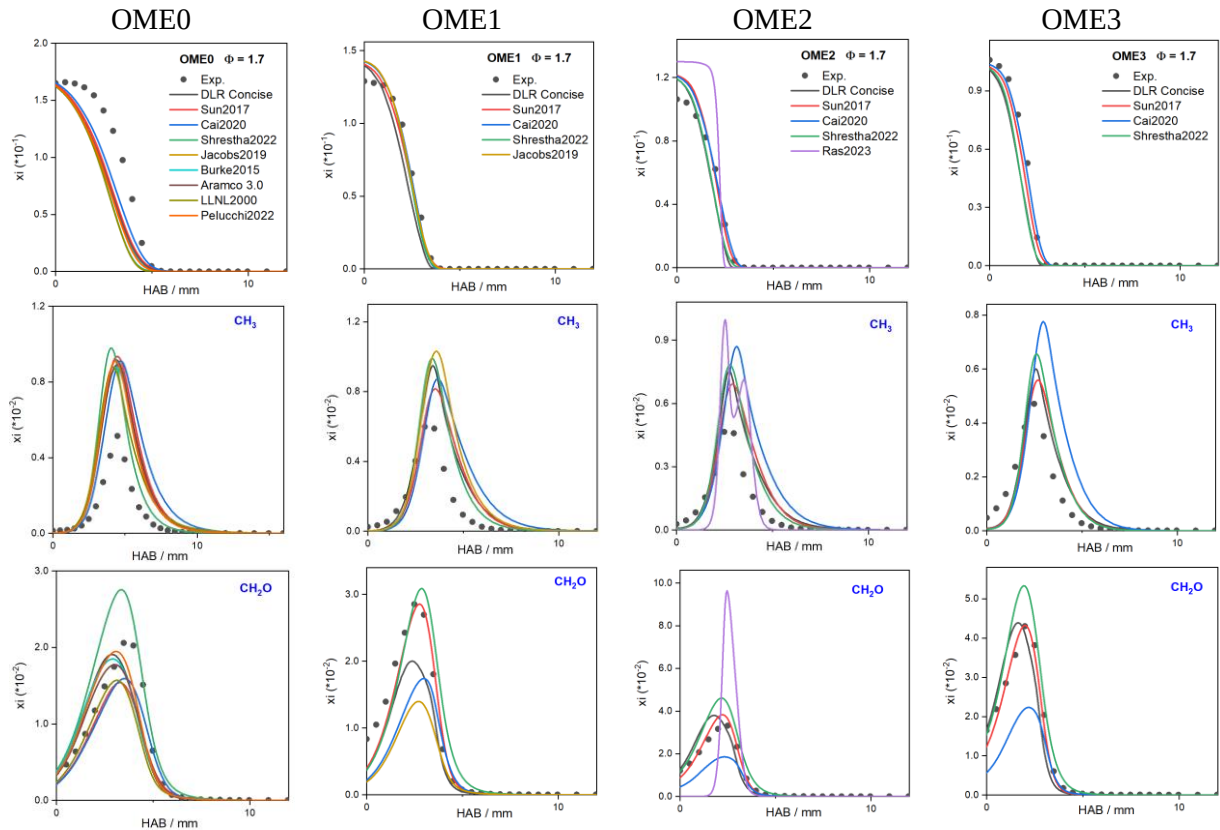


Fig. S74: Predictions of laminar flame speeds of OME4 [Richter2021] compared with literature models.

(2.3) Laminar burner-stabilized flames

In this section major species and important products of OME oxidation is presented. The purpose of this comparison is to present the model prediction of DLR Concise along with various reaction mechanism available in literature. A general observation is, most of the measured data are reproduced by the models. In particular case the model of [Ras2023] predicts fuel conversion much slower than the measurements and other models. At some conditions, for CH_3OH or HOCHO the deviation between experiment and all models is higher than allowed uncertainty limit. In case of large deviation between models and experiments, all models give similar results, e.g. CH_3OH , HOCHO . This observation applies both to the data of [Gaiser2022C] and [Sun2017-OME3].



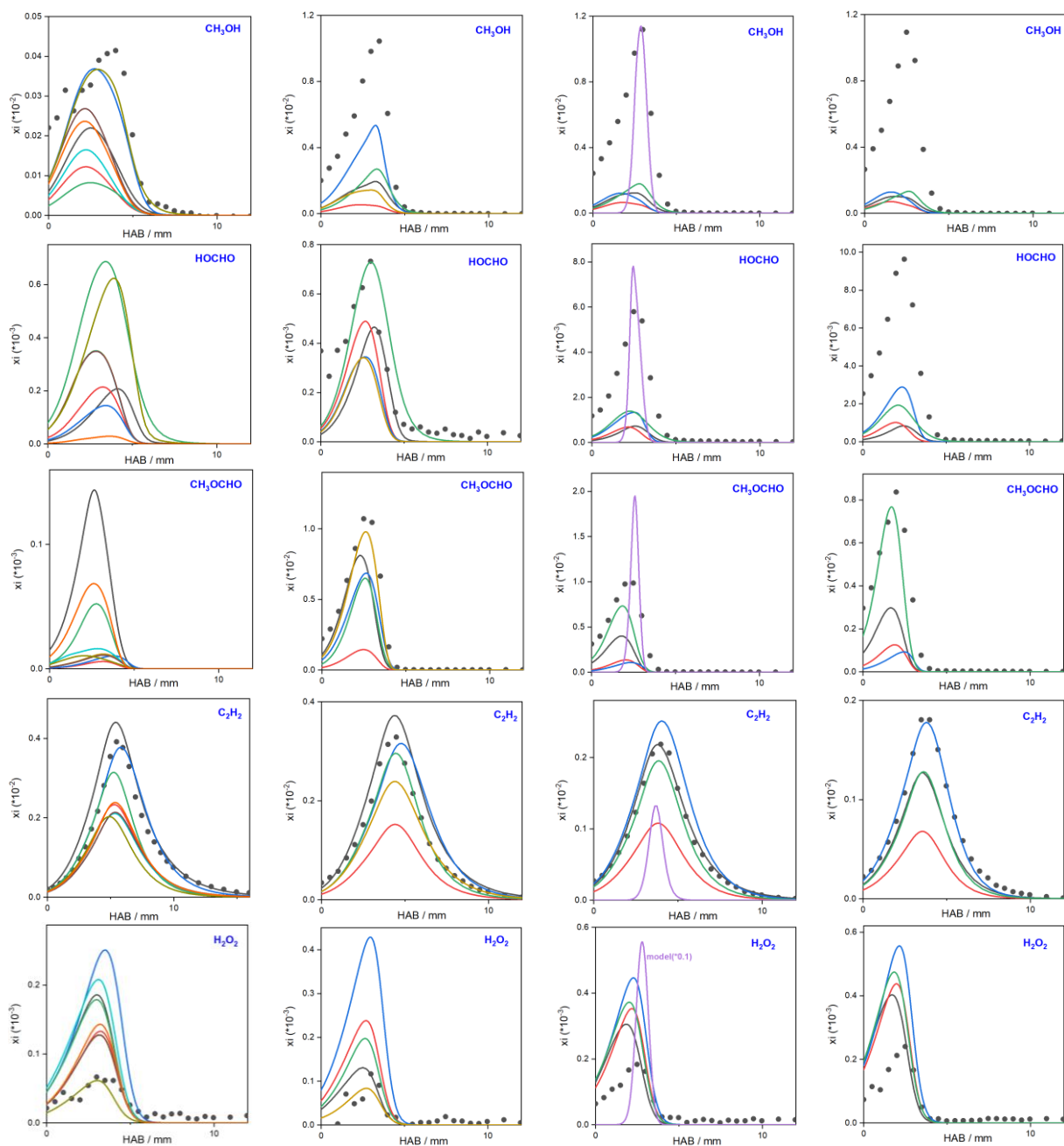
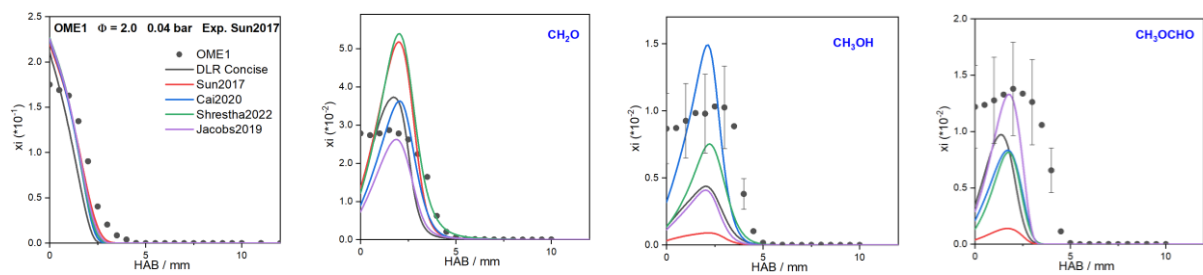


Fig. S75: Comparison of important intermediates and products of OME0-3 oxidation measured in burner-stabilized flames [Gaiser2022C] with DLR Concise and different reaction models from literature.



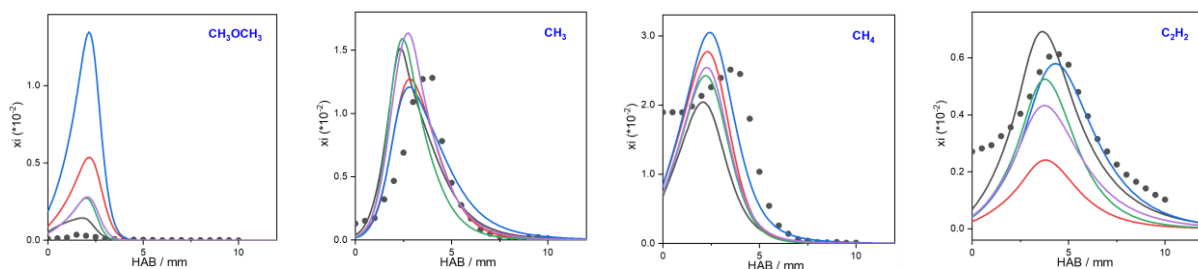
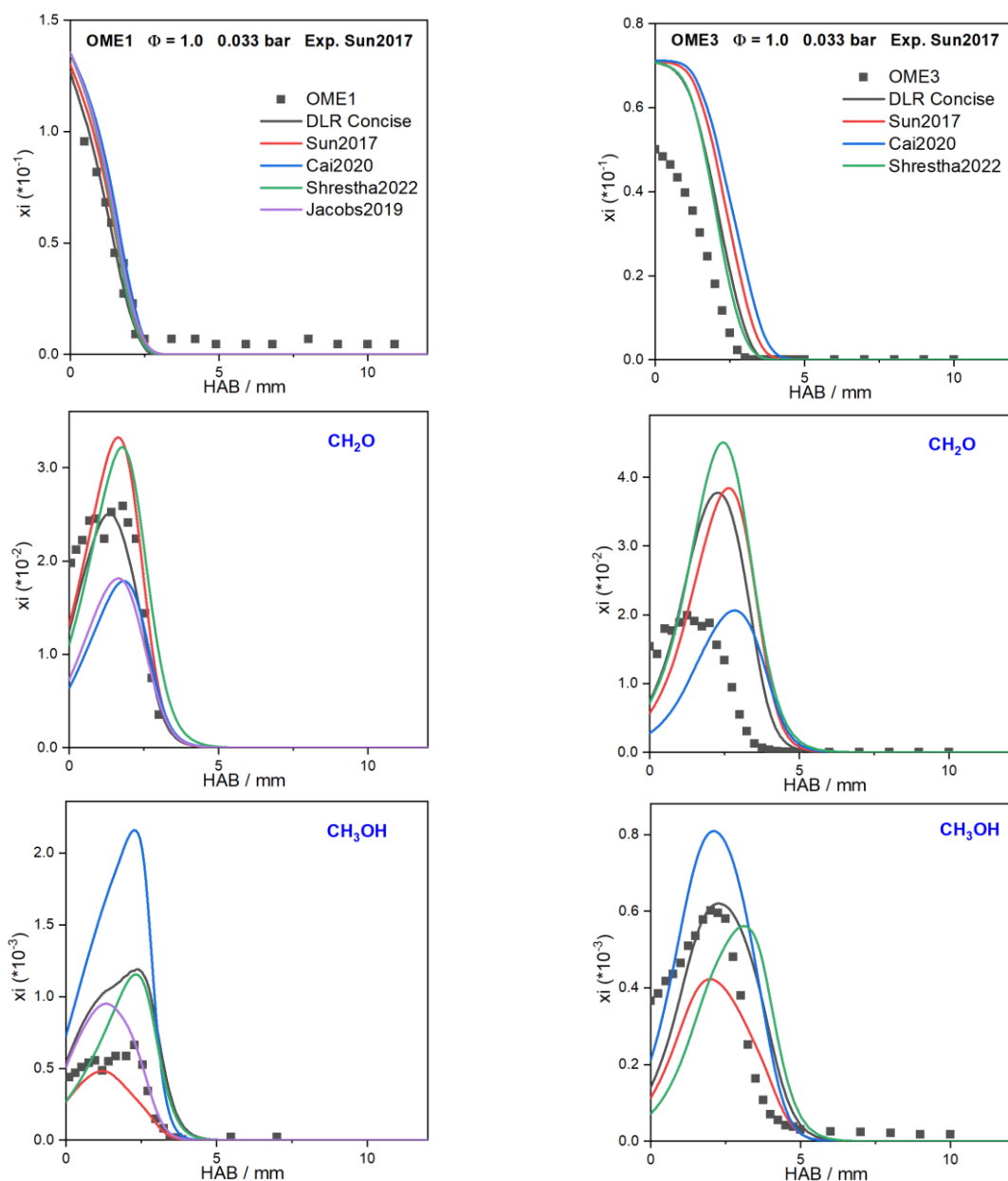


Fig. S76: Comparison of important species measured in OME1 burner-stabilized flames [Sun2017-OME1] with DLR Concise and different reaction models from literature.



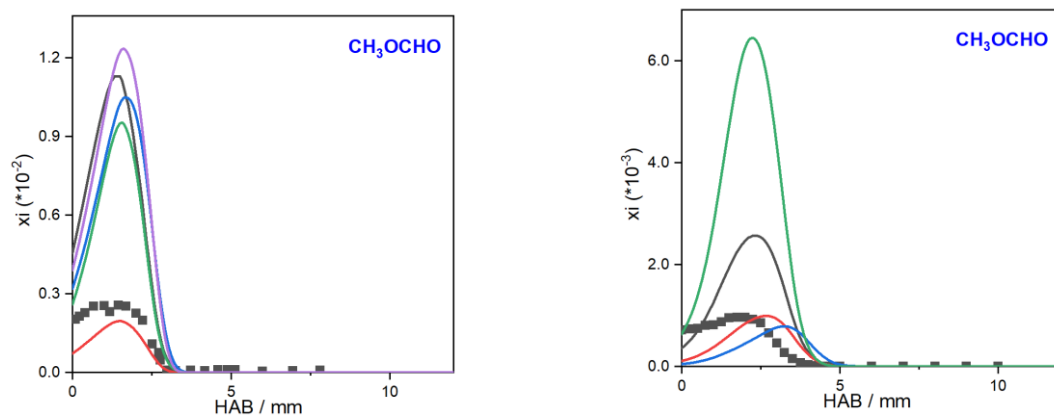
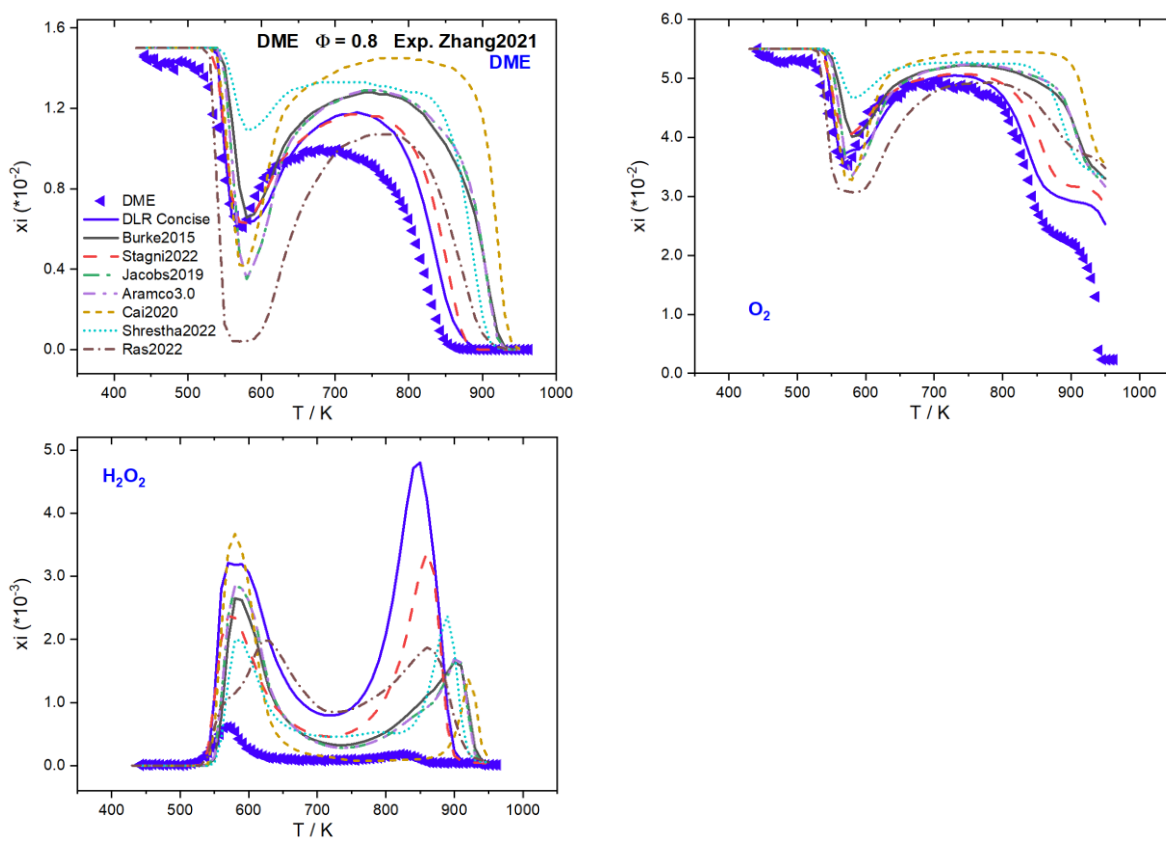


Fig. S77: Comparison of important species measured in OME1 and OME3 burner-stabilized flames [Sun2017-OME3] with DLR Concise and different reaction models from literature.

