Supplementary data

Table S1. Top 5 reactions and their sensitivity coefficients for NO production at lean (ϕ= 0.5) conditions with 0 ppm, 1,000 ppm and 10,000 ppm residual NH_3.

Eq. Ratio	Residual NH_3 [ppm]	Rank	Reaction	Sensitivity Coefficient
Lean (Φ = 0.5)	**0** (Min. NH_3)	1	#72 N+NO=N2+O	0.80493
		2	#161 N2O+O=NO+NO	0.41261
		3	#65 NH+NO=N2O+H	0.1076
		4	#27 HO2+OH<=>H2O+O2	0.10522
		5	#66 NH+NO=N2+OH	0.09251
	1,000	1	#72 N+NO=N2+O	0.05006
		2	#161 N2O+O=NO+NO	0.02593
		3	#65 NH+NO=N2O+H	-0.01987
		4	#27 HO2+OH<=>H2O+O2	-0.00305
		5	#66 NH+NO=N2+OH	0.0044
	10,000 (Max. NH_3)	1	#72 N+NO=N2+O	-0.03282
		2	#161 N2O+O=NO+NO	0.00732
		3	#65 NH+NO=N2O+H	-0.12421
		4	#27 HO2+OH<=>H2O+O2	-0.02643
		5	#66 NH+NO=N2+OH	-3.84E-05

Table S2. Top 5 reactions and their sensitivity coefficients for NO production at rich (ϕ= 2.0) conditions with 0 ppm, 1,000 ppm and 10,000 ppm residual NH_3.

Eq. Ratio	Residual NH_3 [ppm]	Rank	Reaction	Sensitivity Coefficient
Rich (Φ = 2.0)	**0** (Min. NH_3)	1	#1 H2+M<=>H+H+M	0.43829
		2	#166 NH2+NH2=N2H2+H2	0.28185
		3	#2 H2+O<=>H+OH	0.22019
		4	#24 HO2+H<=>OH+OH	0.22388
		5	#25 HO2+H<=>H2+O2	0.18024
	1,000	1	#1 H2+M<=>H+H+M	-0.38361
		2	#166 NH2+NH2=N2H2+H2	-0.24769
		3	#2 H2+O<=>H+OH	-0.20675
		4	#24 HO2+H<=>OH+OH	-0.19087
		5	#25 HO2+H<=>H2+O2	-0.15523
	10,000 (Max. NH_3)	1	#1 H2+M<=>H+H+M	-0.43747
		2	#166 NH2+NH2=N2H2+H2	-0.28902
		3	#2 H2+O<=>H+OH	-0.24706
		4	#24 HO2+H<=>OH+OH	-0.22443
		5	#25 HO2+H<=>H2+O2	-0.18247

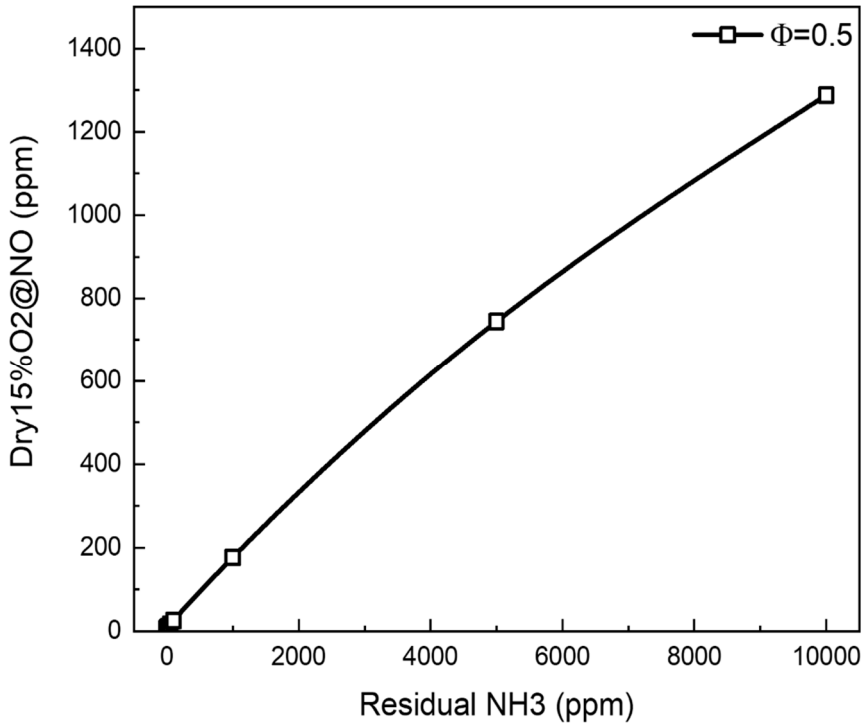

Figure S1. Final NO mole fraction as a function of residual NH_3 in the low-concentration (0–100 ppm) range under fuel-lean (ϕ= 0.5) conditions at 20 atm and 673 K.

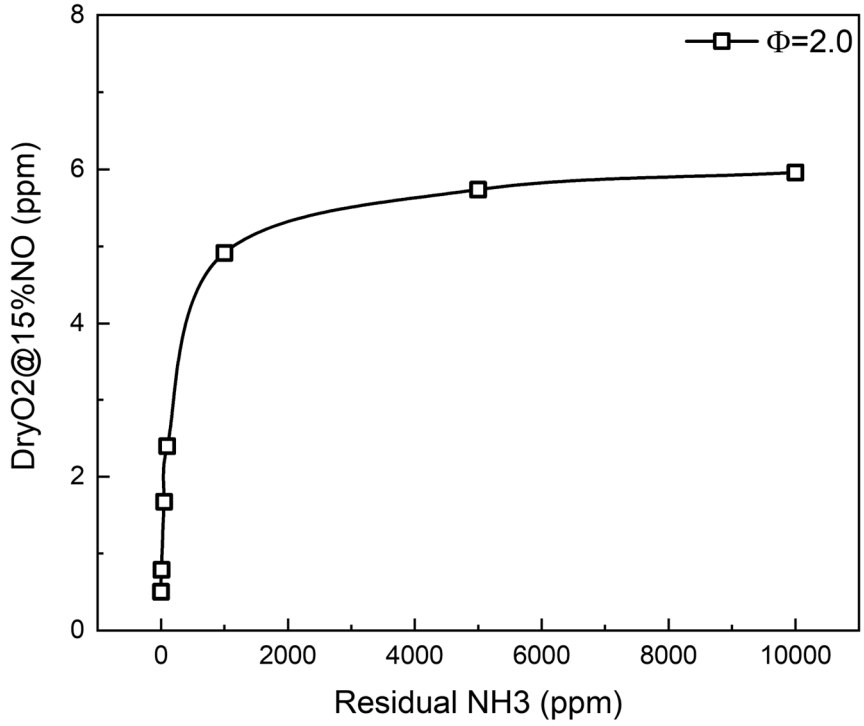

Figure S2. Final NO mole fraction as a function of residual NH_3 in the low-concentration (0–100 ppm) range under fuel-rich (ϕ= 2.0) conditions at 20 atm and 673 K.