Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

Elucidating the structure, redox properties and active entities of high-temperature thermal aged CuO_x-CeO_2 catalysts for CO-PROX

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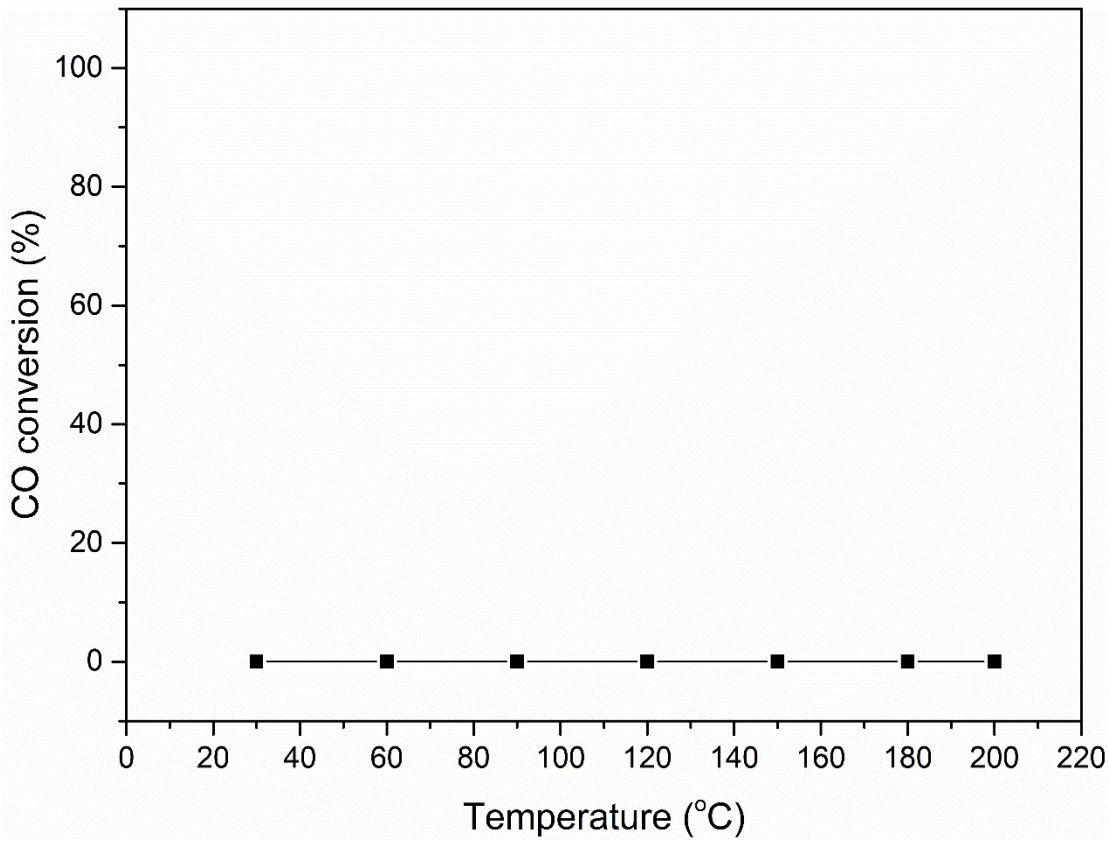

Fig. S1 Catalytic performance of 0.1 g α-Al_2O_3 for CO-PROX (blank experiment).