(2.4) Flow reactor



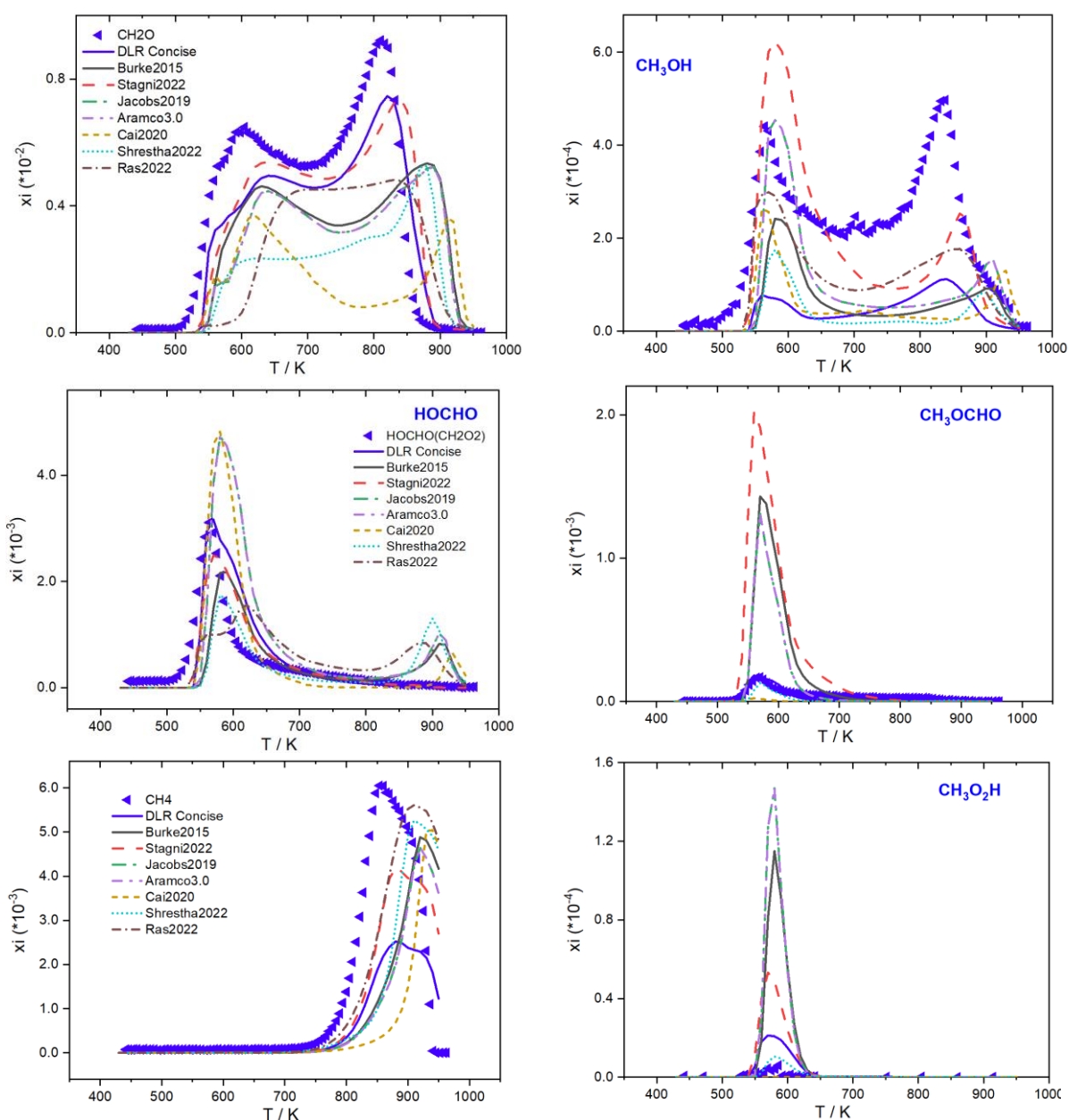
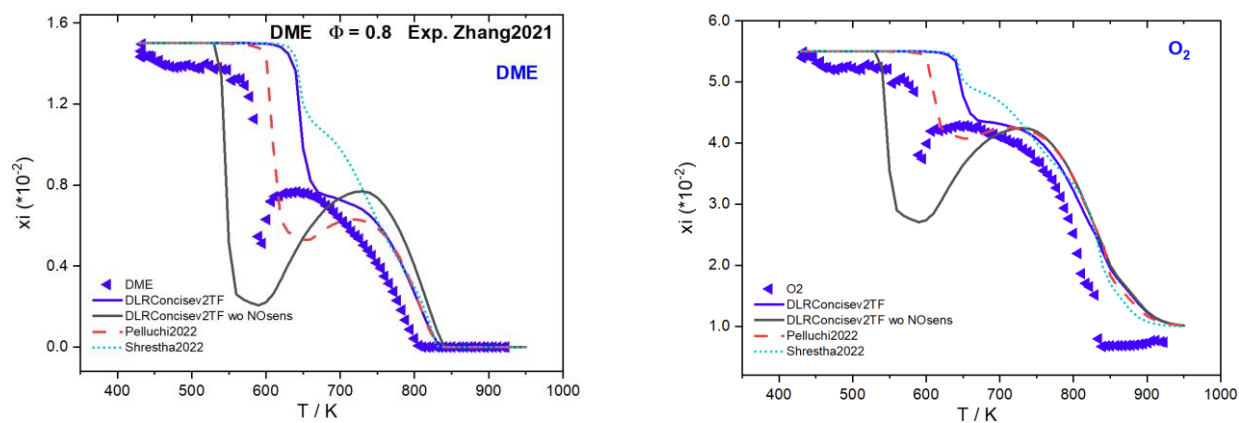
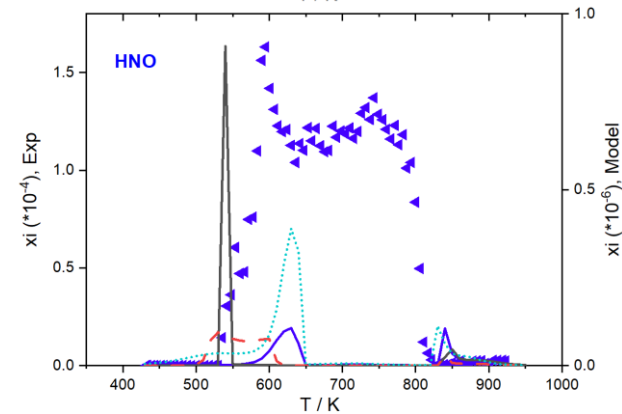
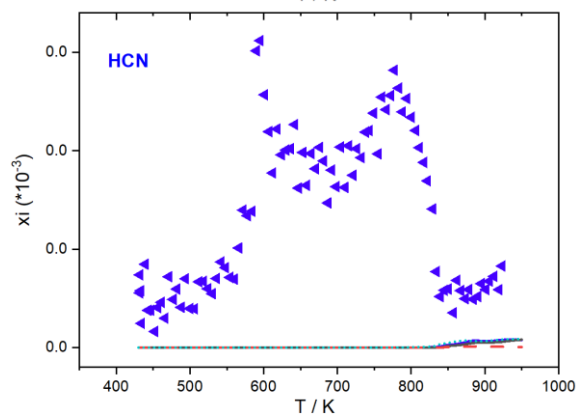
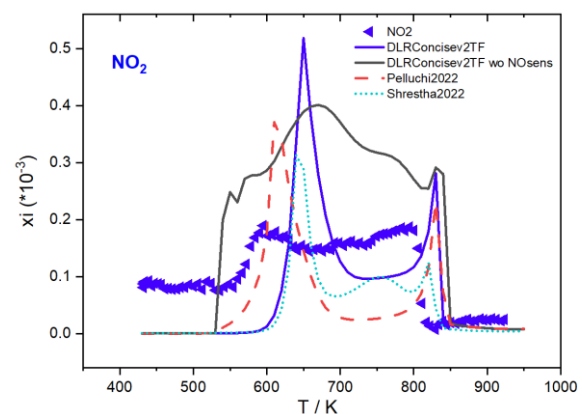
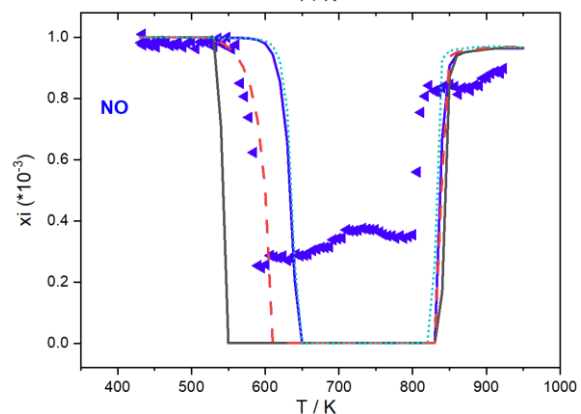
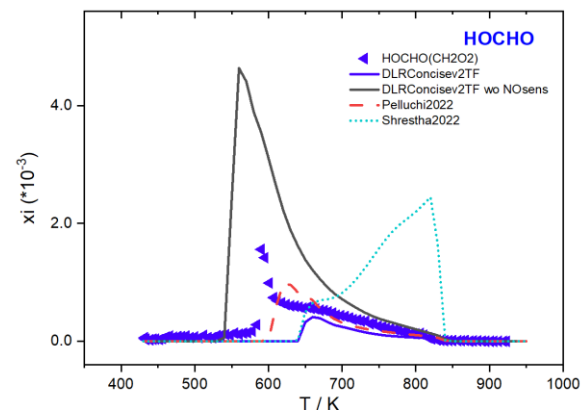
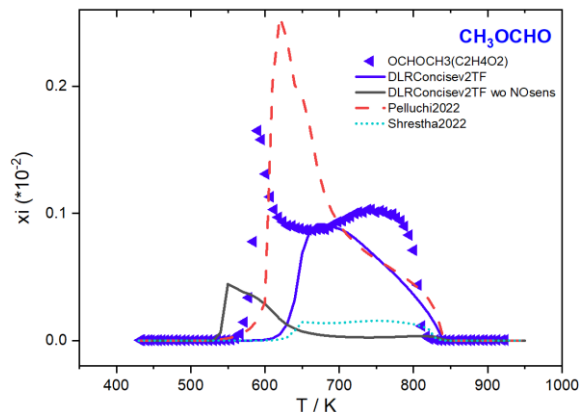
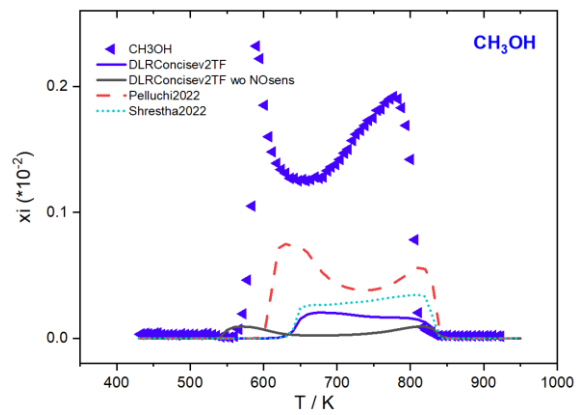
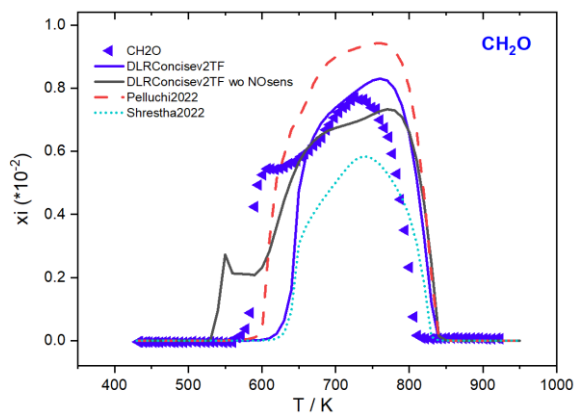


Fig. S78: Predictions of speciation obtained in DME-ONO in flow reactor with different kinetic models [Zhang2021].





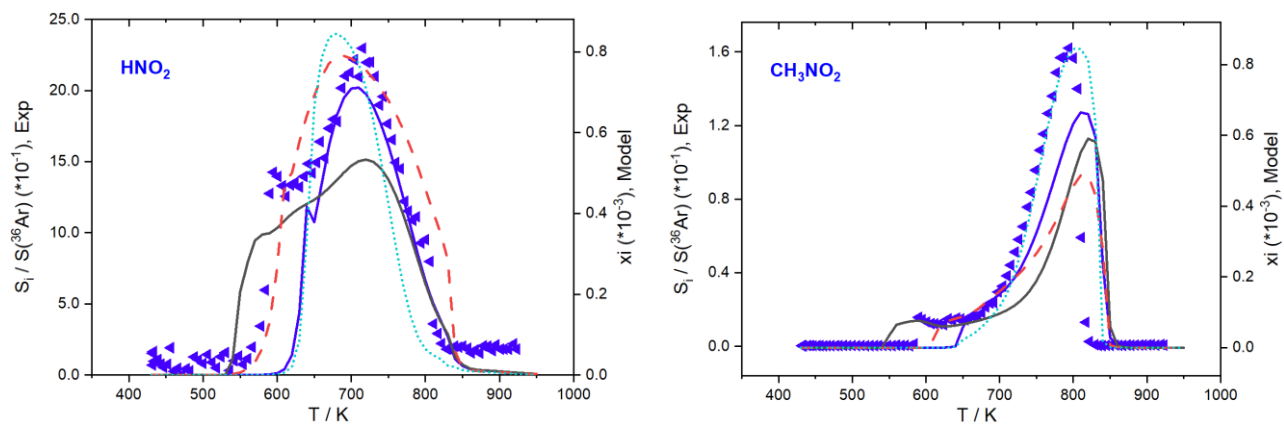
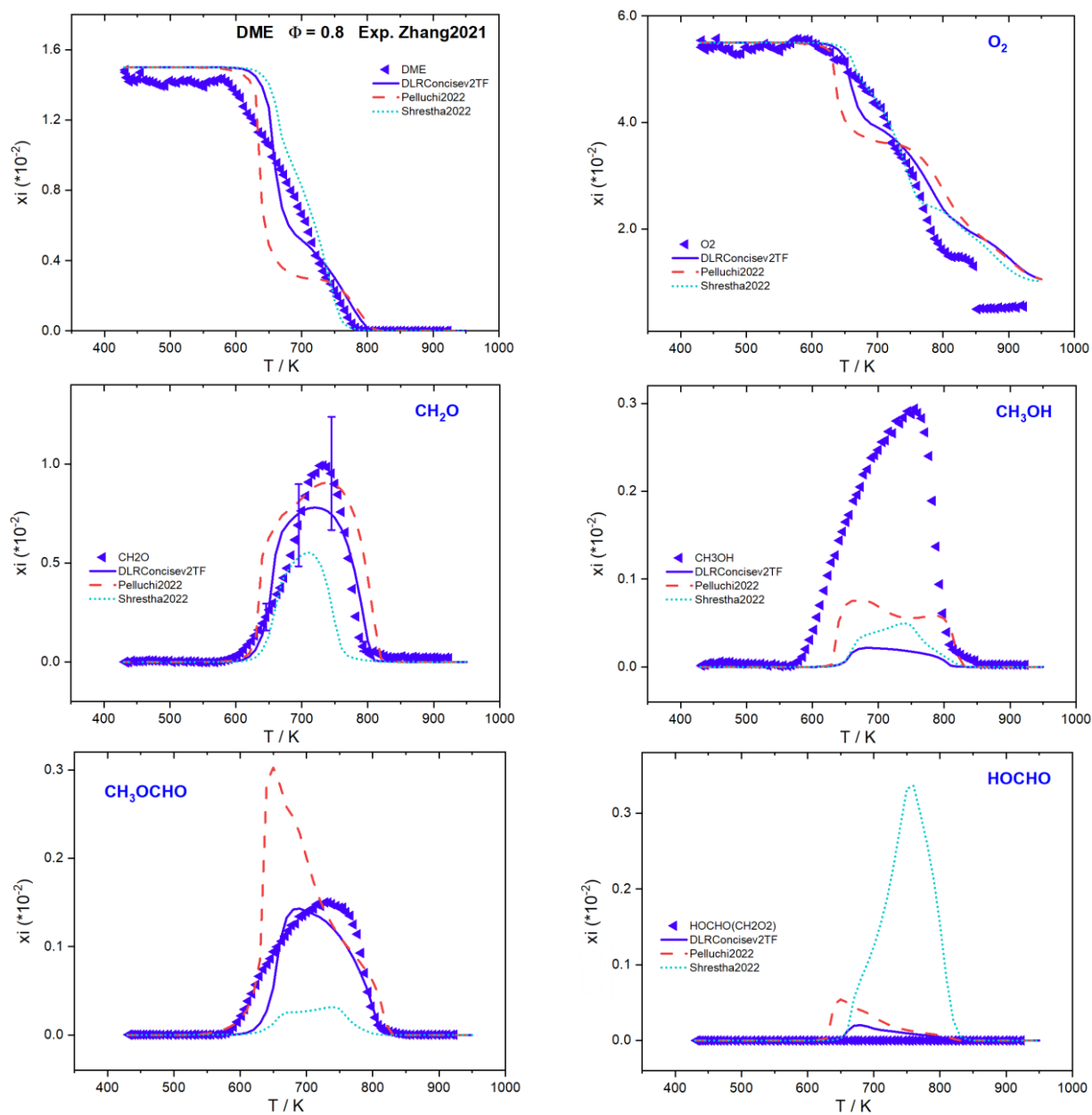


Fig. S79: Predictions of speciation obtained in DME-1000NO mixtures in flow reactor with different kinetic models [Zhang2021]. Comparison of DLR Concise with and without DME-NO interaction.



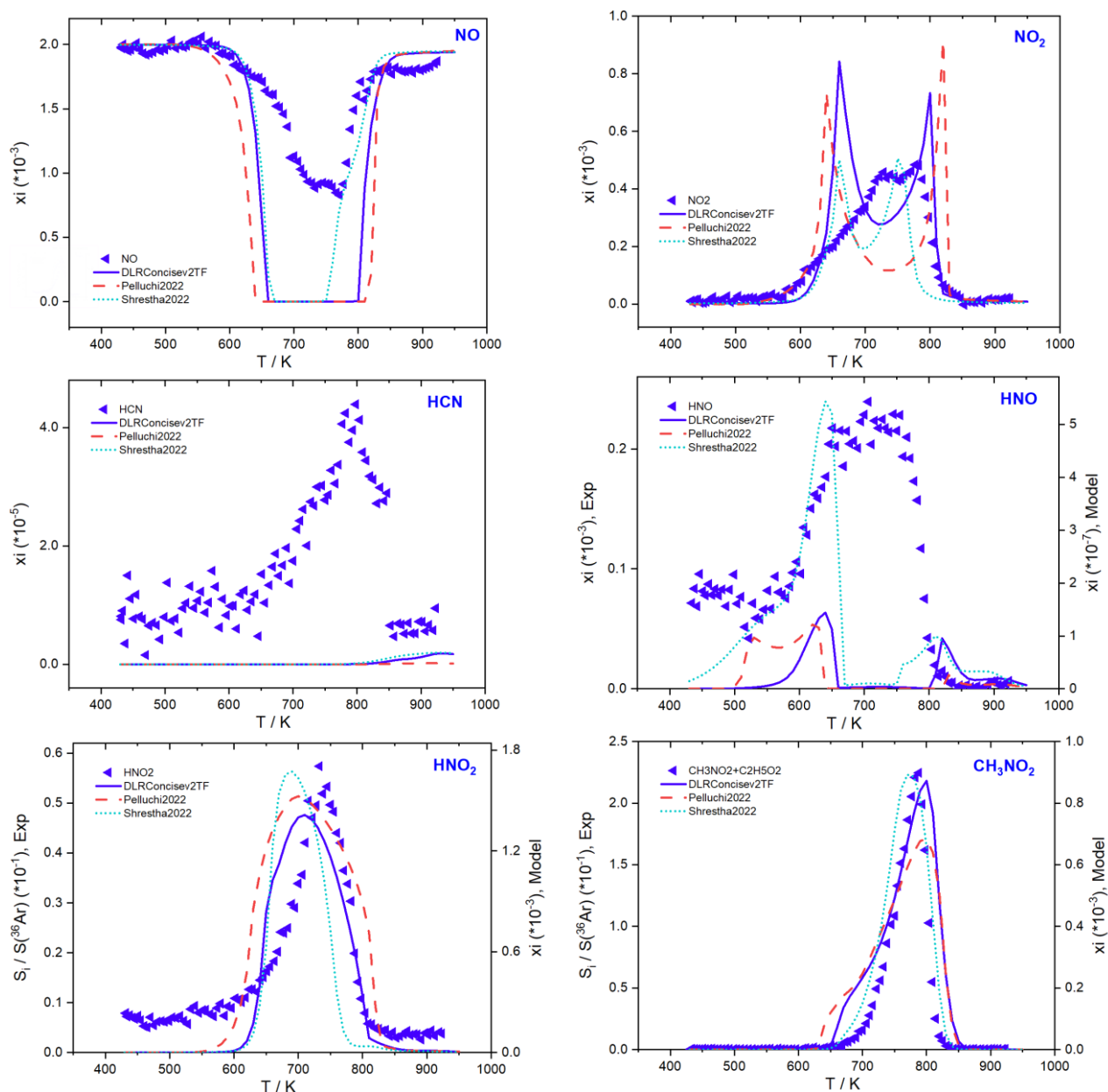
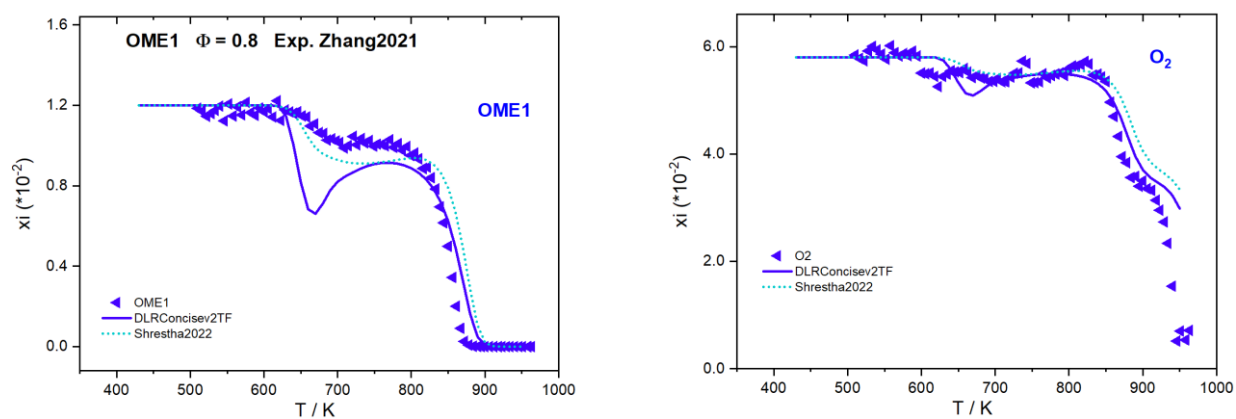


Fig. S80: Predictions of speciation obtained in DME-2000NO mixtures in flow reactor with different kinetic models [Zhang2021].



