An RNN model for biomass gasification chemistry

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Table S1: Biomass composition used to generate the primary product compositions in Step 1 of data generation.

Wood type	Cellulose	Hemicellulose	LIGC	LIGH	LIGO	Ash
Cellulose	1	0	0	0	0	0
Hemicellulose	0	1	0	0	0	0
Lignin 1	0	0	0.54	0.23	0.23	0
Lignin 2	0.0797	0.0349	0.3784	0.3784	0	0.121
Almond shell	0.3724	0.2023	0.0552	0.2865	0.0837	0
Beech wood	0.4537	0.2419	0.0363	0.1021	0.1385	0.0270
Poplar wood	0.4806	0.2611	0.0214	0.0957	0.1325	0.0086
Softwood bark	0.2959	0.1608	0.0707	0.3107	0.1619	0
Beech wood	0.4699	0.2553	0.0347	0.1604	0.0718	0.0080
Maple wood	0.3829	0.2080	0.0511	0.2553	0.0872	0.0155

Table S2: Coefficient of determination (R^2) of the predicted and the test set values for the selected RNN model architectures.

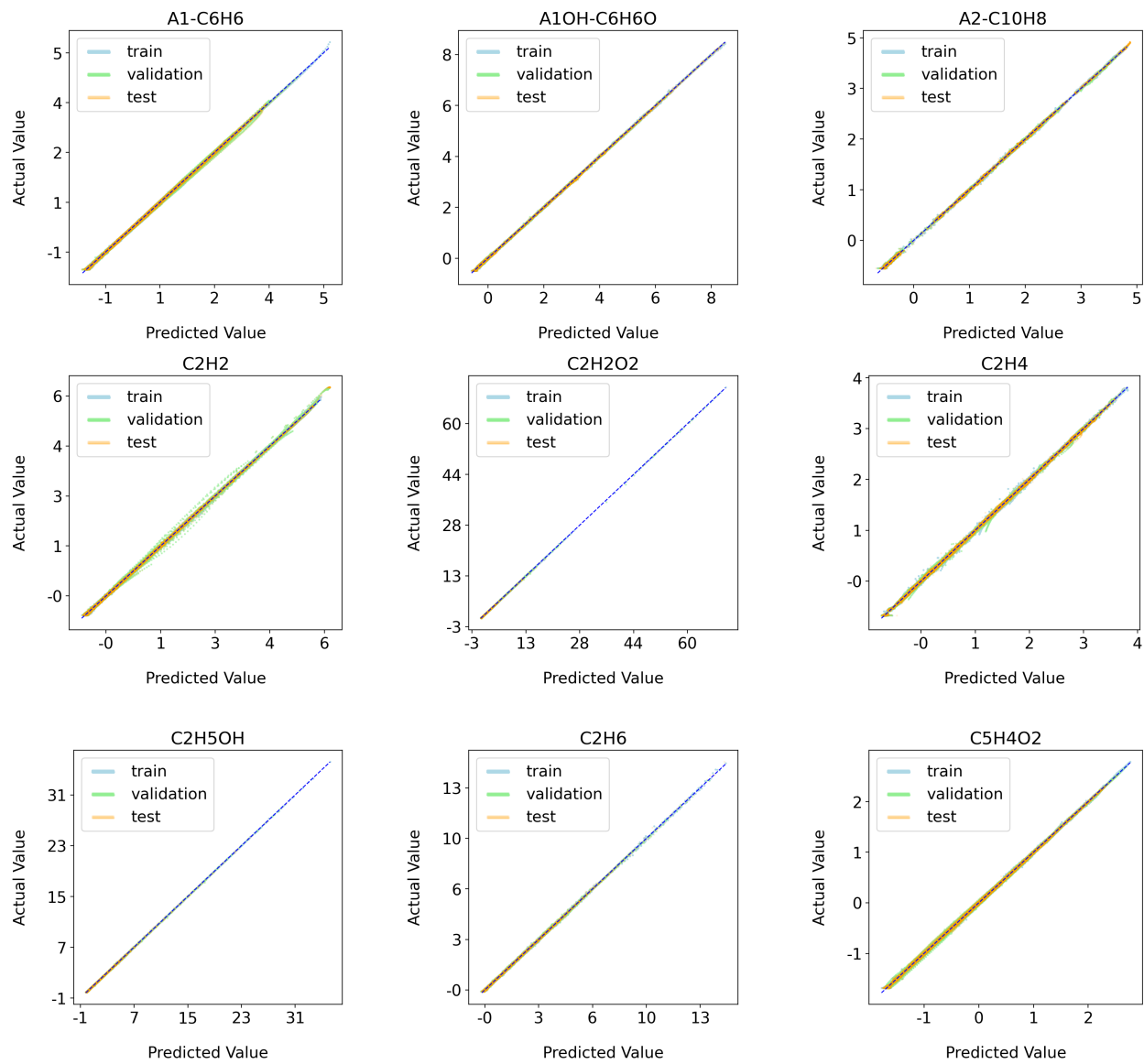| Product species	Model 1	Model 2	Model 3
H2	0.9996	0.9998	0.9999
H2O	0.9997	0.9998	0.9999
CO	0.9996	0.9997	0.9998
CO2	0.9997	0.9997	0.9998
CH2O	0.9993	0.9997	0.9997
CH4	0.9995	0.9996	0.9997
CH3OH	0.9994	0.9996	0.9998
C2H2	0.9993	0.9997	0.9998
CH3CHO	0.9989	0.9998	0.9999
C2H4	0.9995	0.9997	0.9998
C2H6	0.9973	0.9996	0.9998
CH3COCH3	0.9996	0.9998	0.9998
A1-C6H6	0.9995	0.9997	0.9998
C5H6	0.9990	0.9996	0.9997
A2-C10H8	0.9997	0.9998	0.9999
A1OH-C6H6O	0.9995	0.9998	0.9999
LVG-C6H10O5	0.9927	0.9997	0.9999
HMFU-C6H6O3	0.9985	0.9997	0.9999
C5H4O2	0.9997	0.9998	0.9998
C2H2O2	0.9933	0.9996	0.9999
HAA-C2H4O2	0.9929	0.9996	0.9999
XYLOSE	0.9984	0.9997	0.9998
C11H12O4	0.9996	0.9998	0.9998
C8H10O3	0.9995	0.9997	0.9998
COUMARYL	0.9964	0.9997	0.9999
C2H5OH	0.9979	0.9996	0.9998
HCOOH	0.9996	0.9997	0.9998