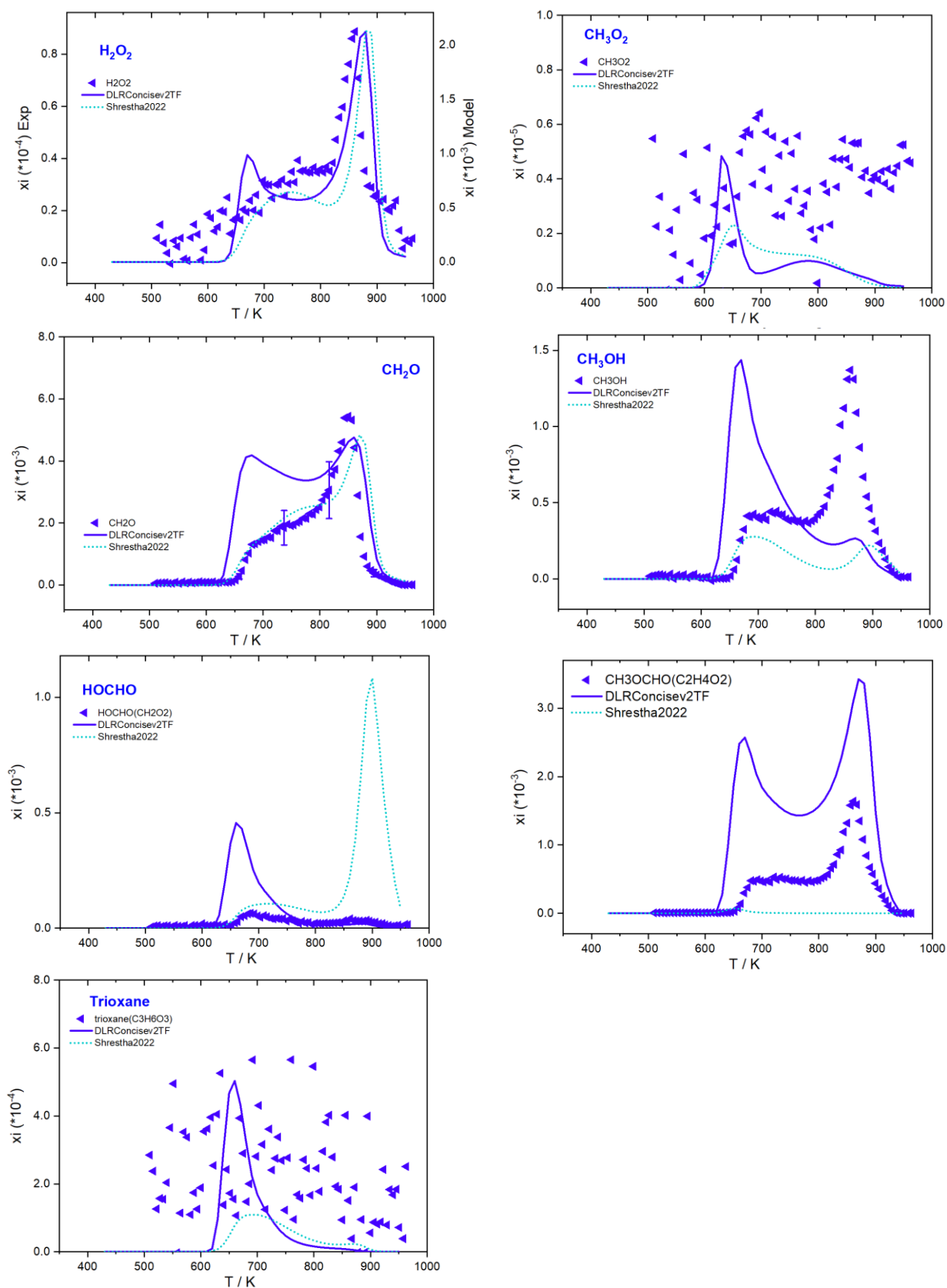
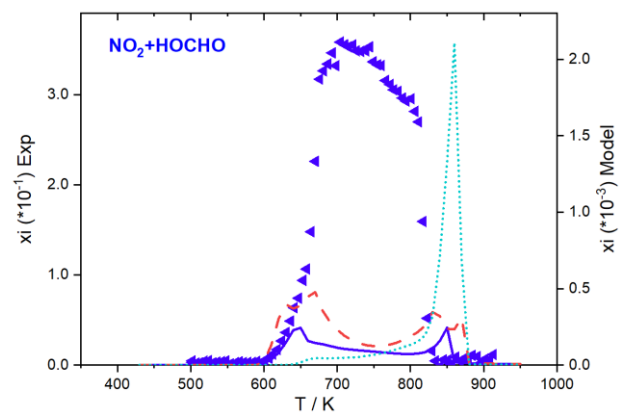
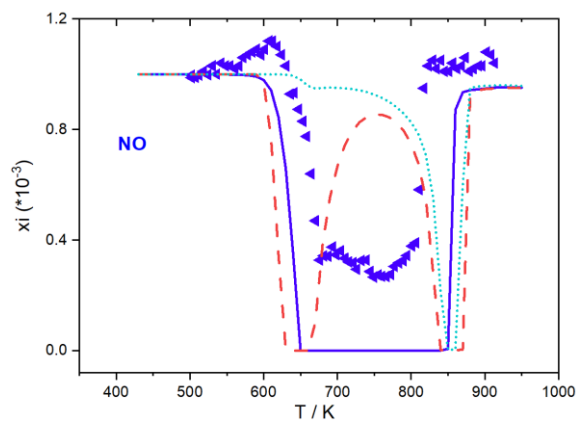
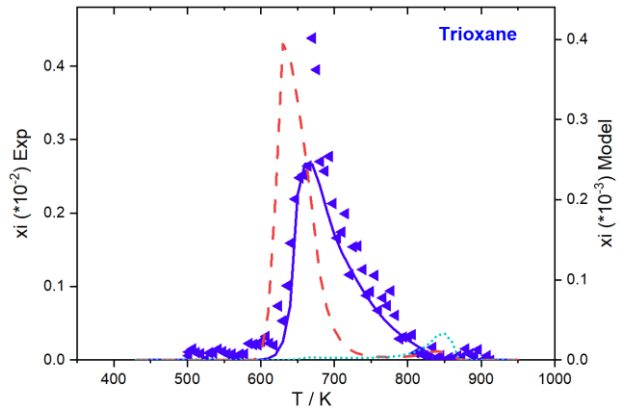
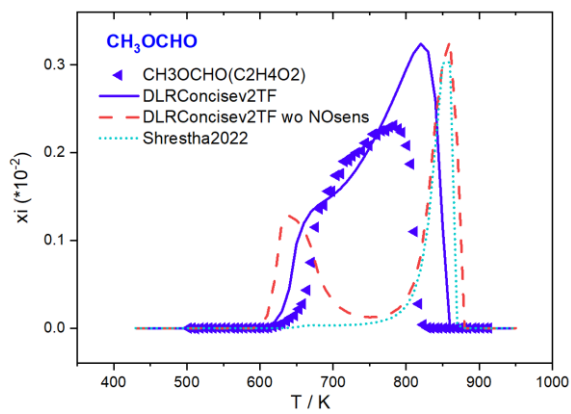
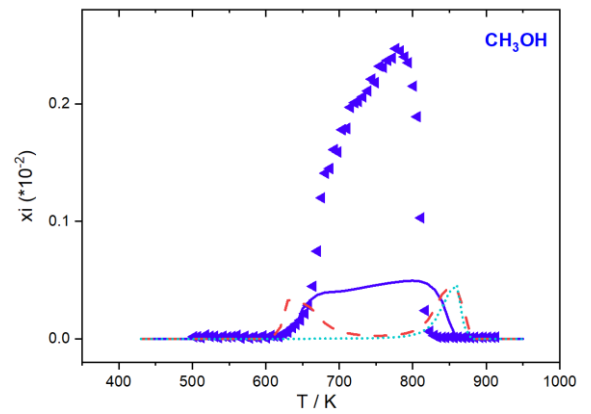
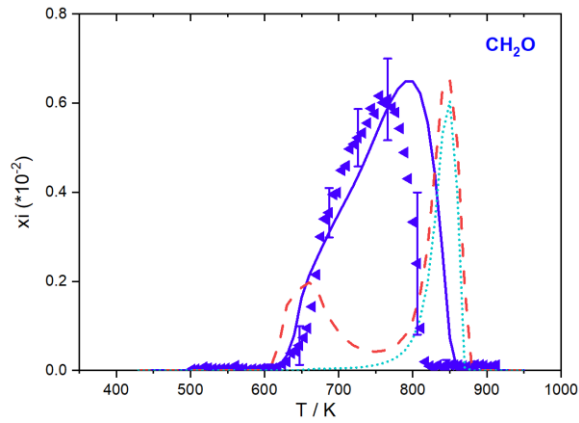
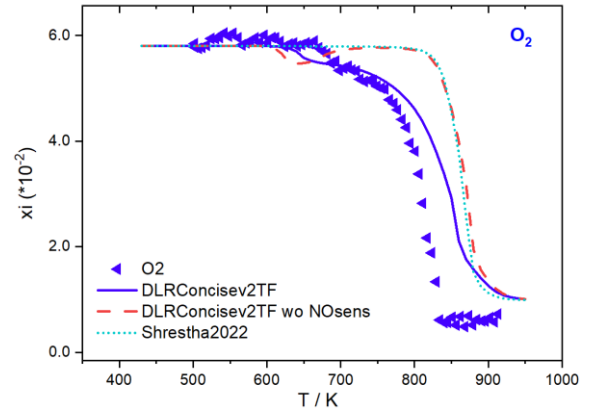
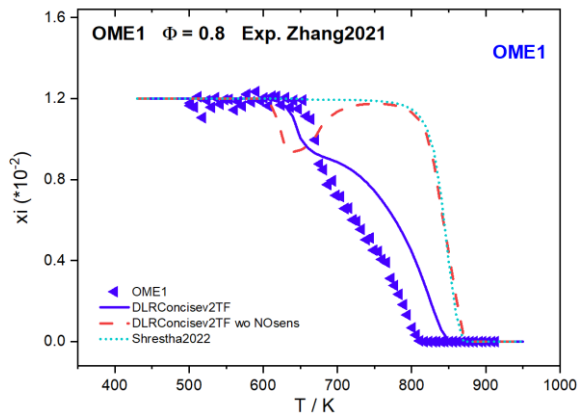


Fig. S81: Predictions of speciation obtained in OME1-ONO mixtures in flow reactor with different kinetic models [Zhang2021].



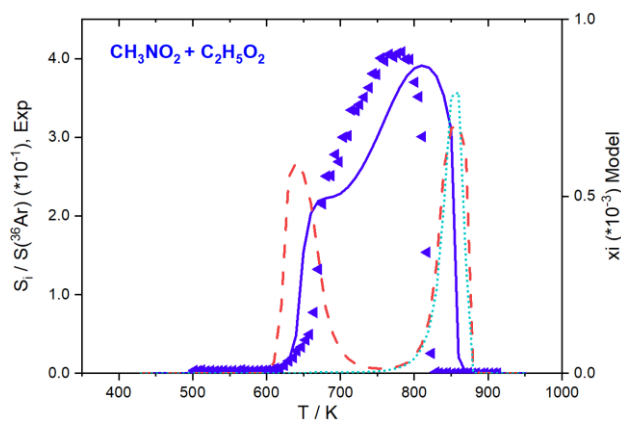
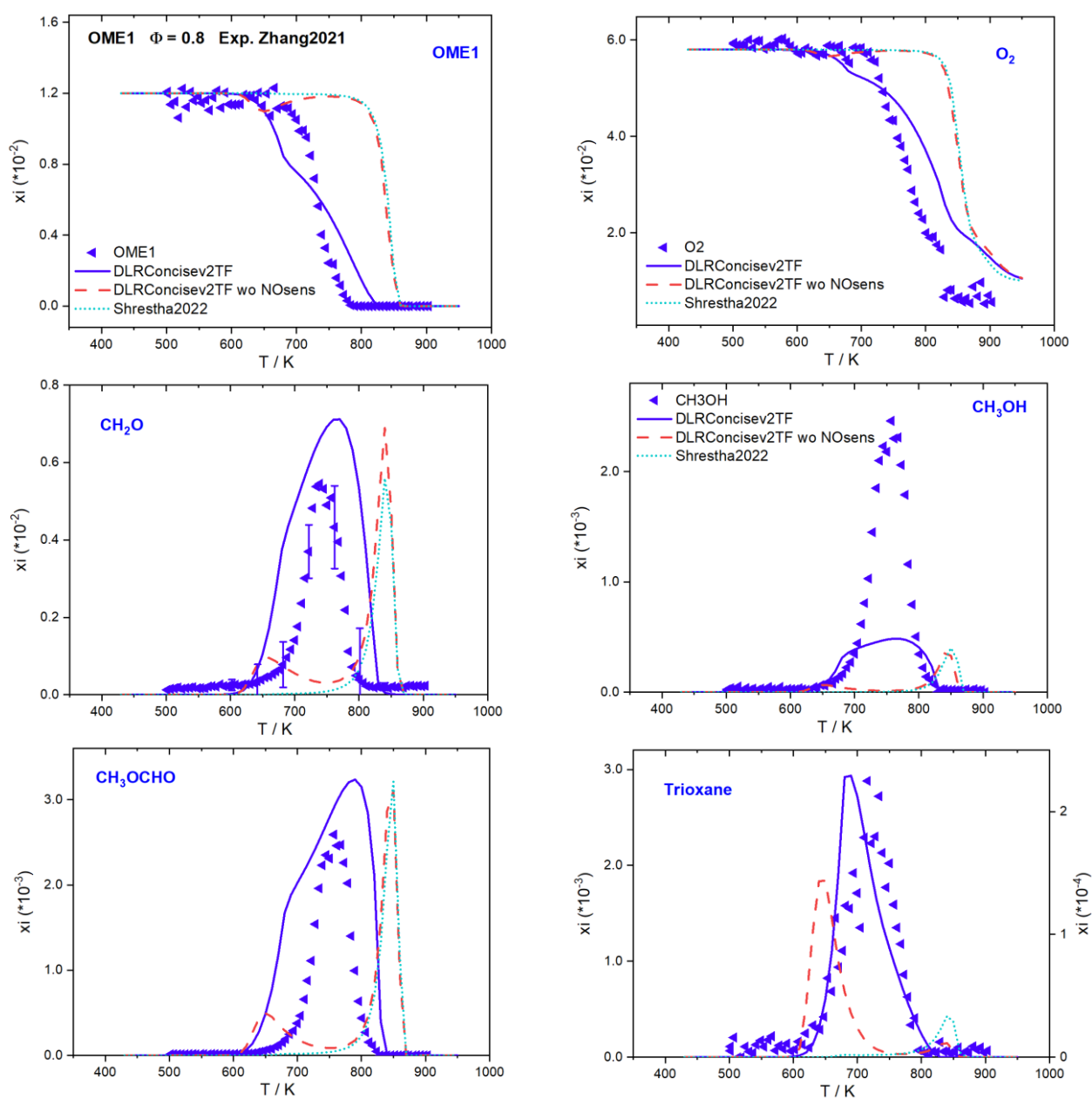


Fig. S82: Predictions of speciation obtained in OME1-1000 NO mixtures in flow reactor with different kinetic models [Zhang2021]. Comparison of DLR Concise with and without OME1-NO interaction.



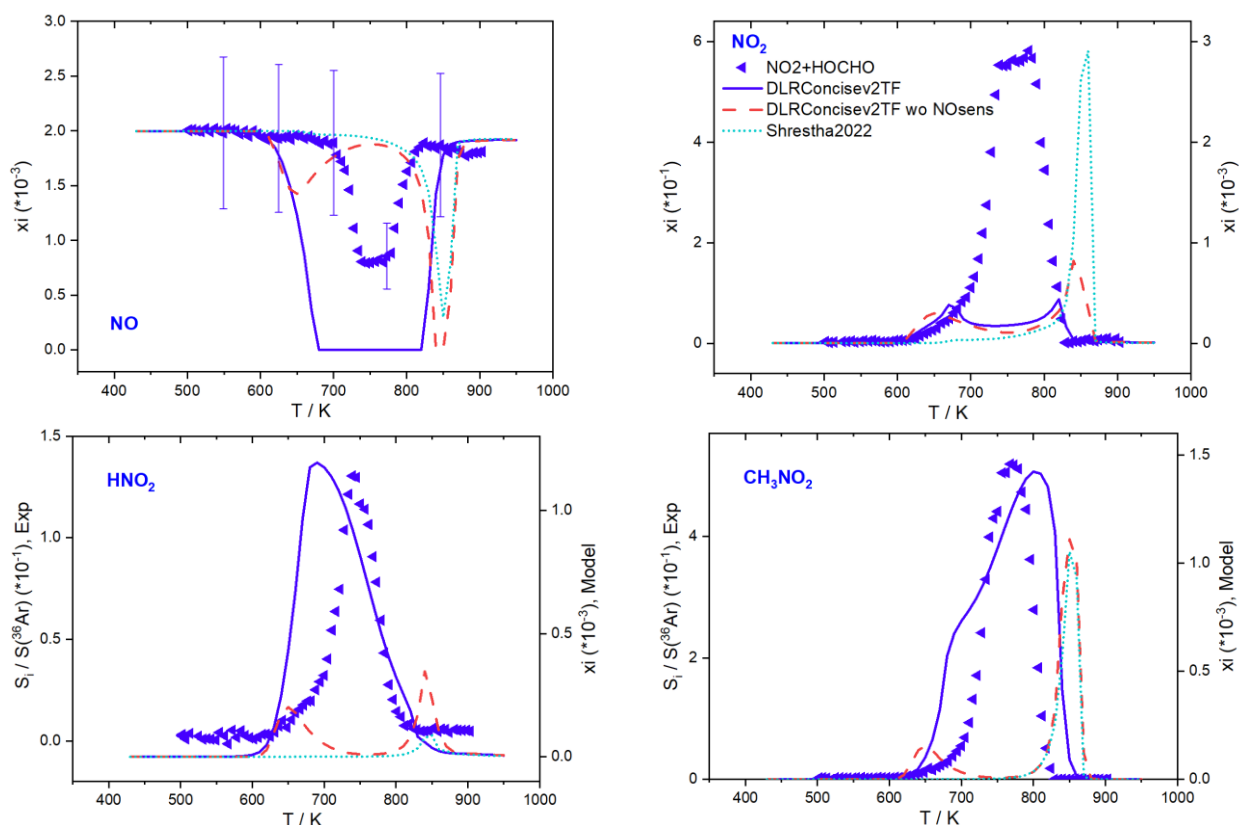
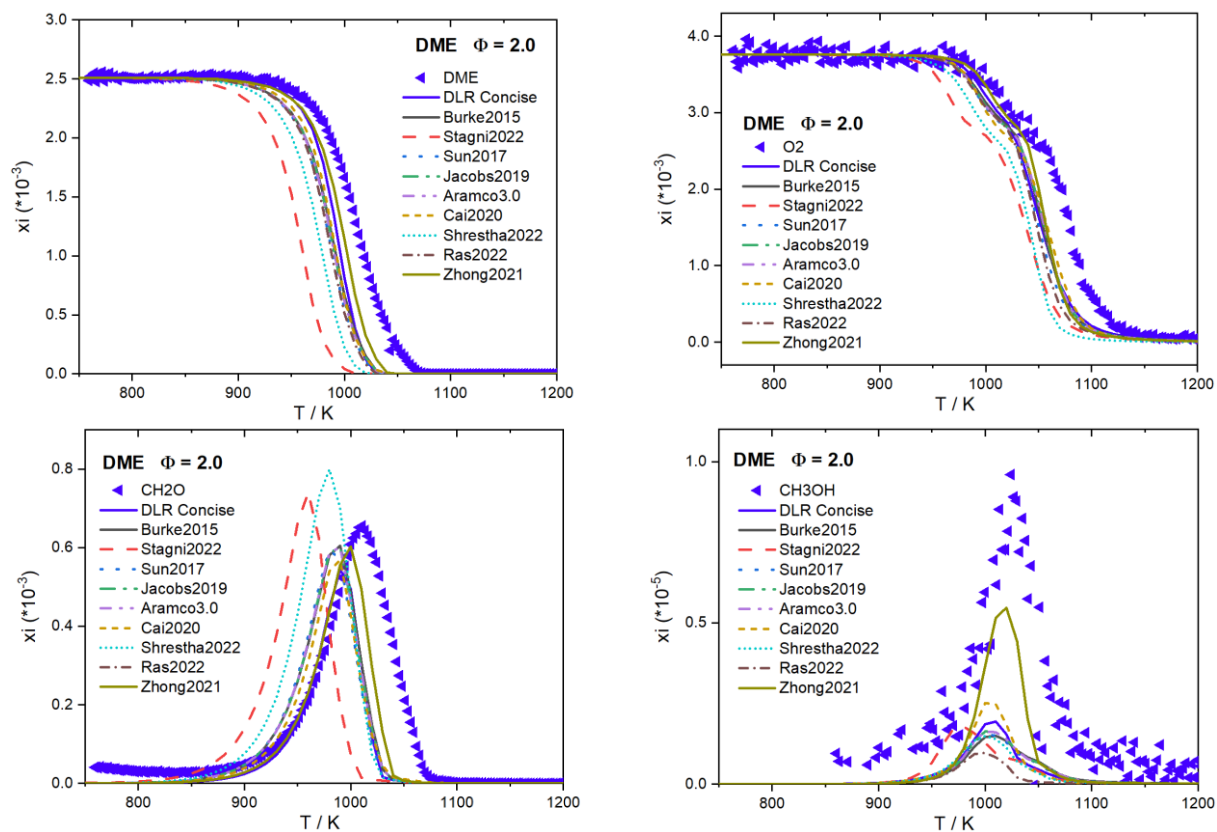


Fig. S83: Predictions of speciation obtained in OME1-2000NO mixtures in flow reactor with different kinetic models [Zhang2021]. Comparison of DLR Concise with and without OME1-NO interaction.



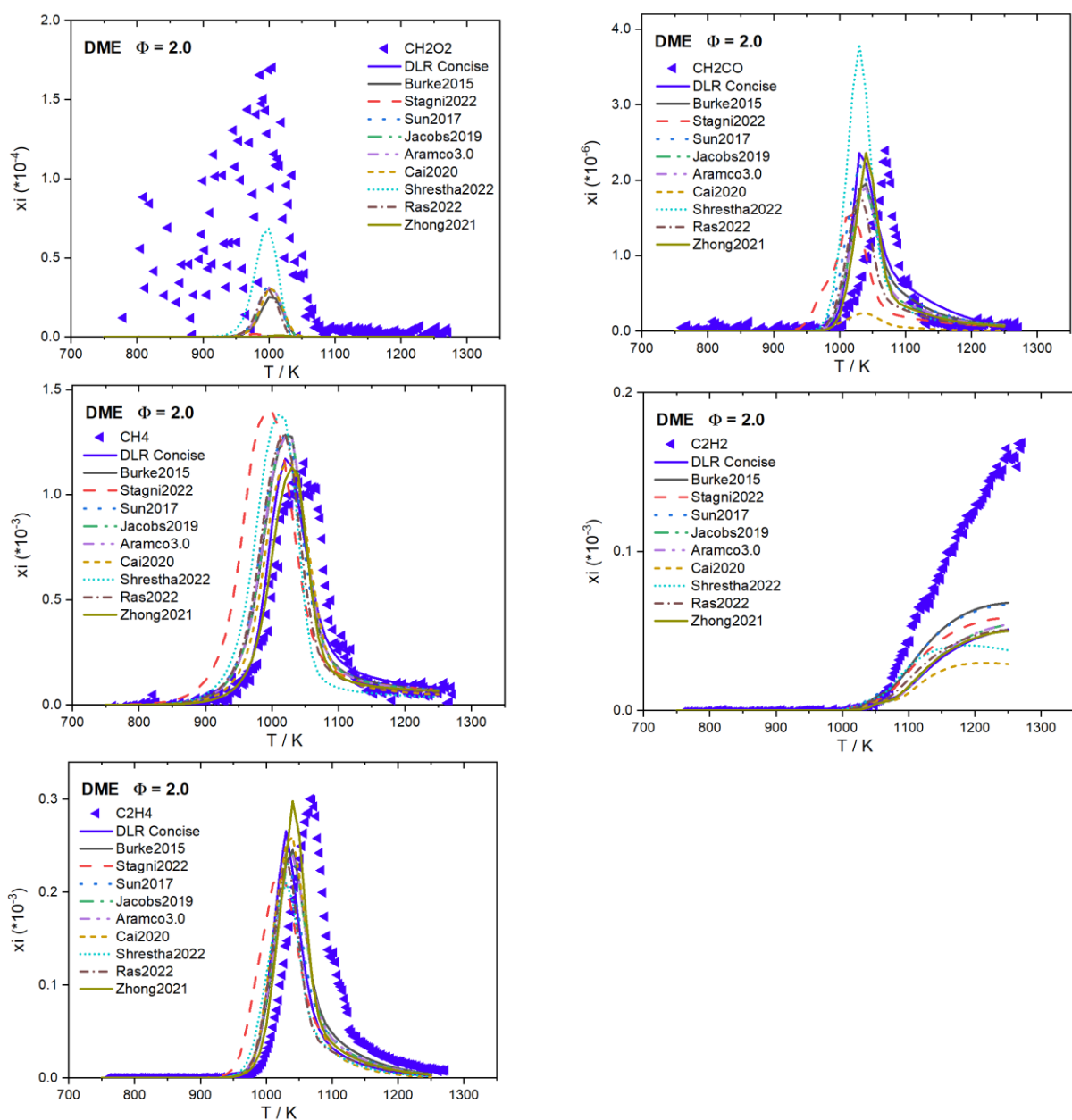
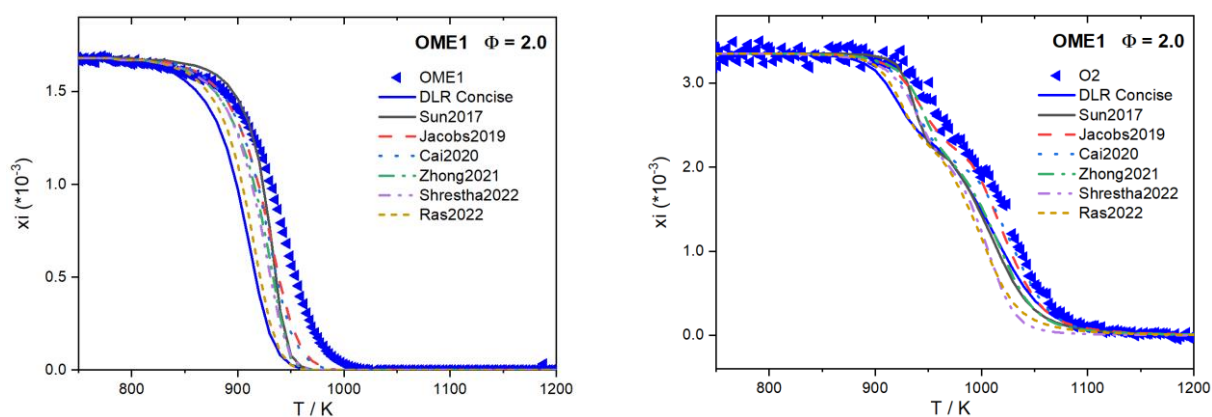


Fig. S84: Predictions of speciation obtained in DME in flow reactor with different models [Gaiser2022F].