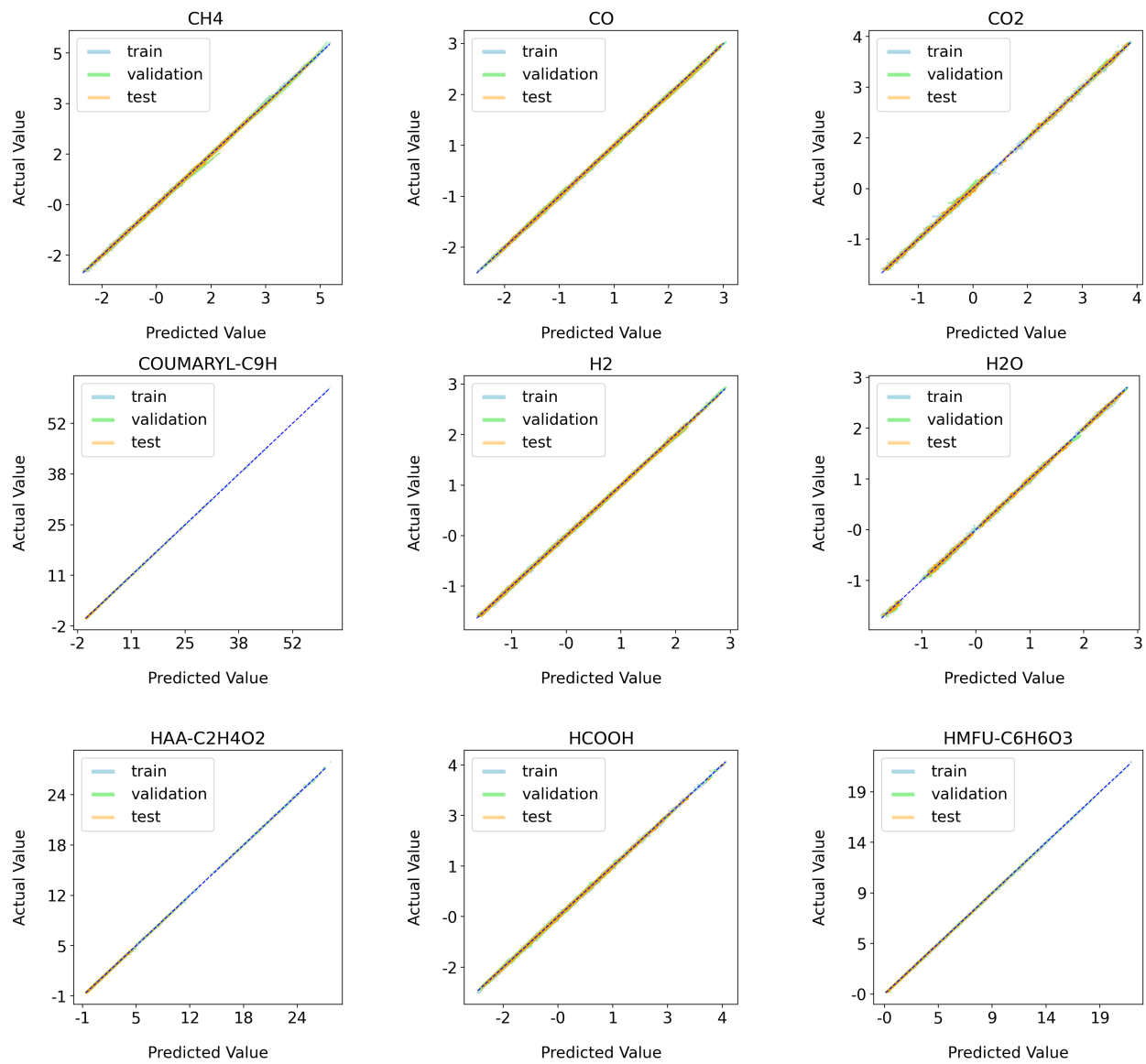Figure S1: Parity plots for individual species using Model 3 (1 to 9).