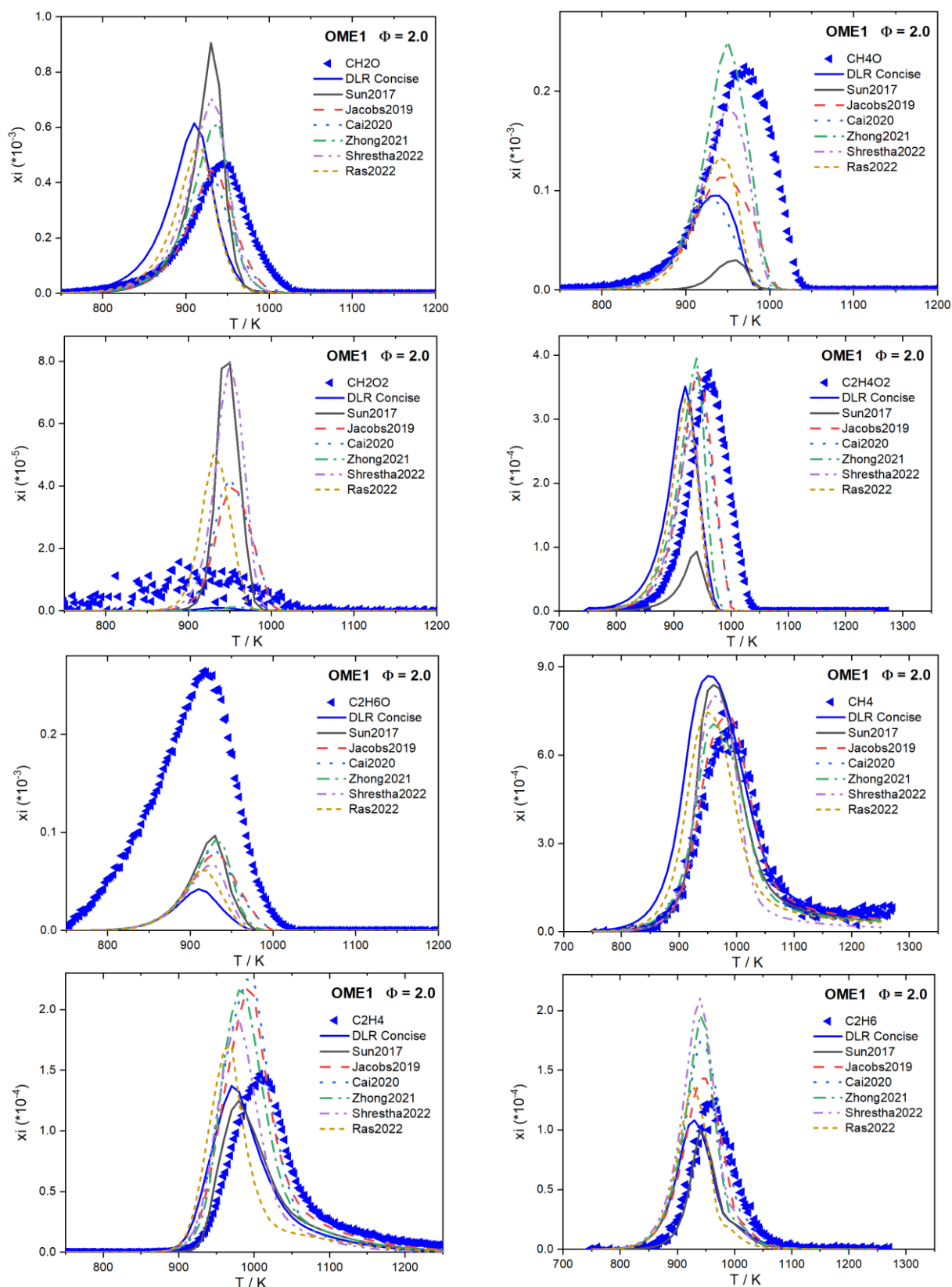
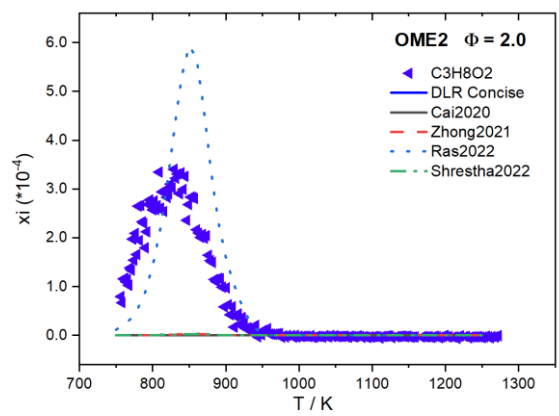
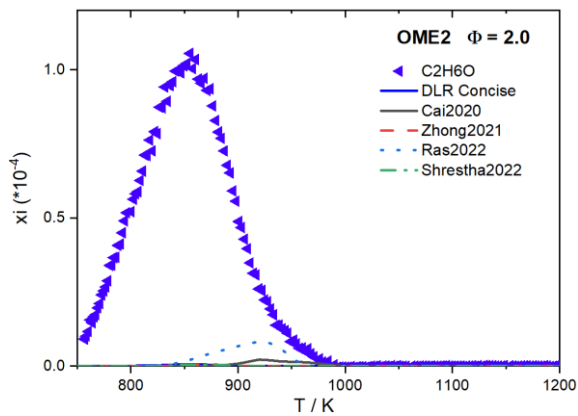
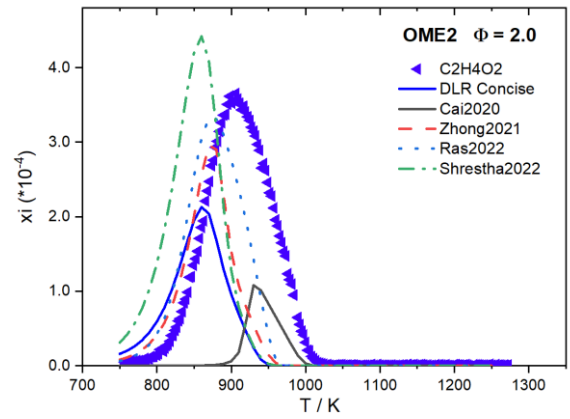
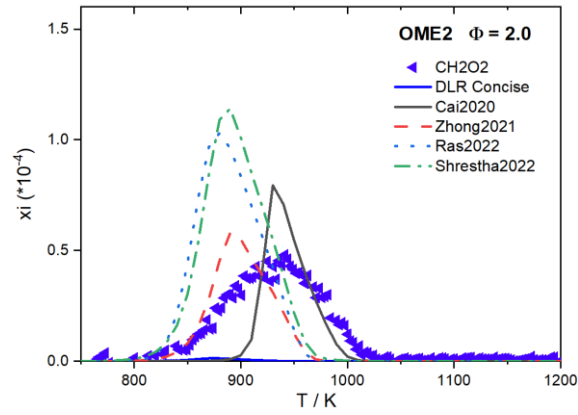
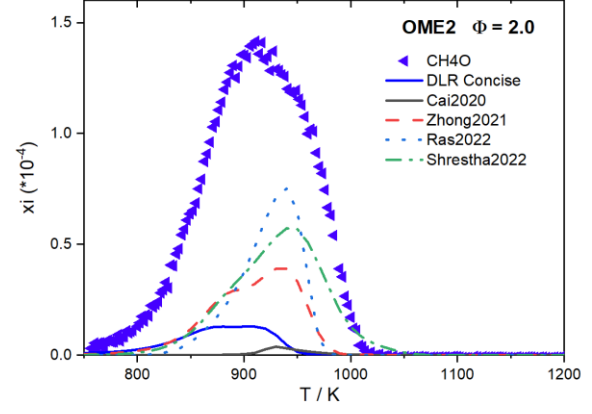
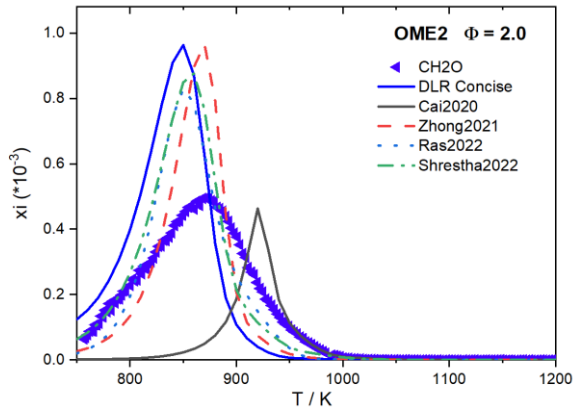
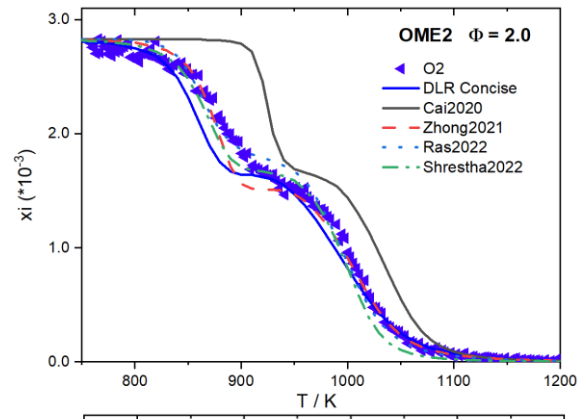
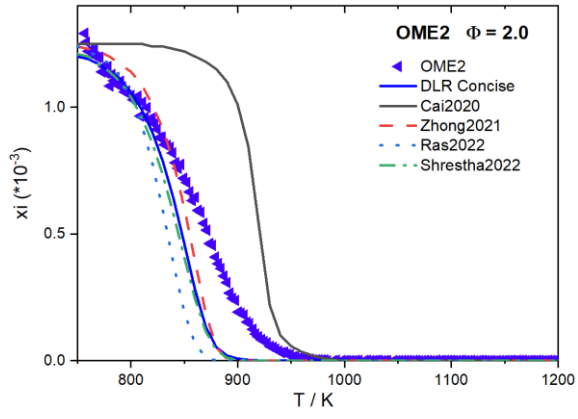


Fig. S85: Predictions of speciation obtained in OME1 in flow reactor with different models [Gaiser2022F].



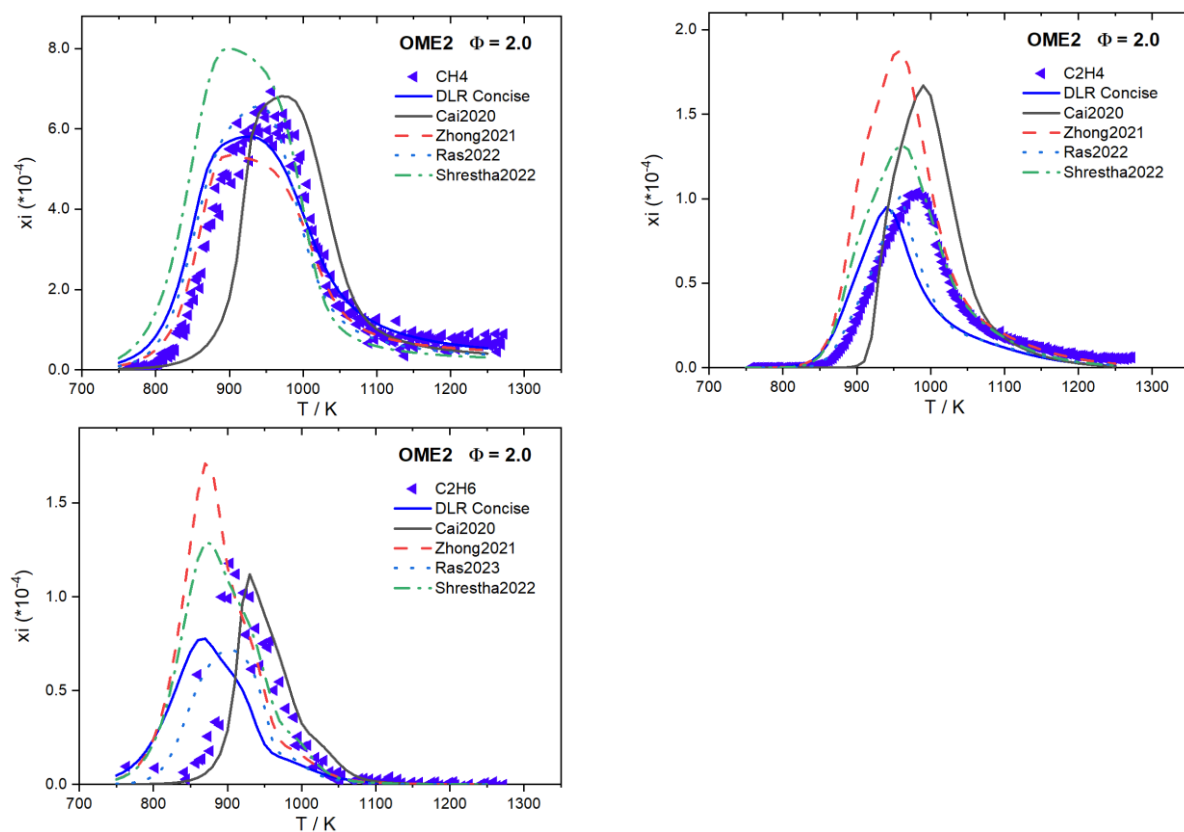
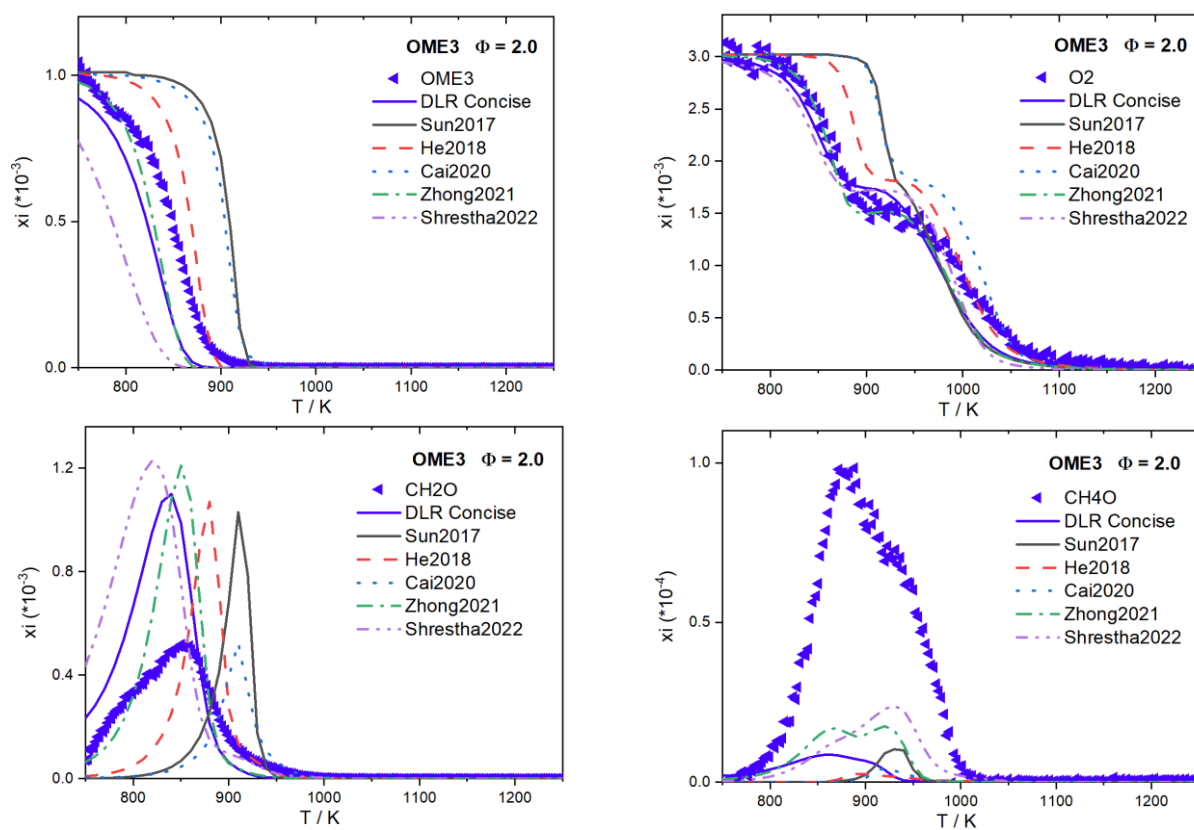


Fig. S86: Predictions of speciation obtained in OME2 in flow reactor with different models [Gaiser2022F].



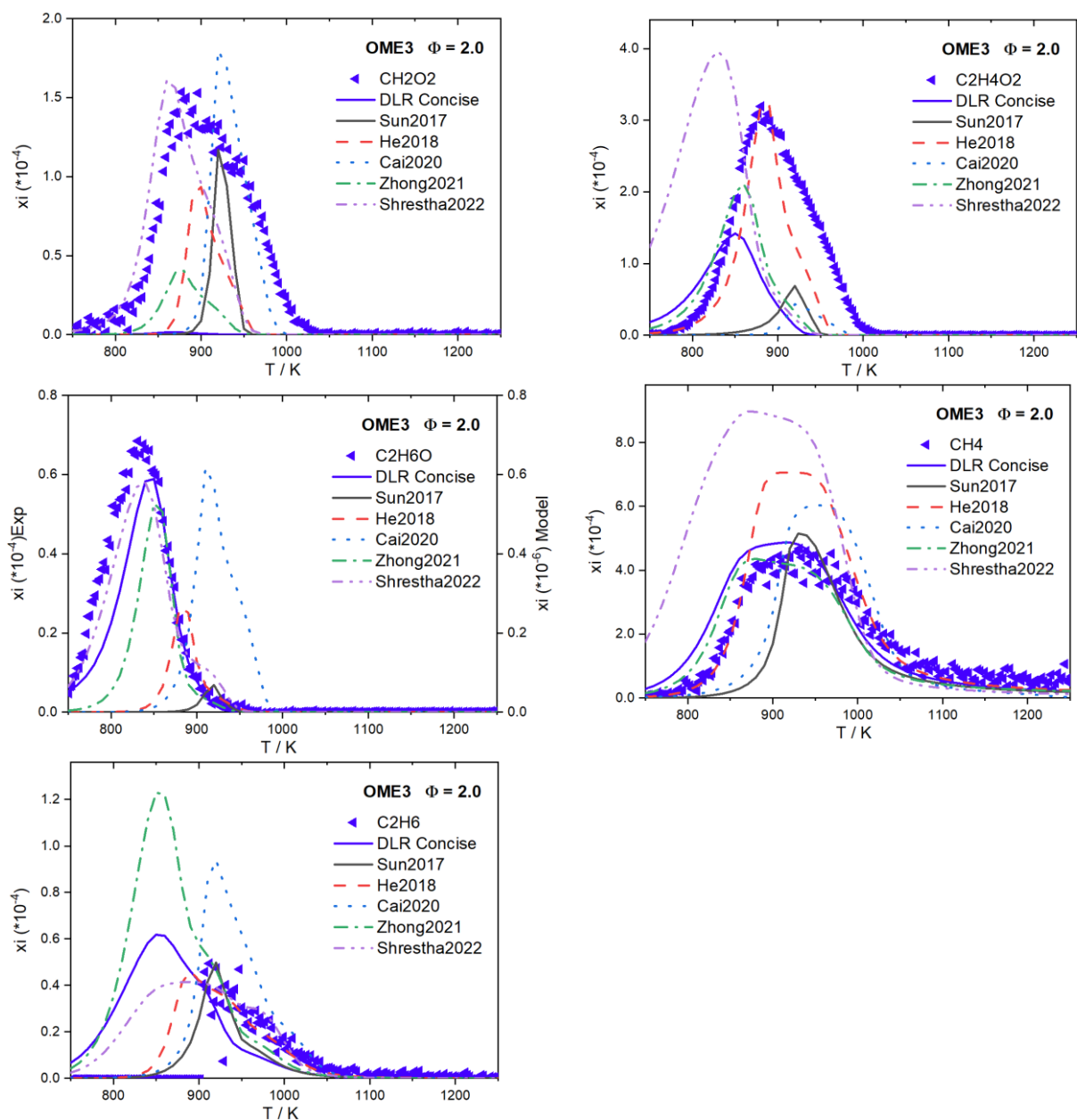
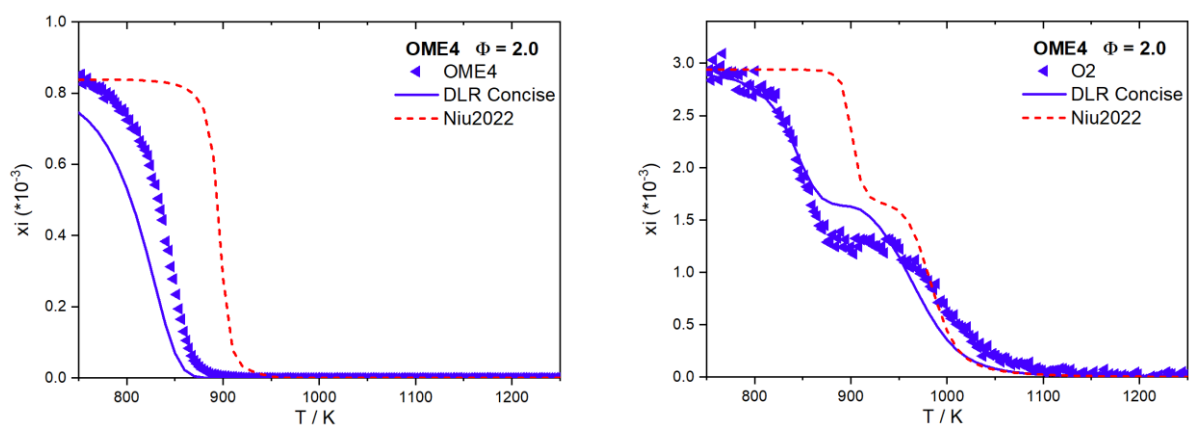


Fig. S87: Predictions of speciation obtained in OME3 in flow reactor with different models [Gaiser2022F].