Figure S2: Parity plots for individual species using Model 3 (10 to 18).
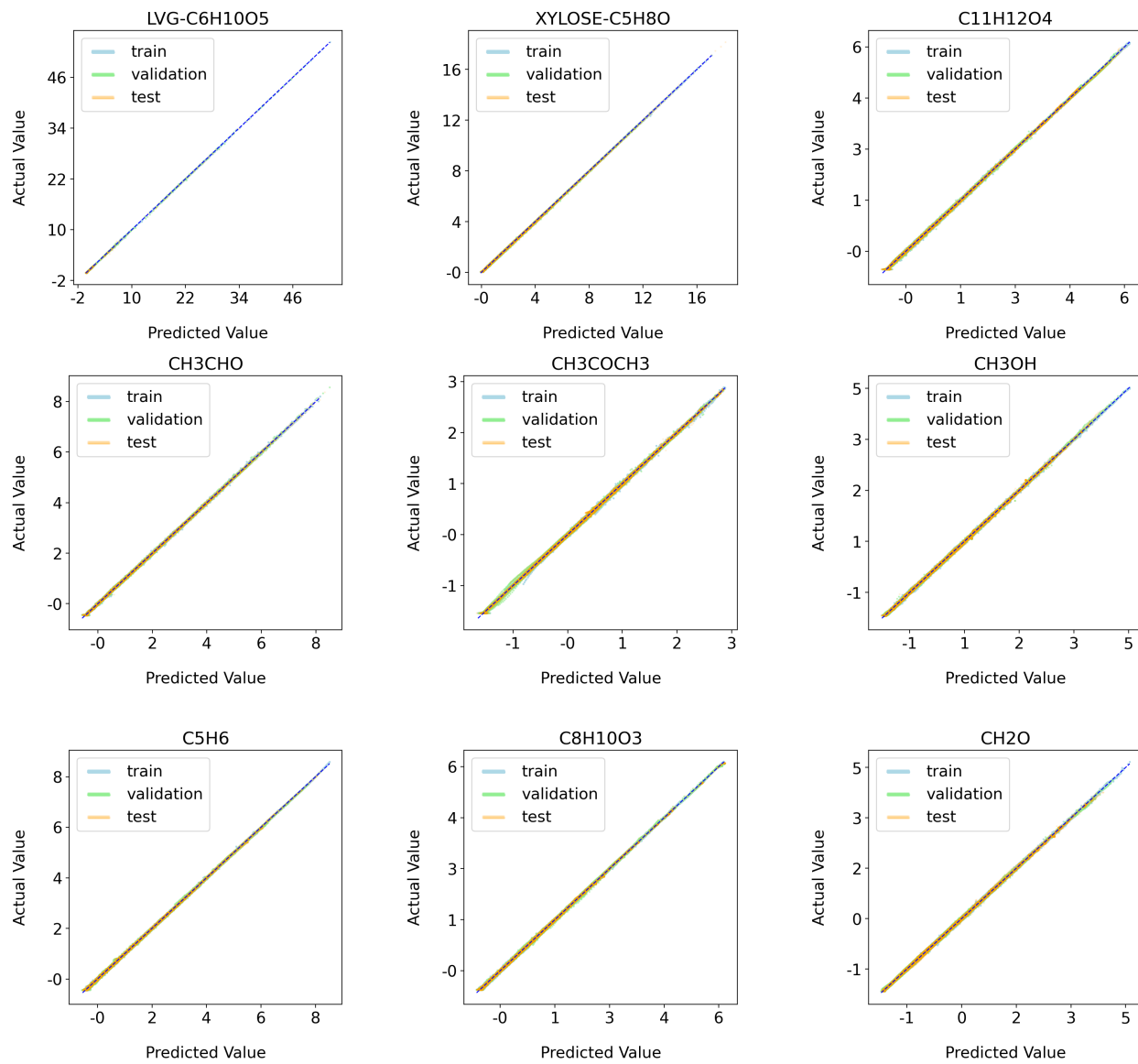
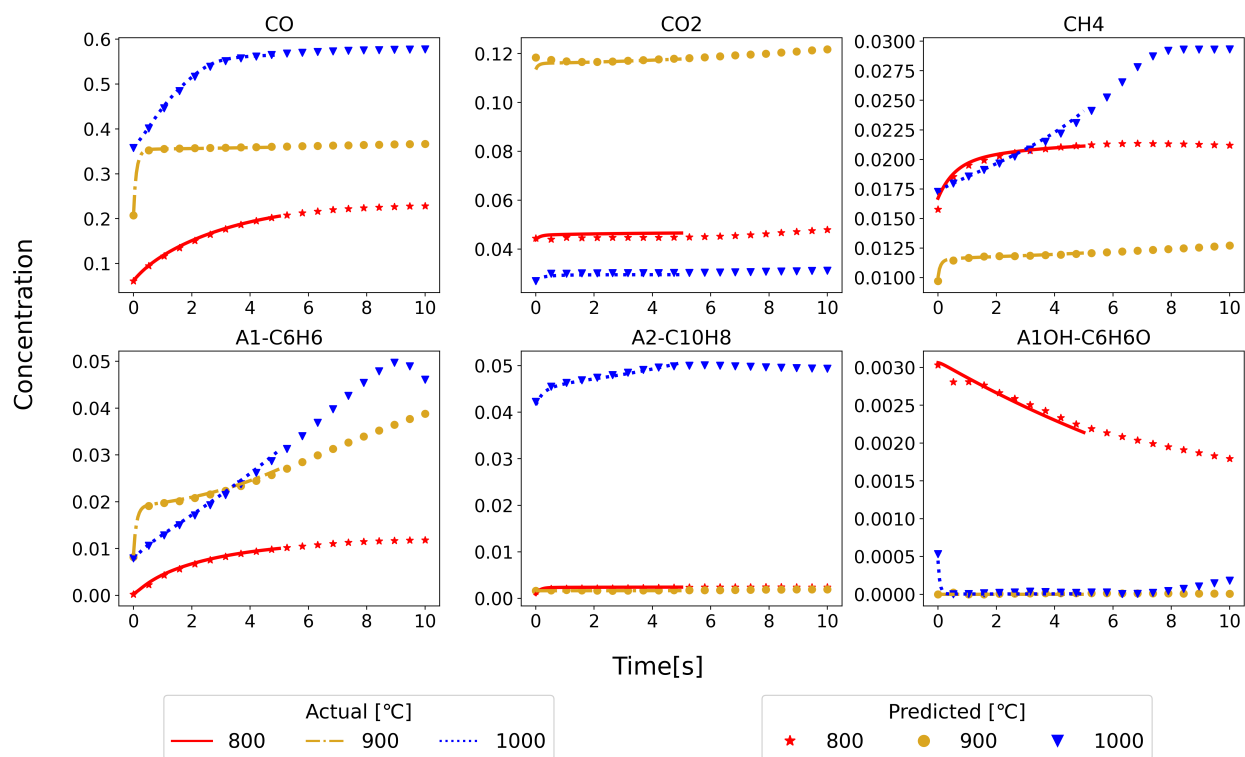Figure S3: Parity plots for individual species using Model 3 (19 to 27).

Figure S4: Comparison of the mass fraction profiles of major chemical species predicted by Model 3 (symbols) and test set data (solid lines) for different temperatures. Model predictions are made till ten seconds and the test data profiles are till five seconds.