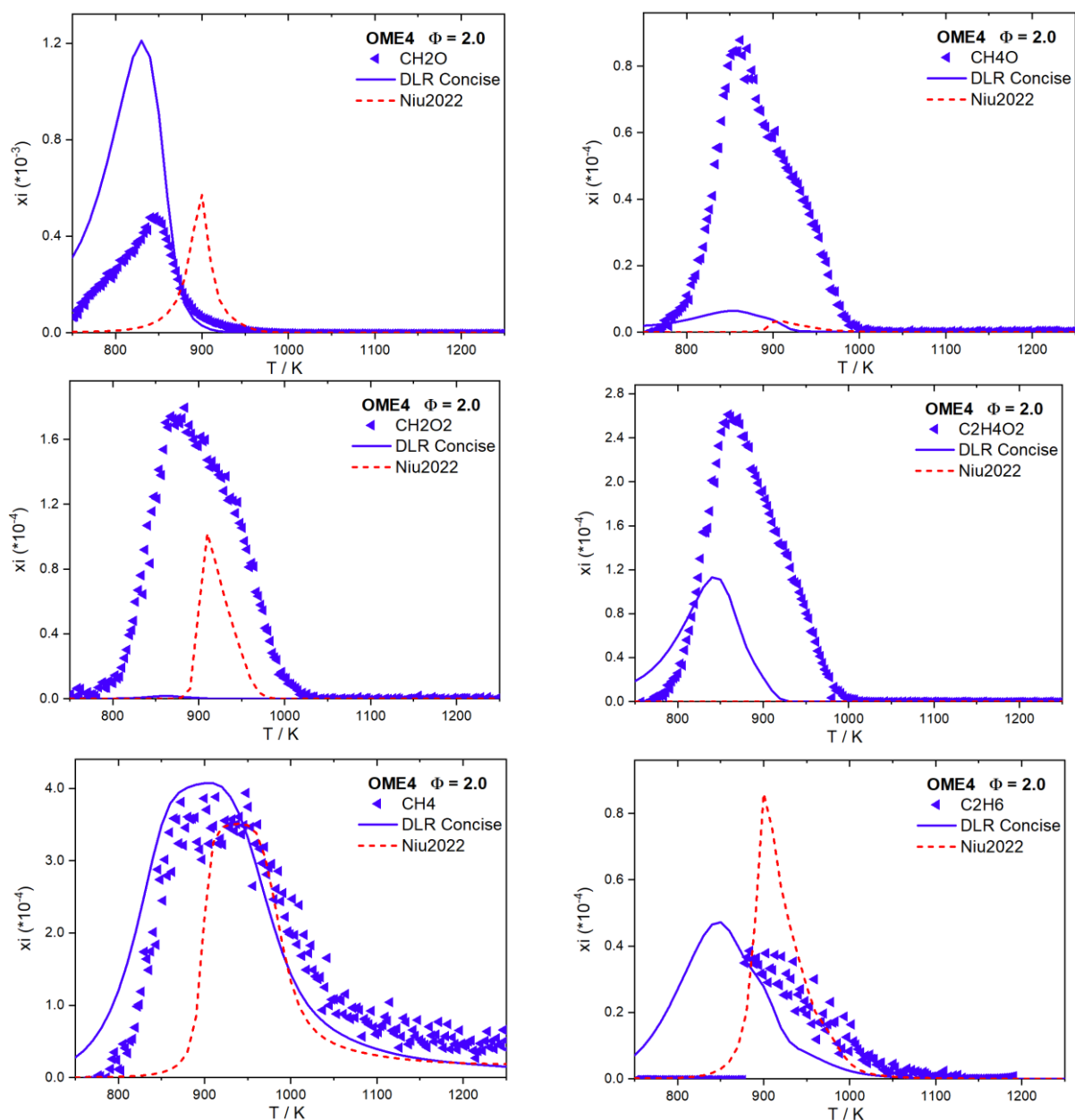
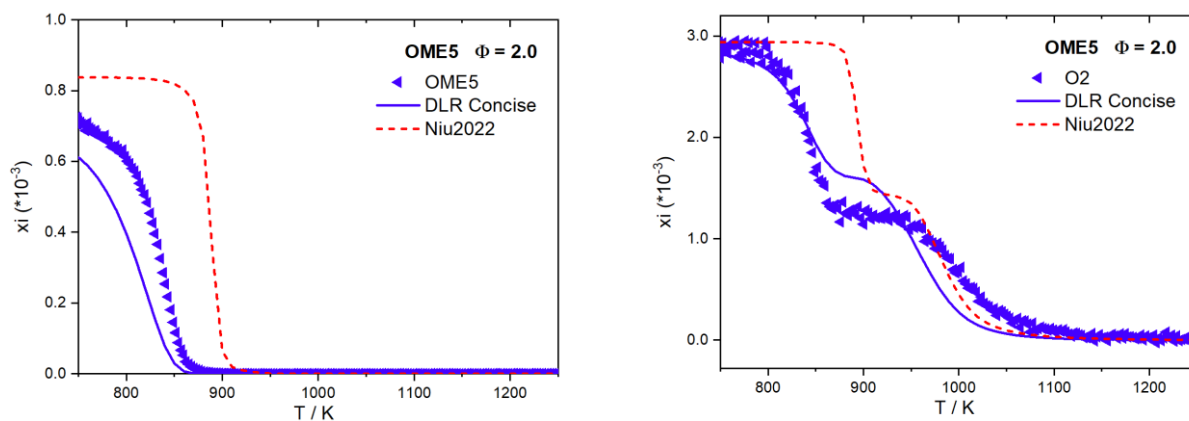


Fig. S88: Predictions of speciation obtained in OME4 in flow reactor with different models [Gaiser2022F].



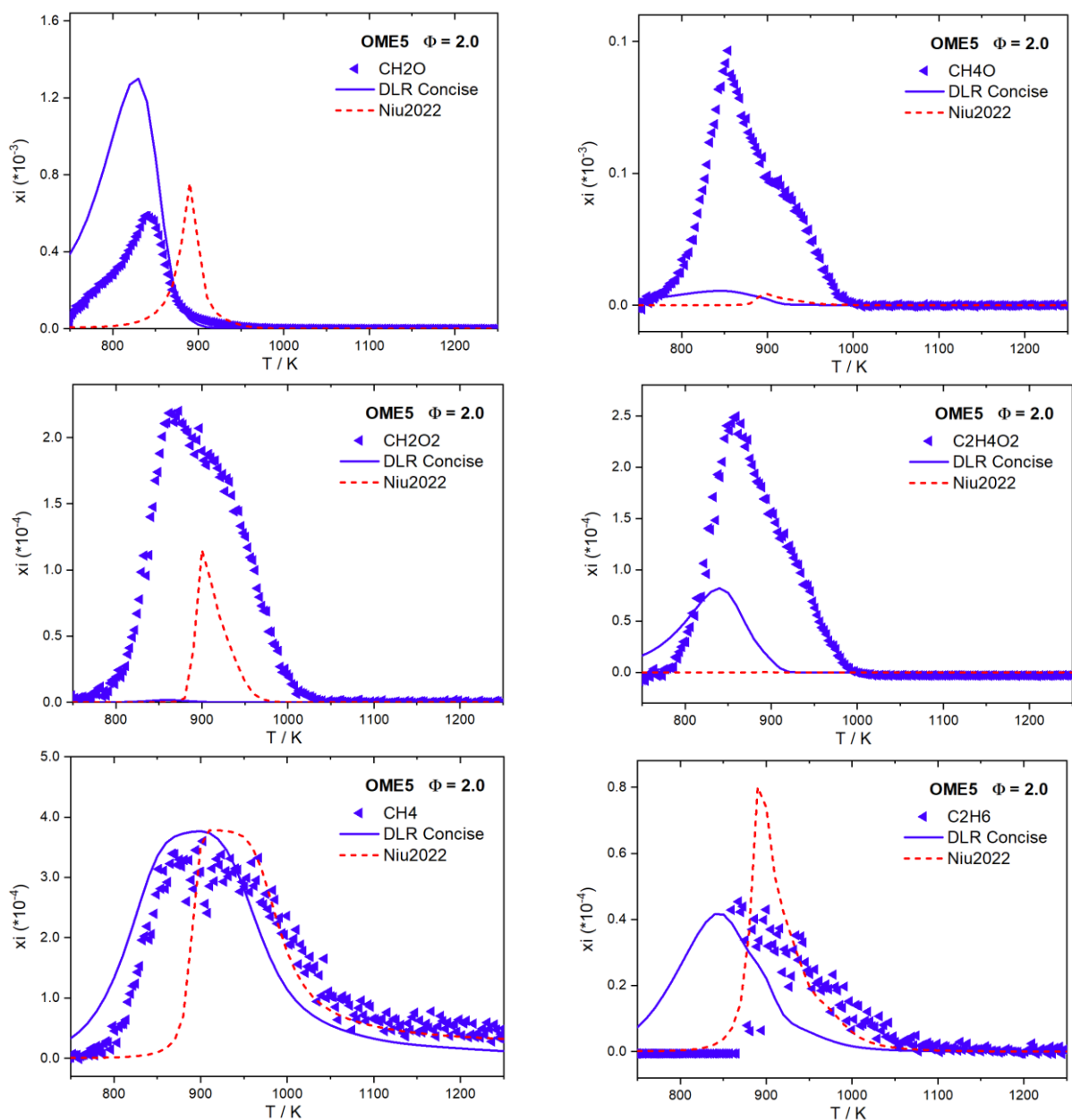
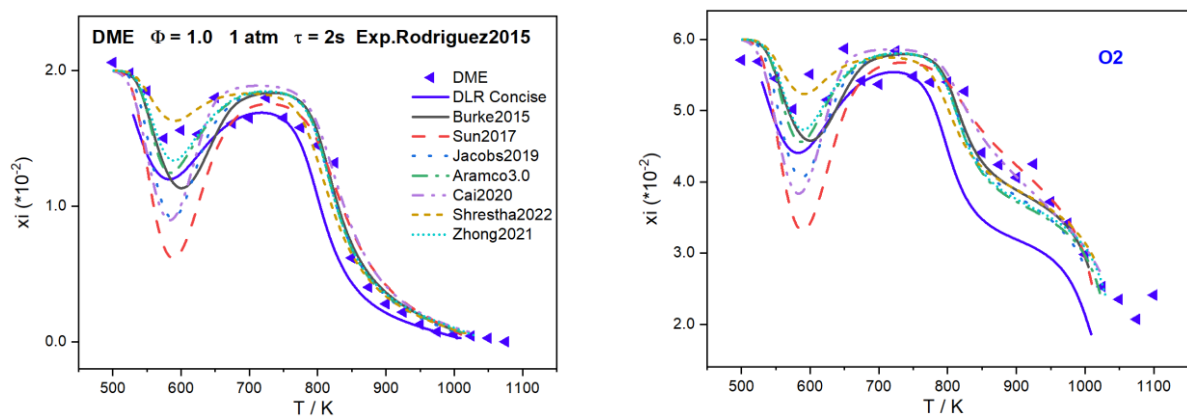


Fig. S89: Predictions of speciation obtained in OME5 in flow reactor with different models [Gaiser2022F].

(2.5) Jet-stirred reactor (JSR)



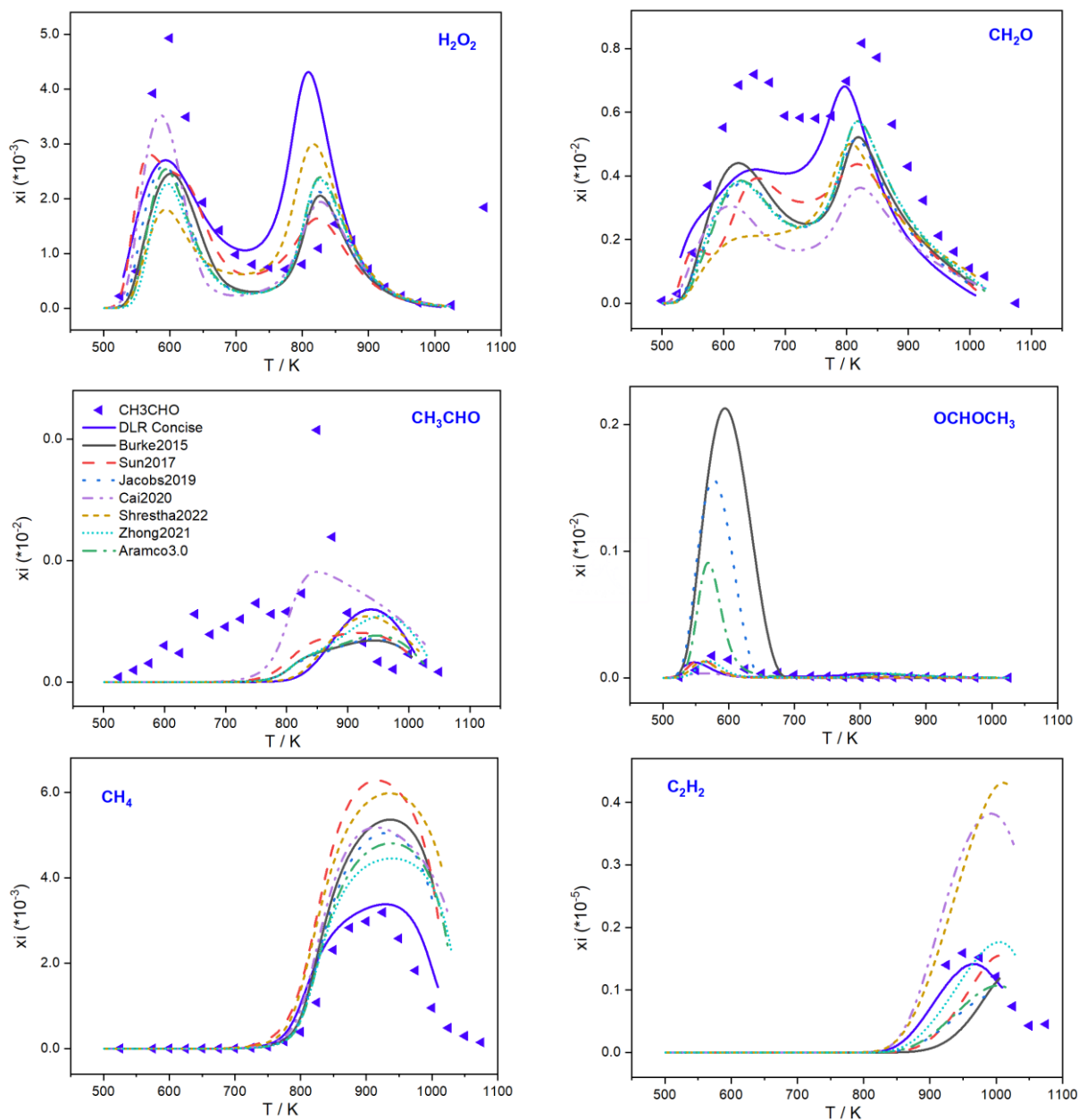
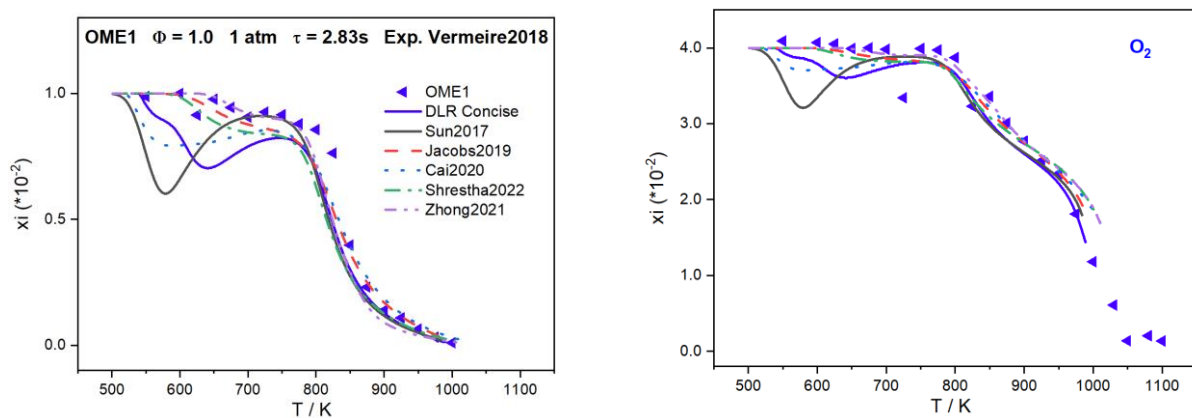


Fig. S90: Predictions of speciation obtained in DME in JSR with different models [Rodriguez2015].



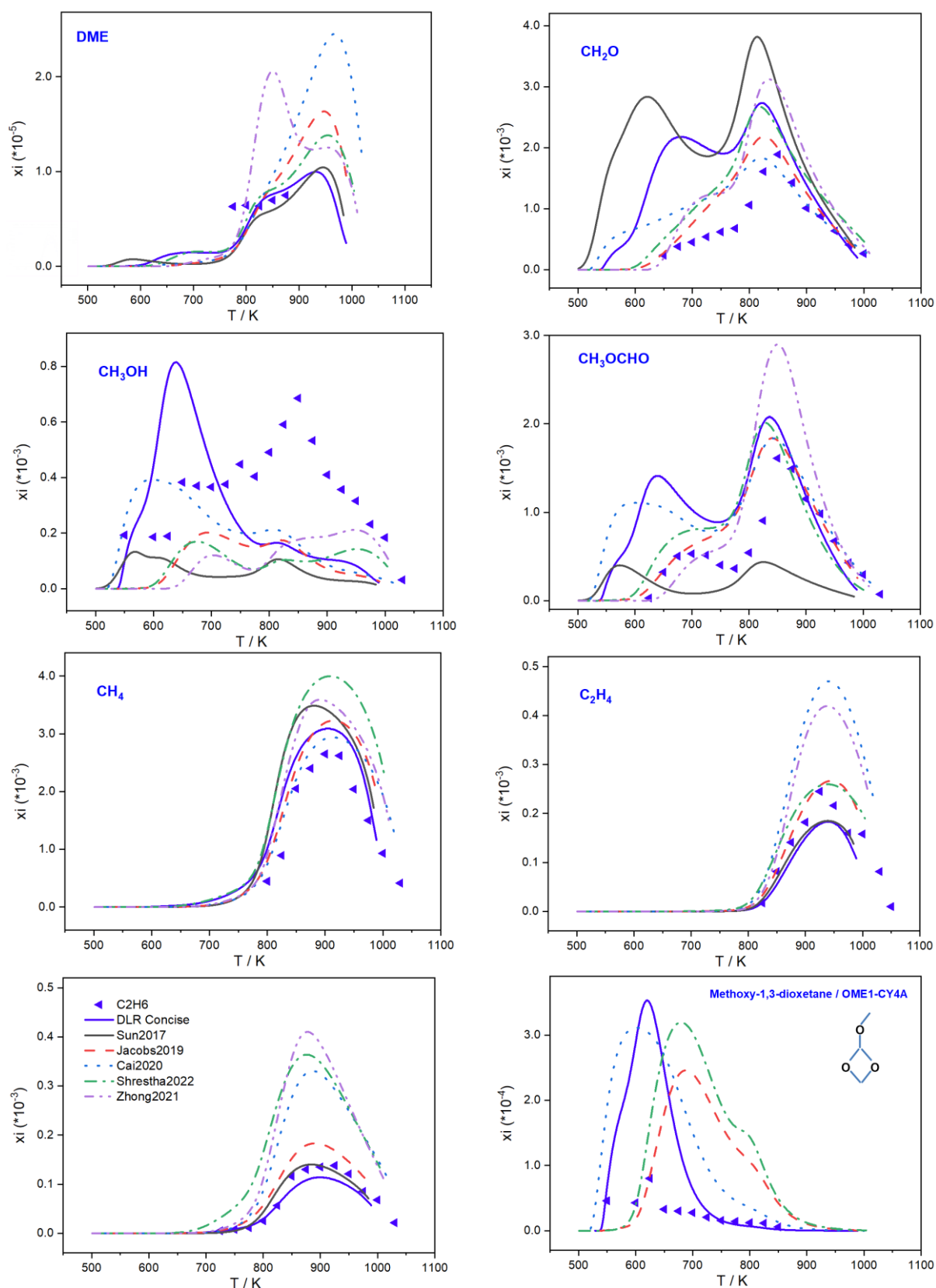


Fig. S91: Predictions of speciation obtained in OME1 in JSR with different models [Vermeire2018].

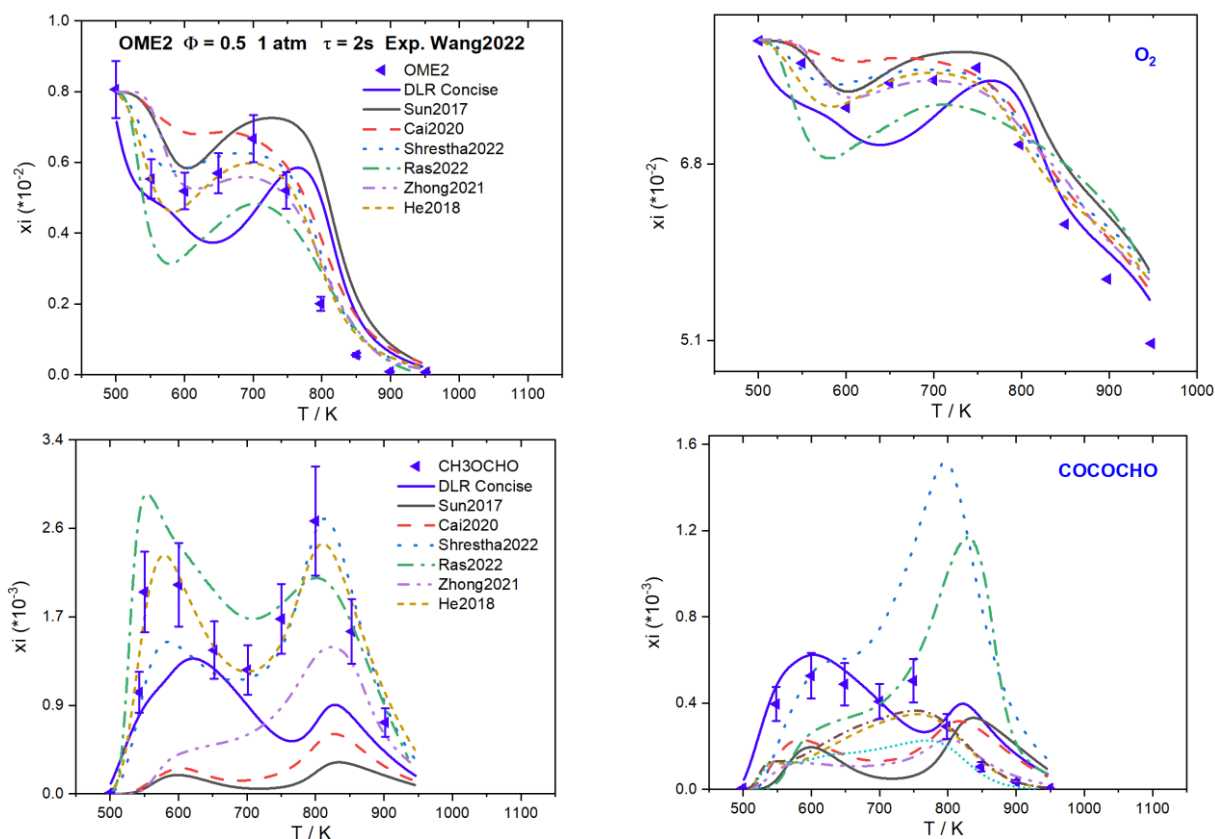


Fig. S92: Predictions of speciation obtained in OME2 in JSR with different models [Wang2022].

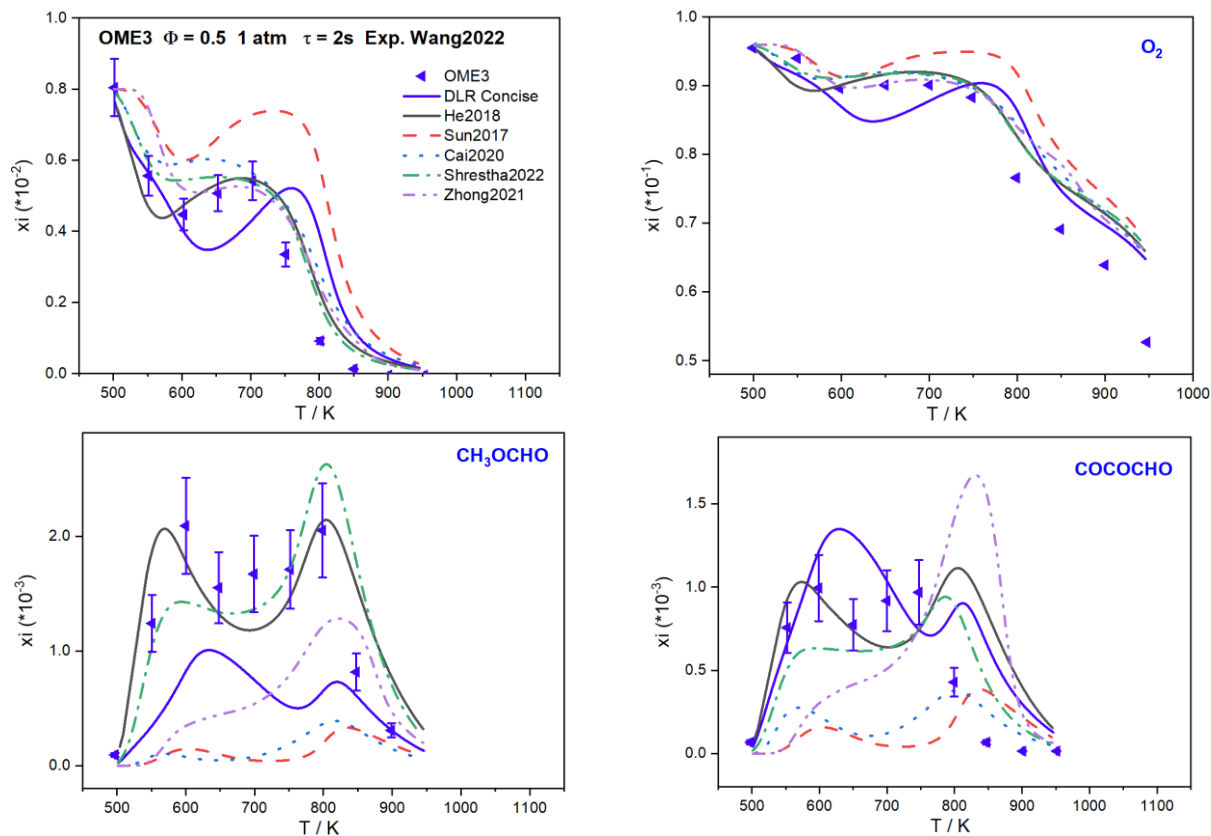


Fig. S93: Predictions of speciation obtained in OME3 in JSR with different models [Wang2022].

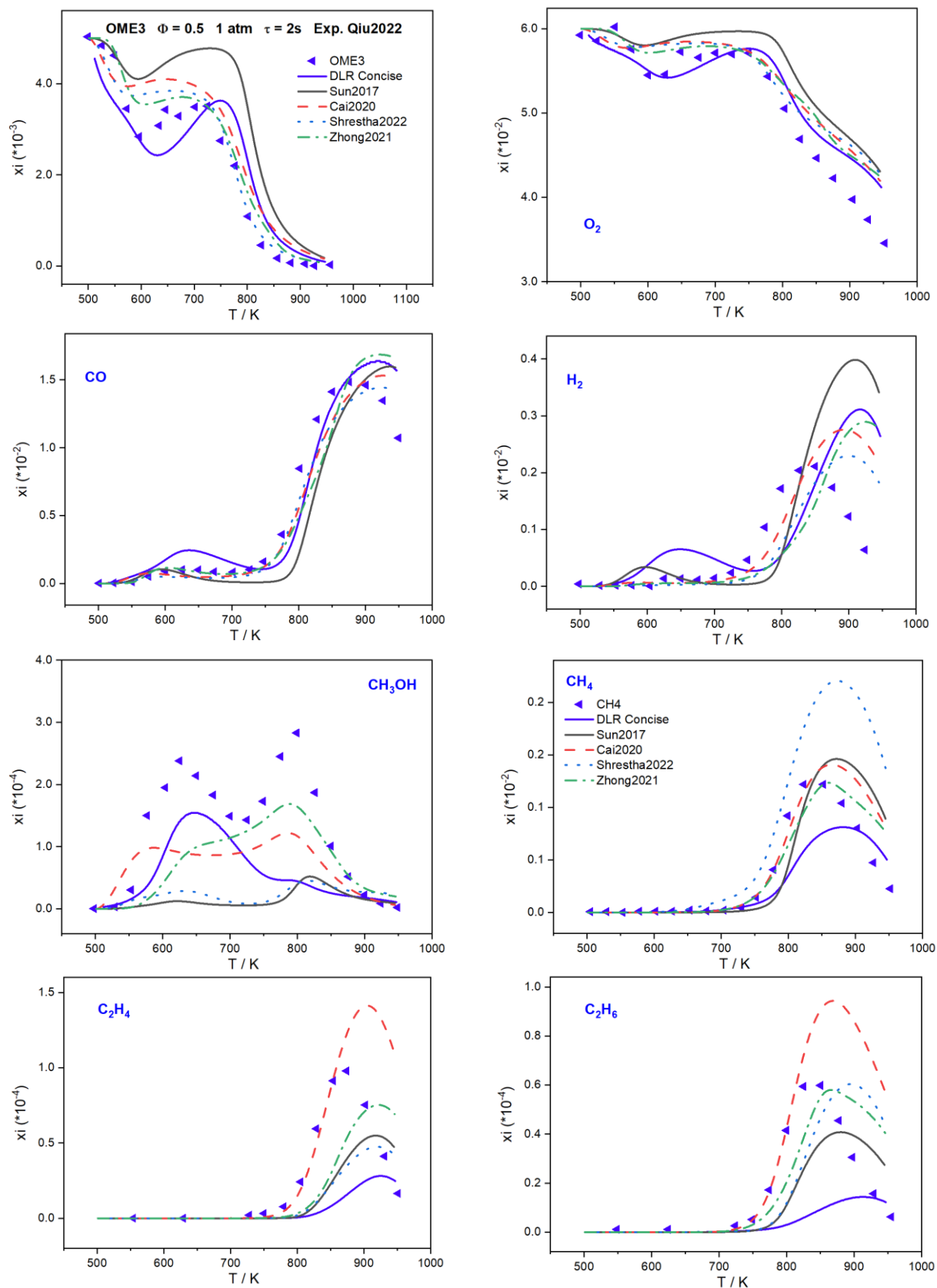


Fig. S94: Predictions of speciation obtained in OME3 in JSR with different models [Qiu2022].

(S3) Direct Comparison of OMEs for visualization

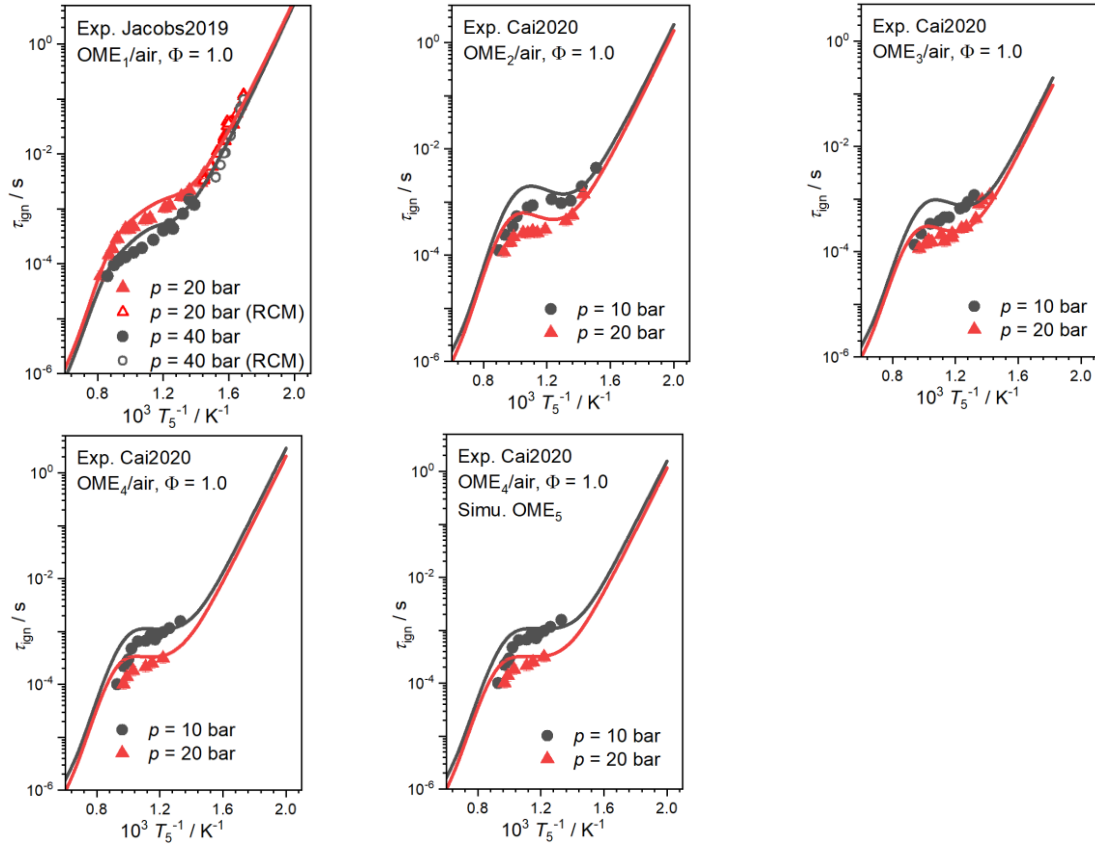
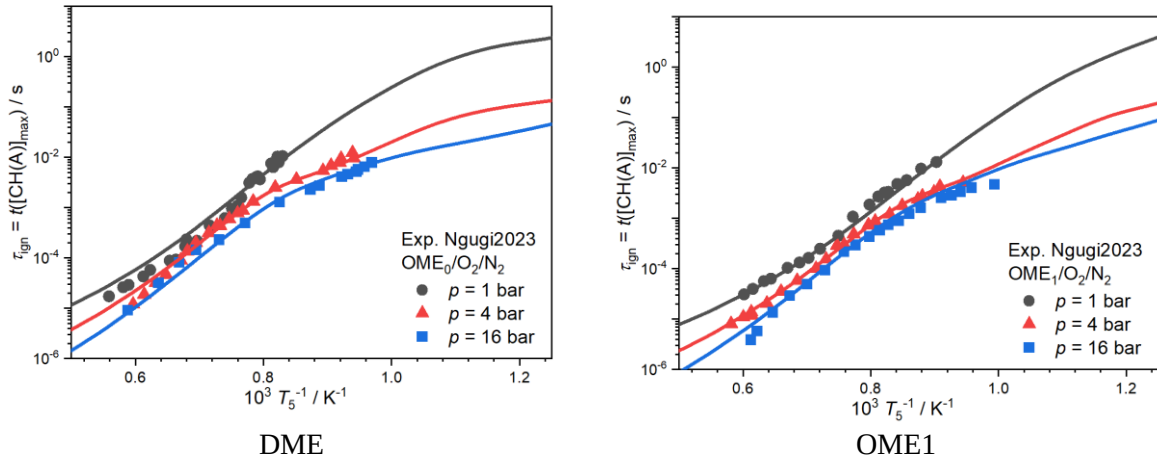


Fig. S95: Ignition delay times of OME1-OME5 from [Jacobs2019, Cai2020]. No experiments are available for OME5, therefore the OME5 model is compared with OME4 experiments.



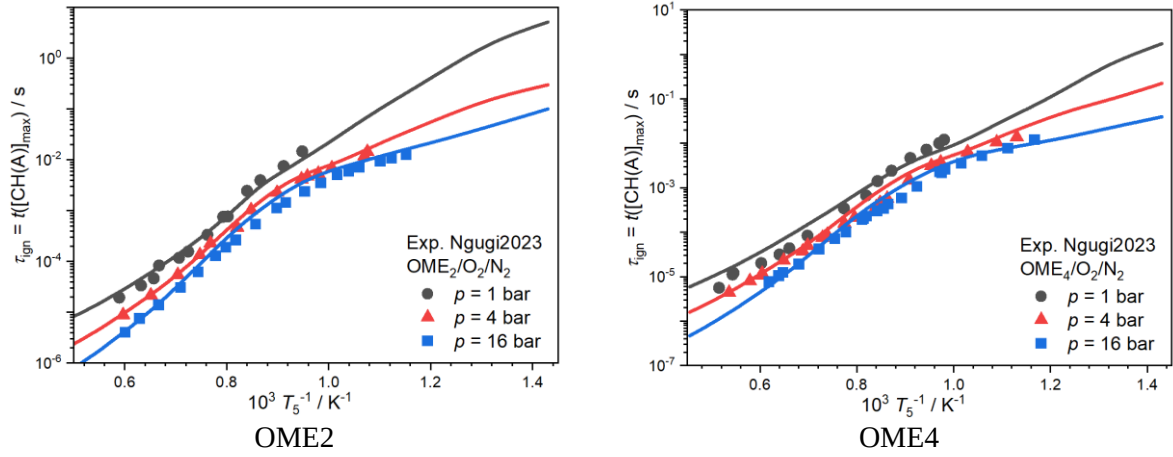


Fig. S96: Ignition delay times of OME0-OME4 from [Ngugi2023].

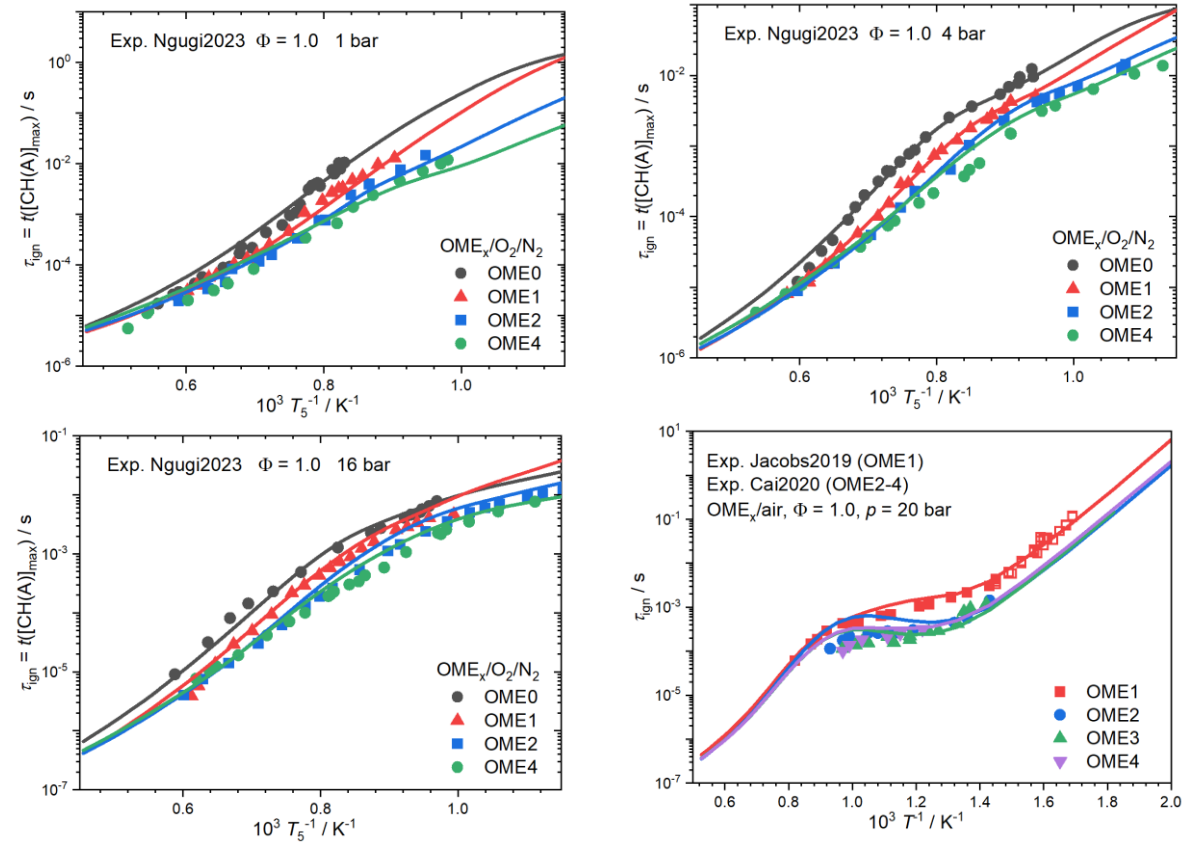
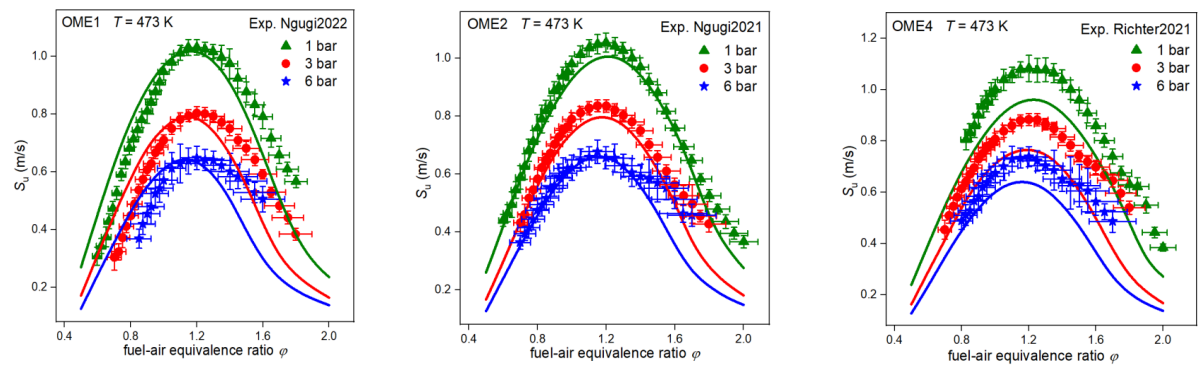


Fig. S97: Relative comparison of DLR Concise model predictions of ignition delay times of OME0-OME4 [Ngugi2023, Cai2020].



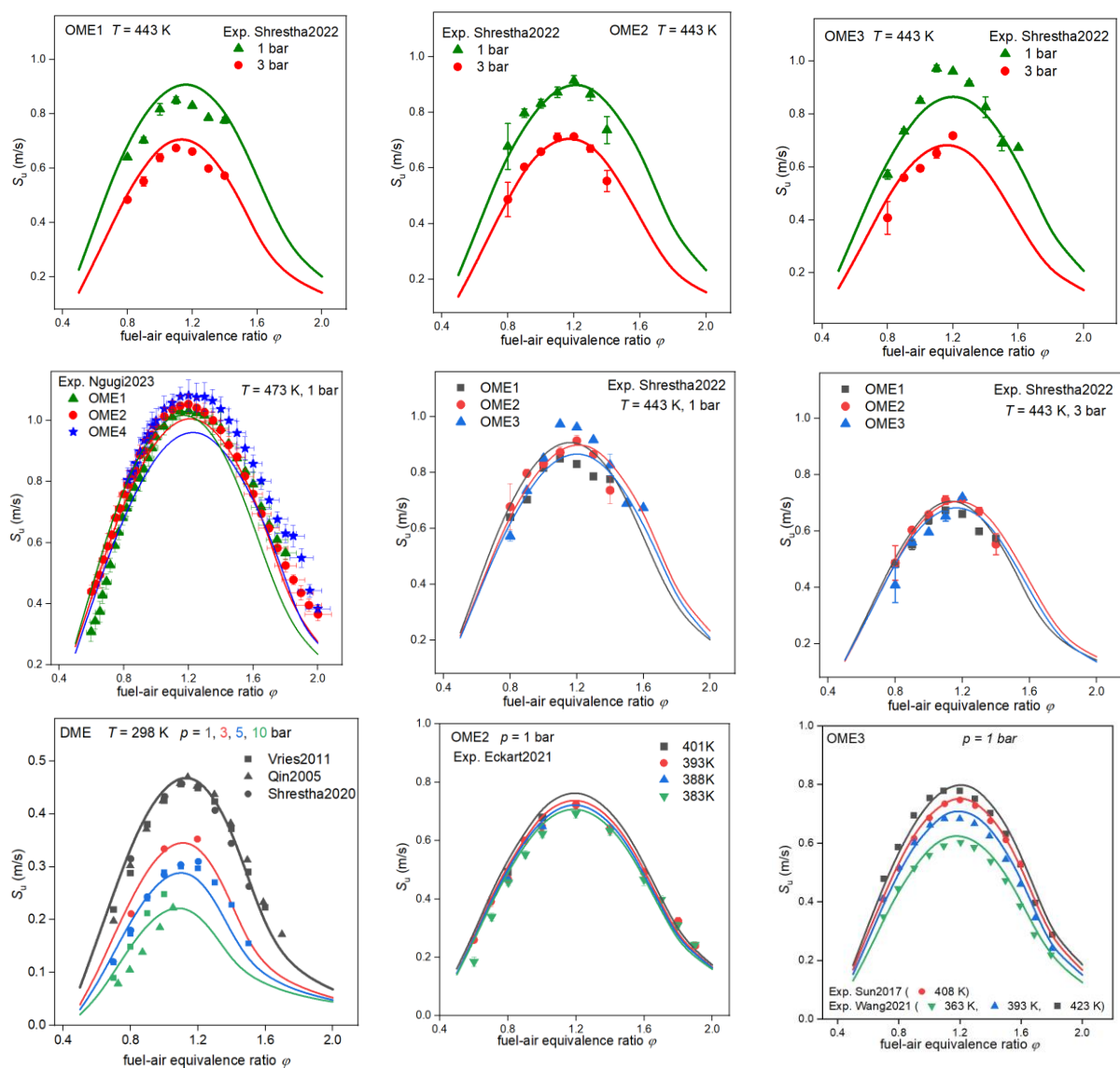
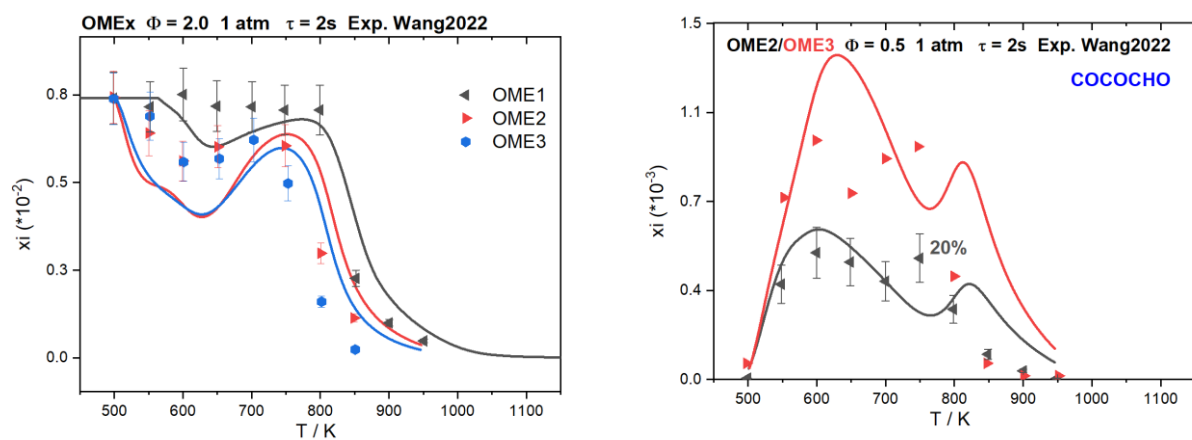


Fig. S98: Comparison of flames speeds as function of OME_x, preheat temperature or pressures.



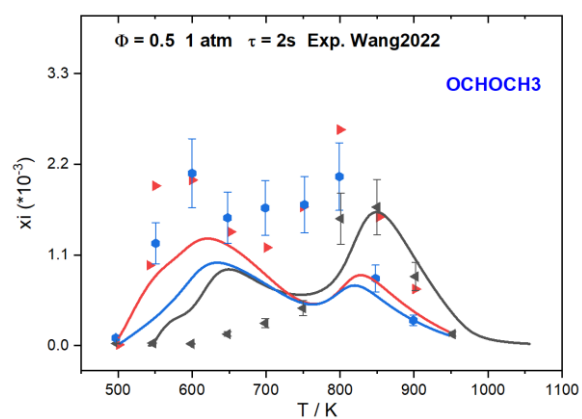


Fig. S99: Comparison of oxidation of OME1 to OME3 in JSR [Wang2022].

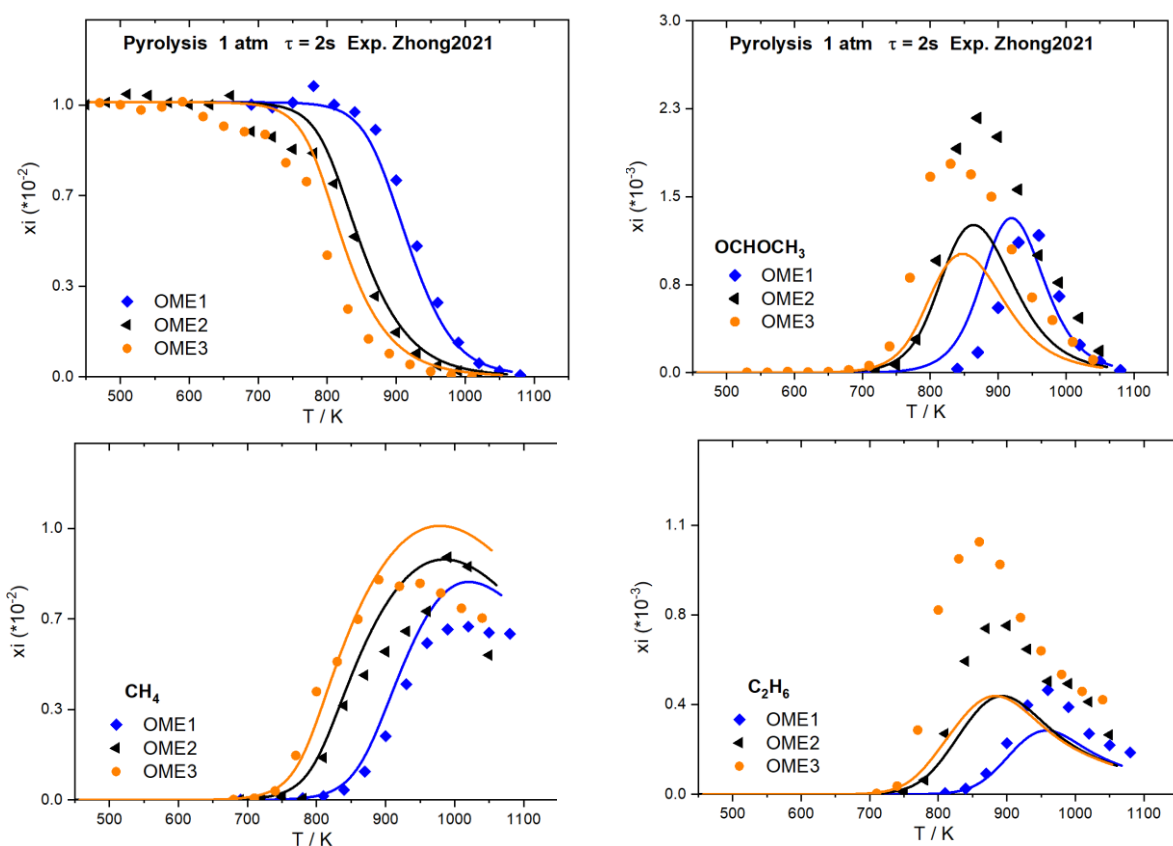


Fig. S100: Comparison of OME1-OME3 pyrolysis in JSR [Zhong2021].

(S4) Reaction routes of OME0-5 (high and low T) in DLR Concise

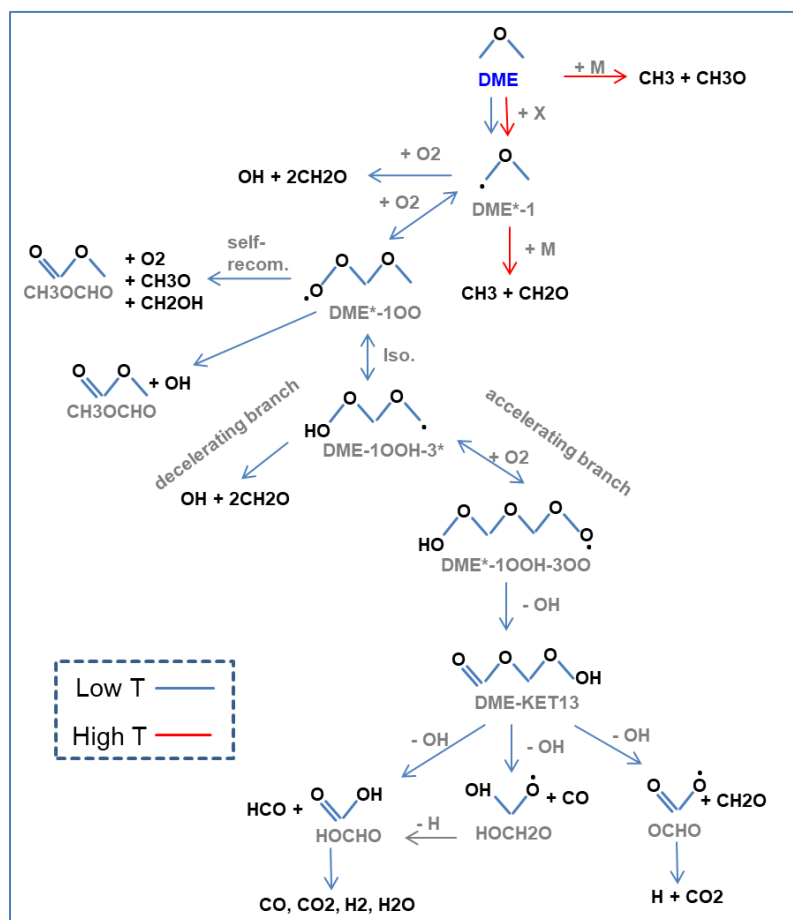


Fig. S101: Reaction routes of DME in DLR Concise.

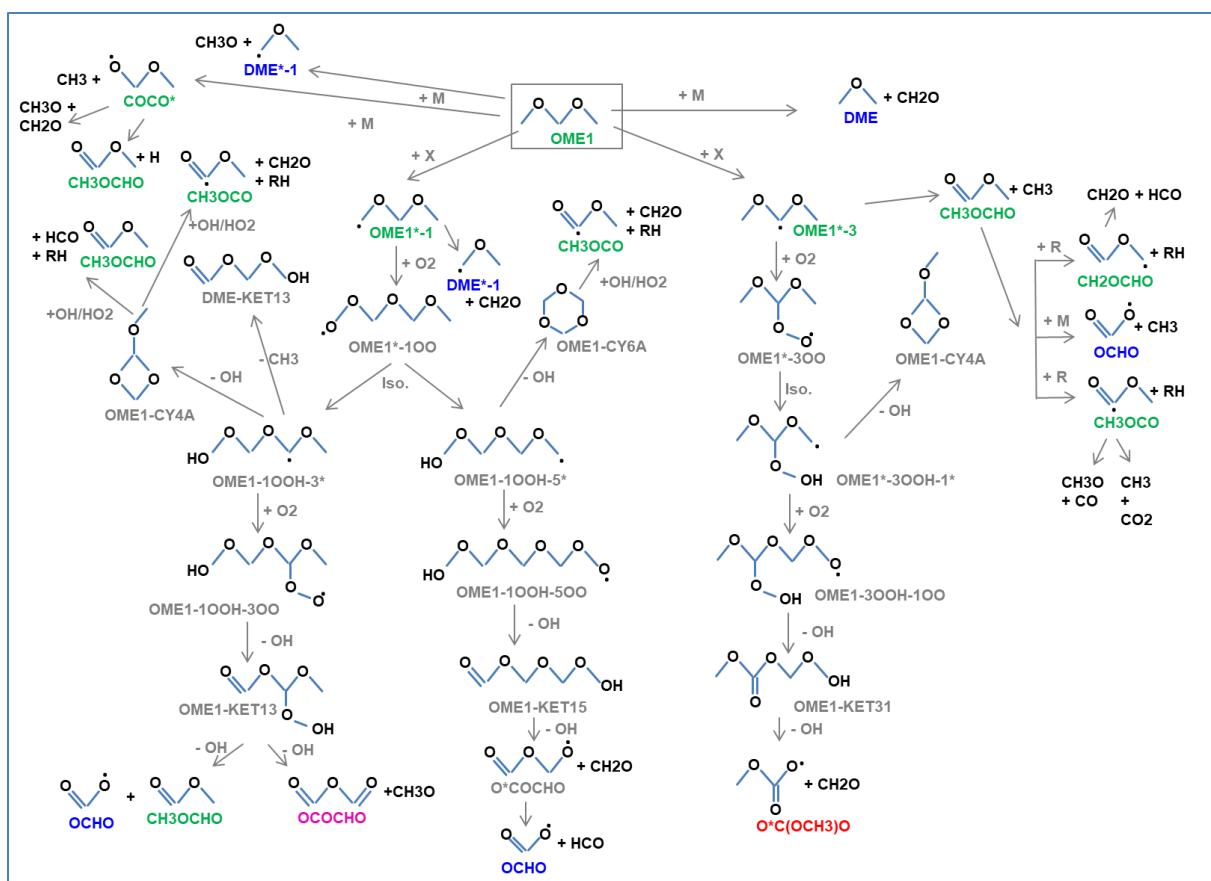


Fig. S102: Reaction routes of OME1 in DLR Concise.

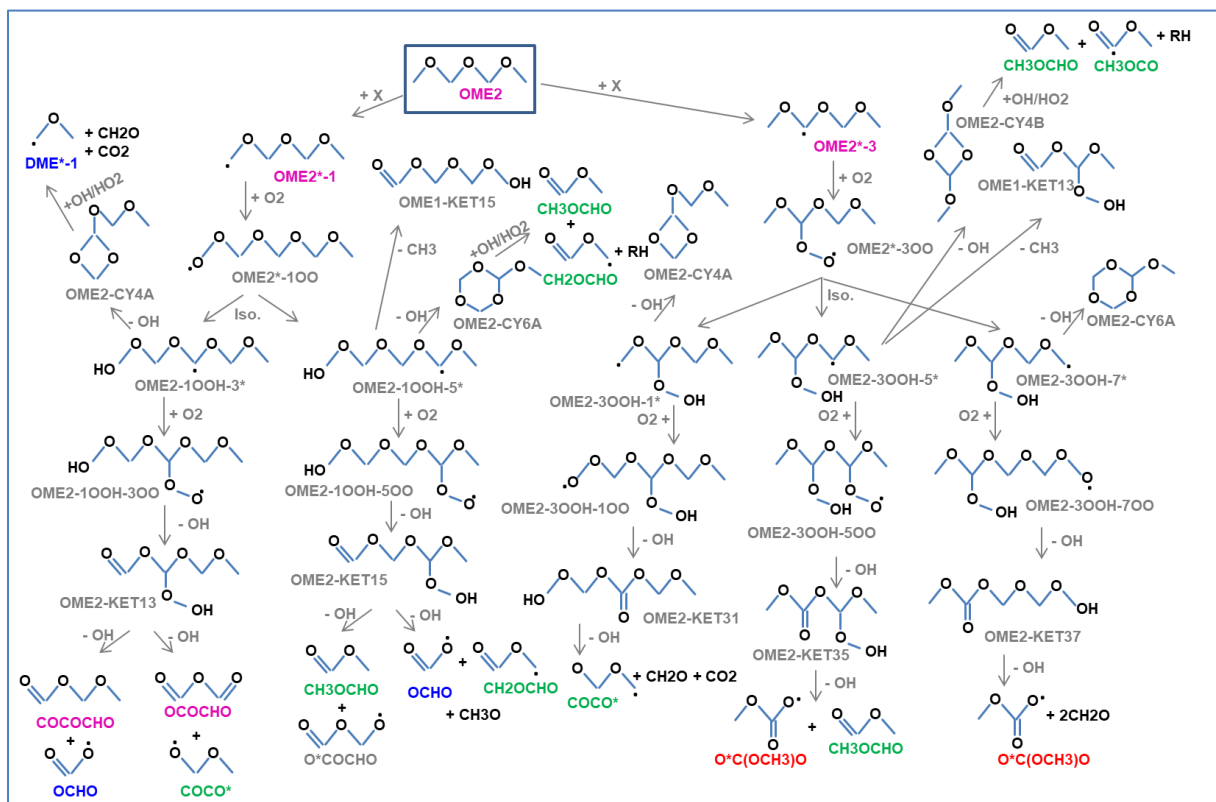
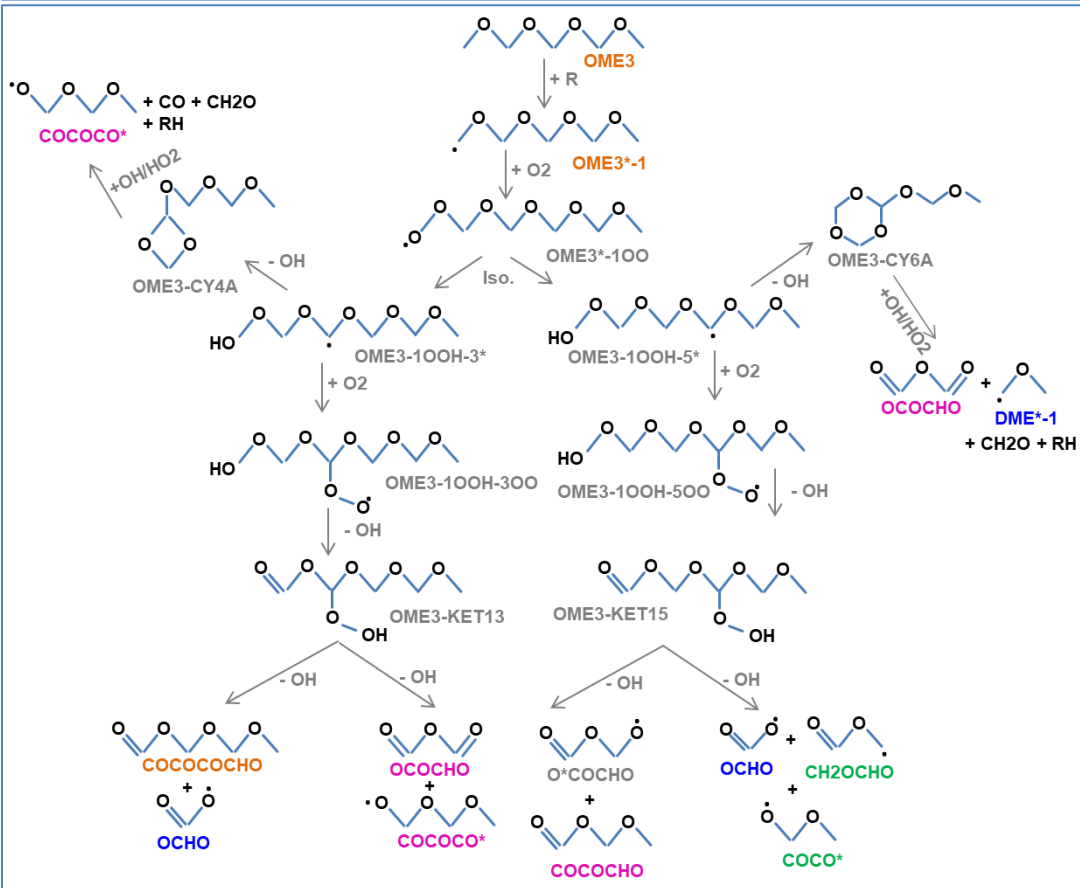
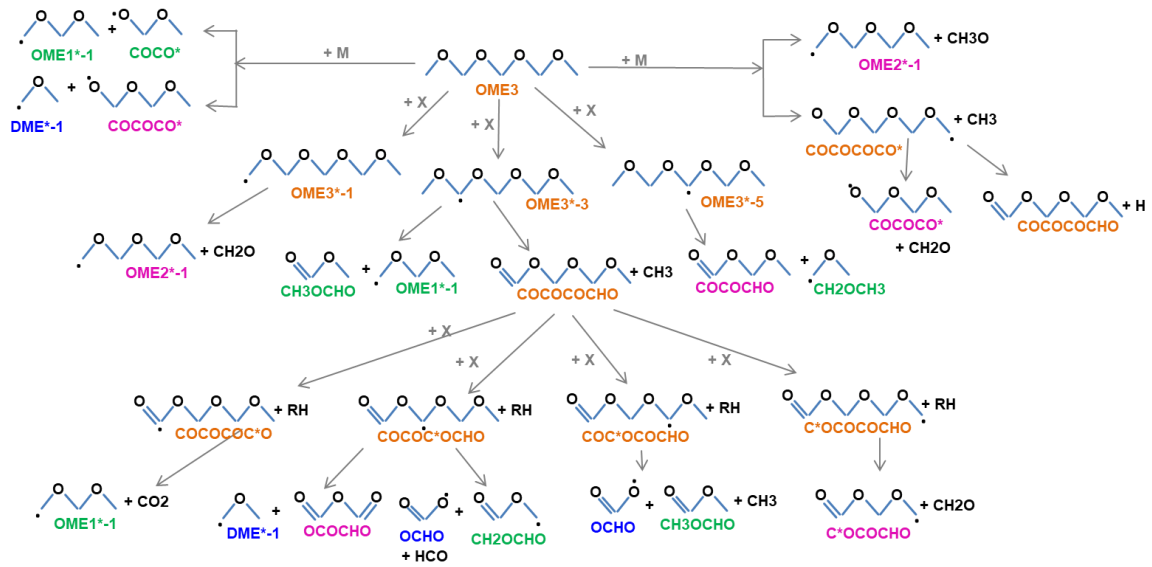


Fig. S103: Reaction routes of OME2 in DLR Concise.

OME₃ = POMDME3 (PolyOxy-Methylene-DiMethyl-Ether-3)



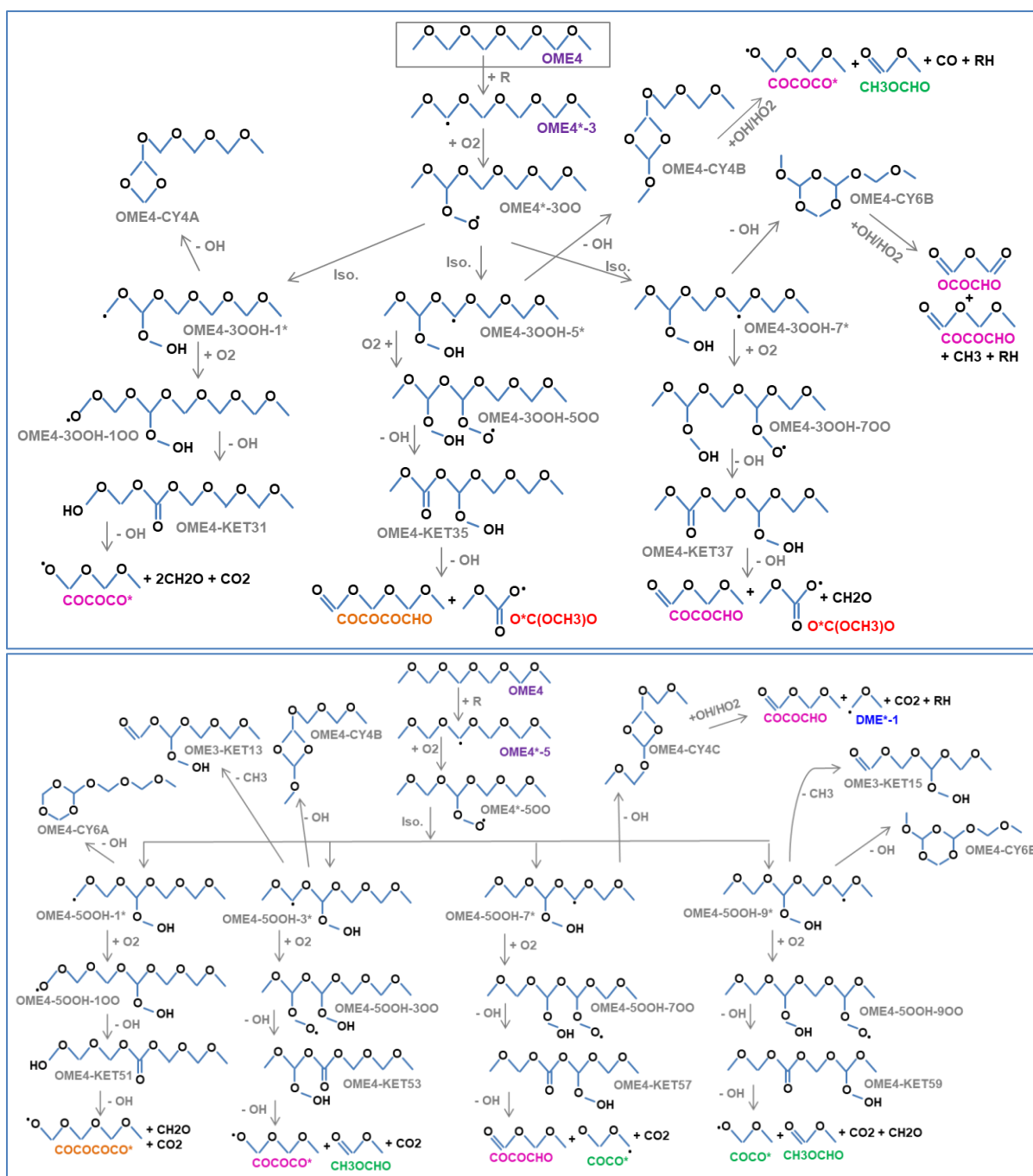
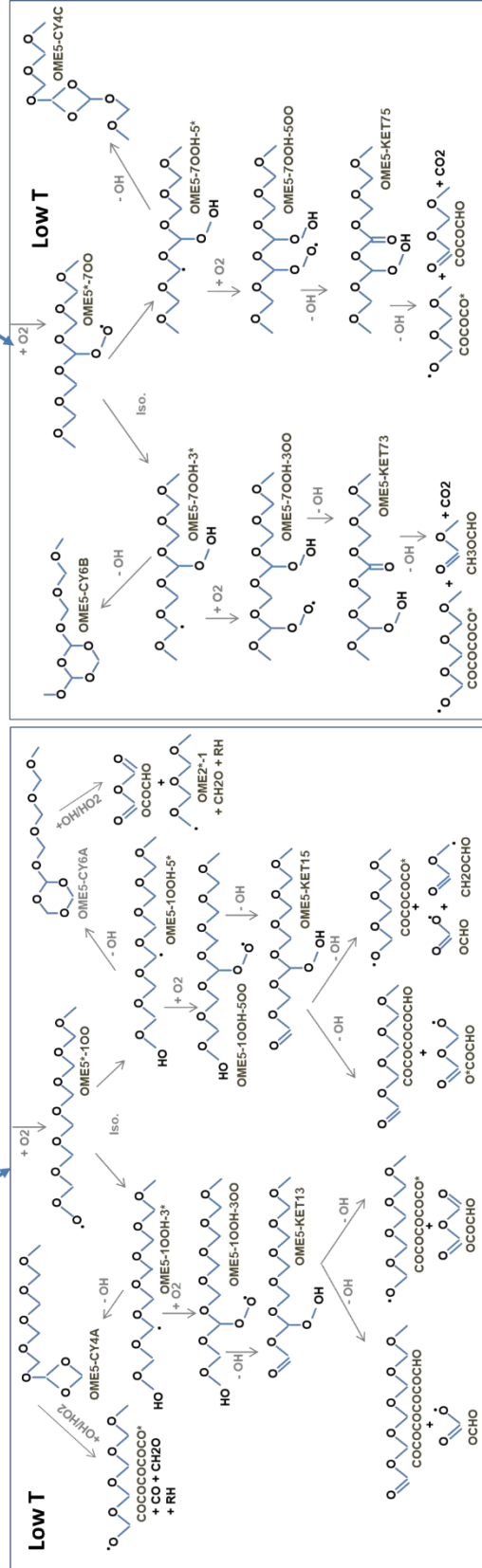
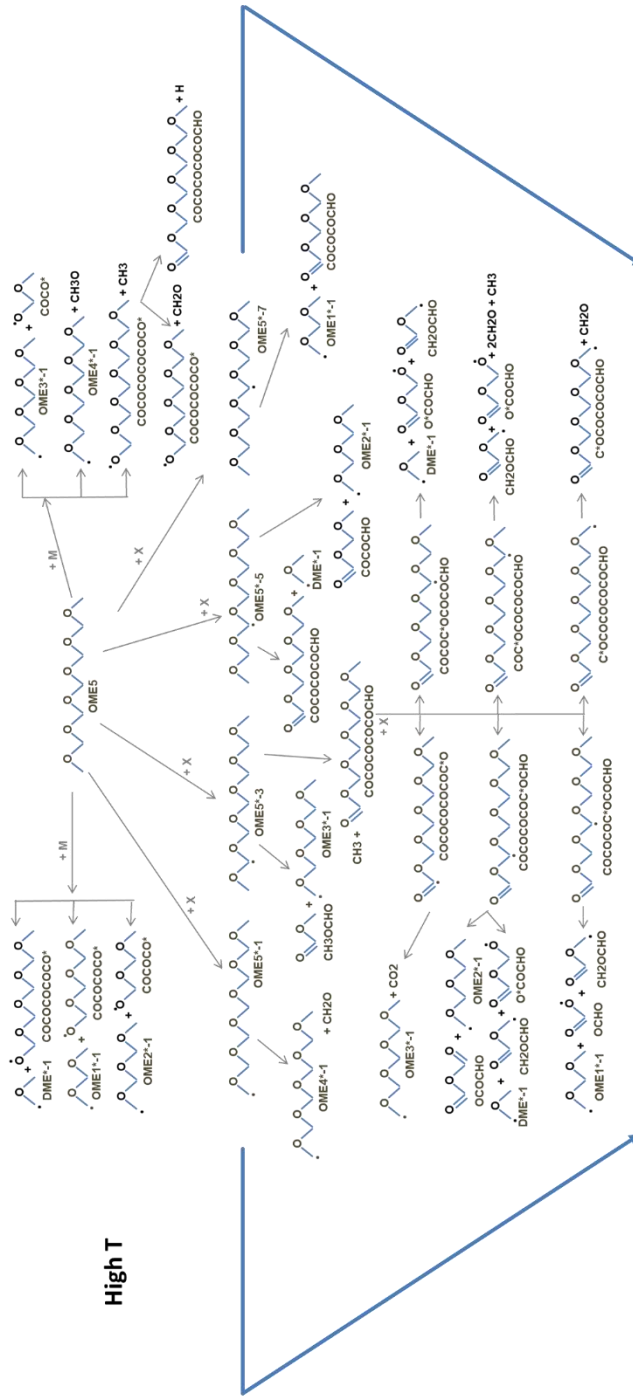


Fig. S105: Reaction routes of OME4 in DLR Concise.



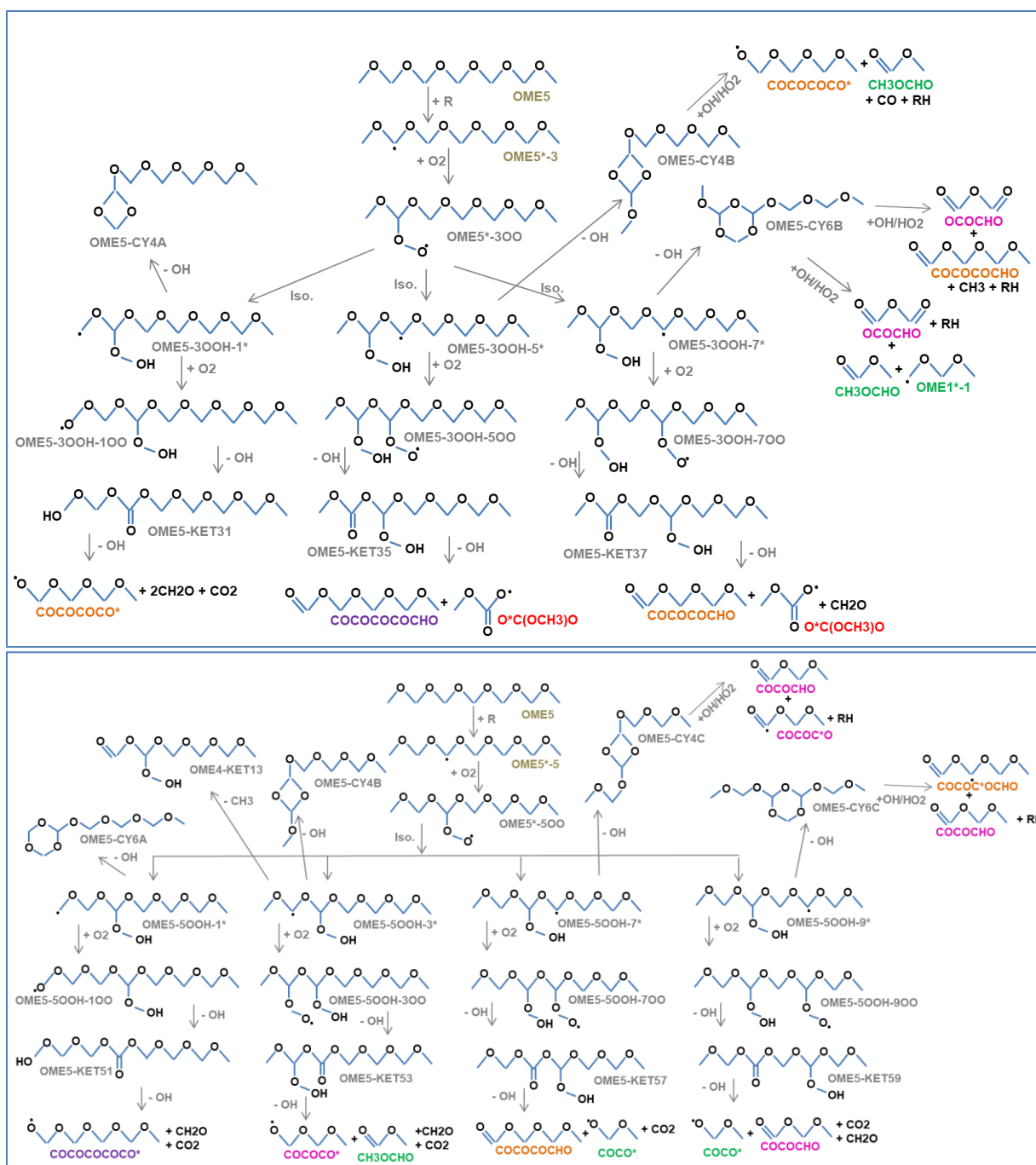
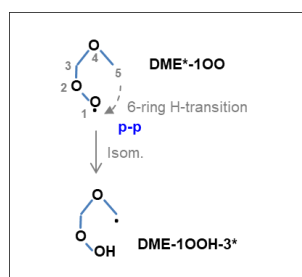
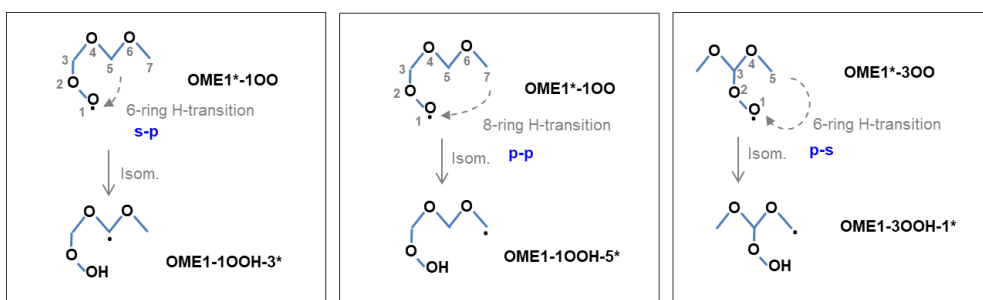


Fig. S106: Reaction routes of OME5 in DLR Concise.

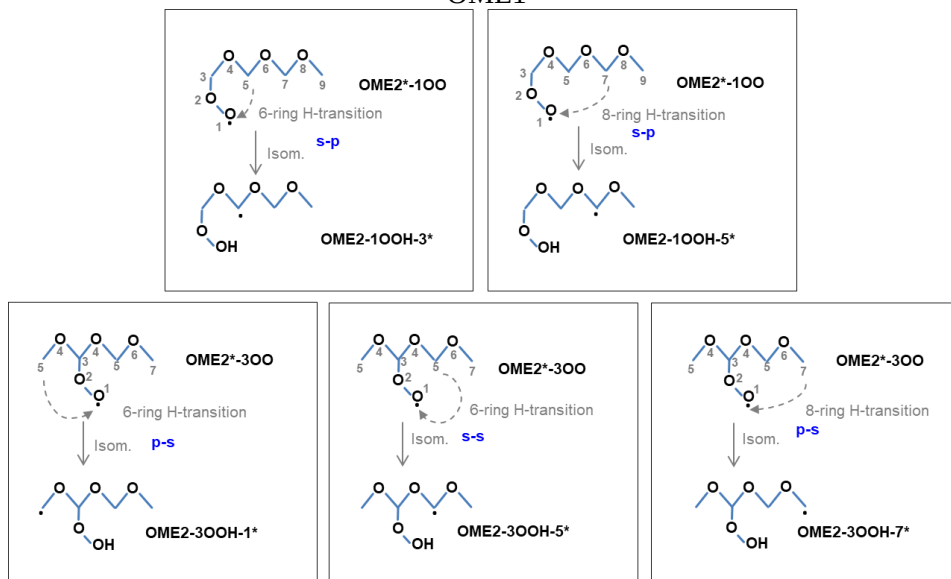
(S5) Intramolecular H-transfer possibilities in OMEs - RO2 to QOOH



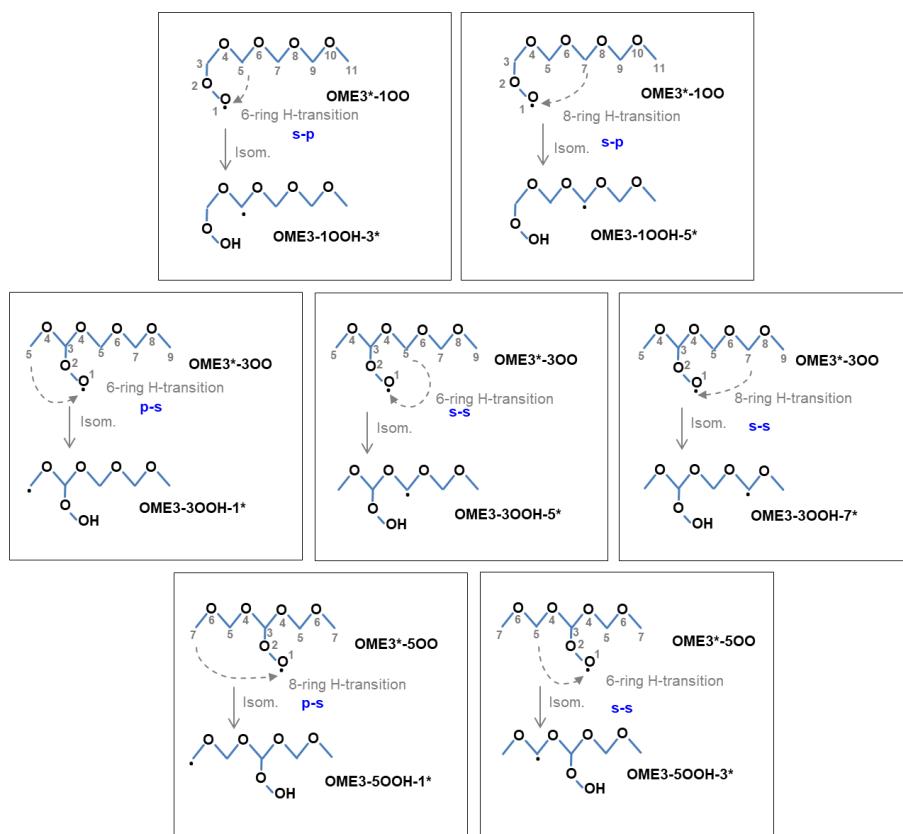
DME



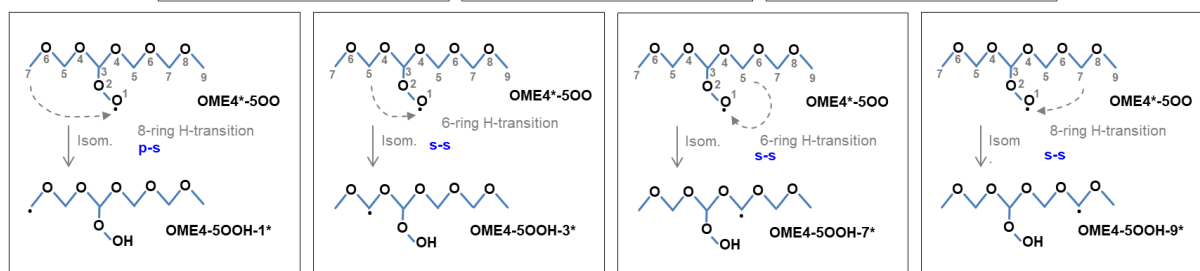
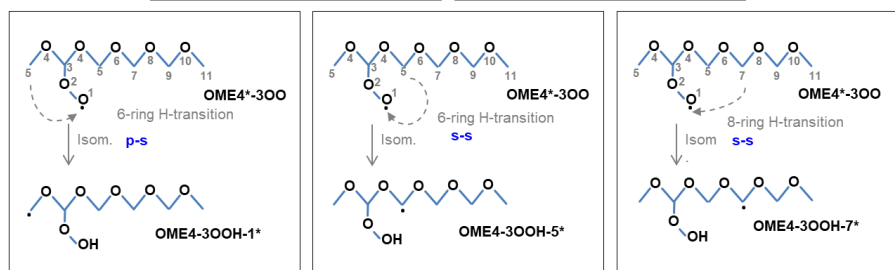
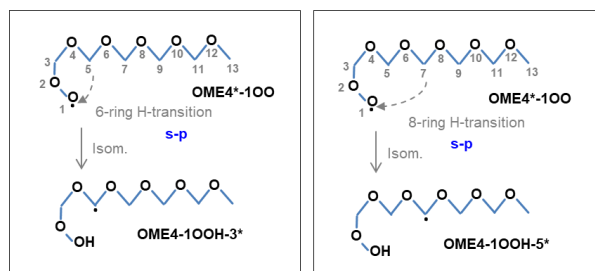
OME1



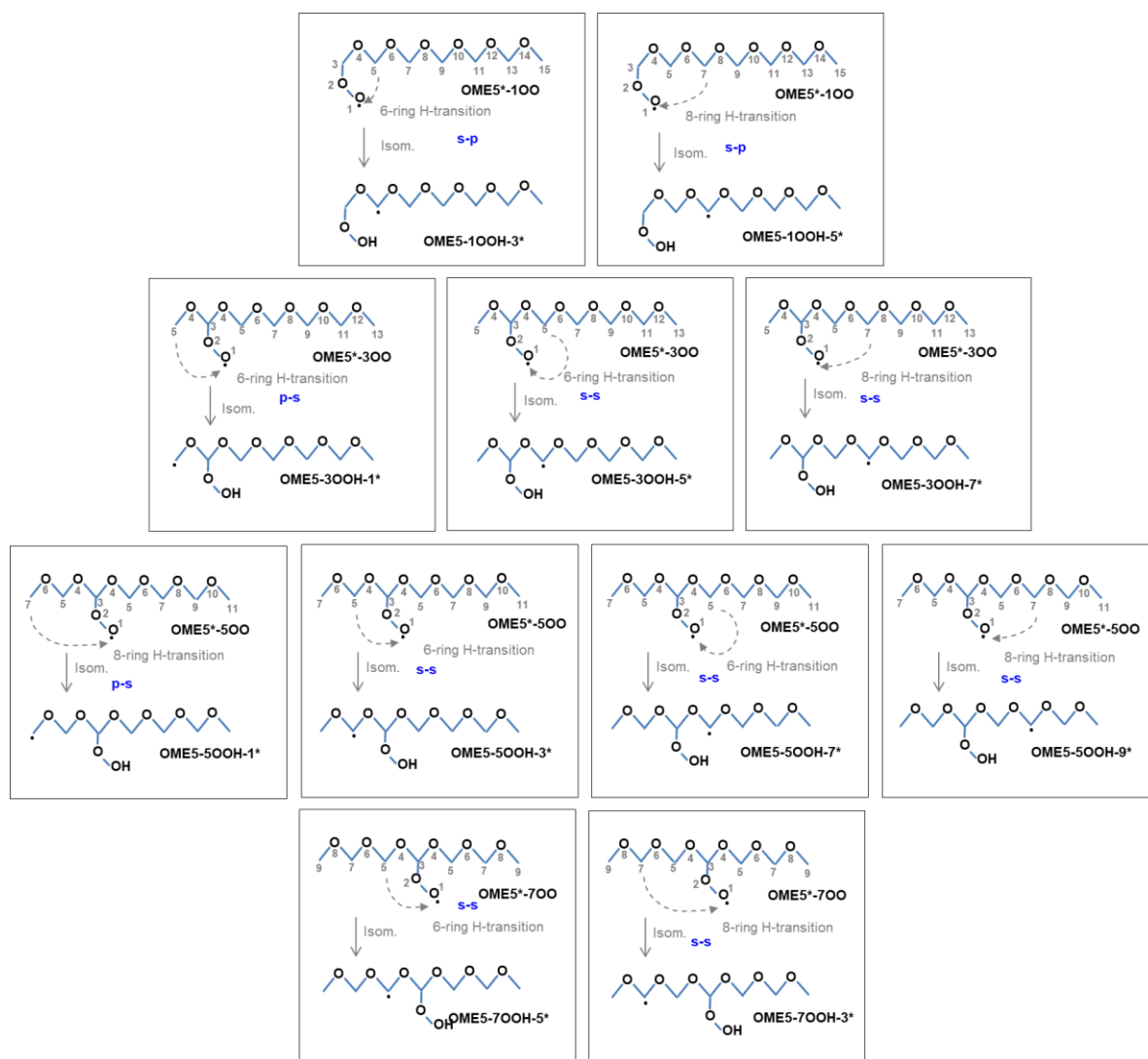
OME2



OME3



OME4



OME5

Fig. S107: Intramolecular H-transfer possibilities in OMEs during isomerization reaction of RO₂ to QOOH

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