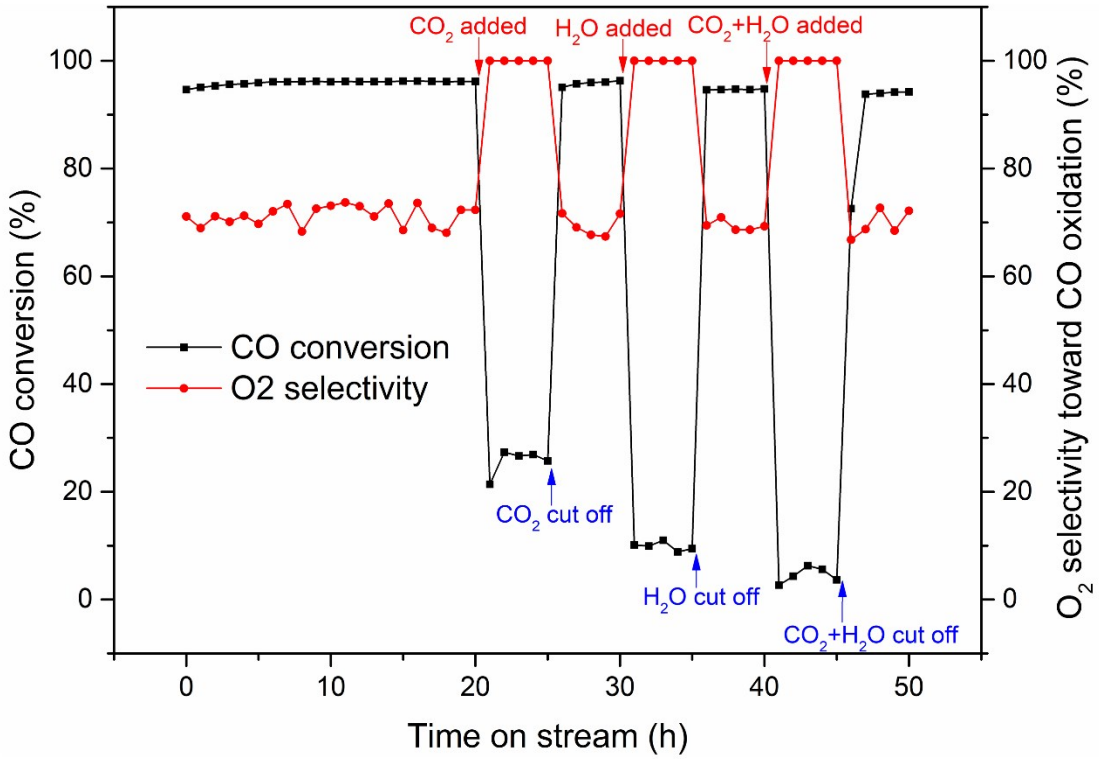

Fig. S2 Catalytic performance of 7CuCe catalyst under 50 h CO-PROX reaction at 80 ^{o}C with H_2O or/and CO_2 added.

Table S1 Copper content of the CuO_x-CeO_2 catalysts analyzed by ICP-AES.

Catalyst	Copper content (wt%)
1CuCe	0.7
2CuCe	1.2
5CuCe	3.3
7CuCe	4.8
10CuCe	7.1
15CuCe	11.2

Table S2 Structure parameters of the CuO_x-CeO_2 catalysts with 7% Cu content and different calcination temperature.

Catalyst	Weight percentage of crystalline CuO phase (%)	Lattice parameter of CeO_2 (Å)	Grain size[a] (Å)	Microstrain[a] (10^{-3})
7CuCe-200	0.4	5.4104	38.0/32.7/36.2	10.4/5.70/9.46
7CuCe-300	0.2	5.4121	42.3/39.1/41.4	8.14/4.55/7.41
7CuCe-400	0.3	5.4128	51.9/49.8/51.3	5.46/3.19/4.99
7CuCe-500	0.5	5.4127	63.8/62.6/63.4	3.98/2.77/3.72
7CuCe-600	0.9	5.4123	77.4/76.8/77.2	2.62/1.95/2.47
7CuCe-700	4.3	5.4100	139/153/142	1.07/1.93/1.33

[a]The crystalline size and microstrain of the three crystal planes of CeO_2 basic grain, which are {111}, {100} and {110} from left to right.

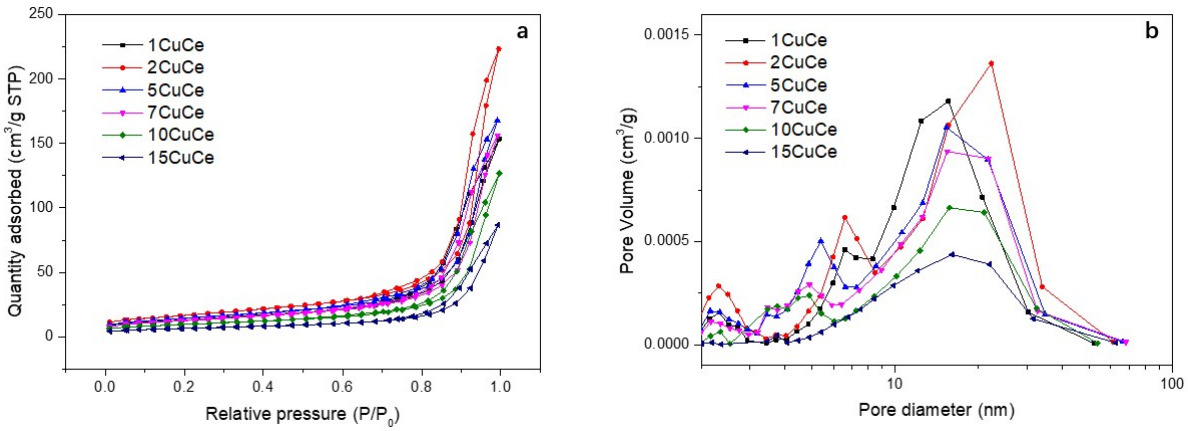

Fig. S3 N_2 adsorption-desorption isotherms (a) and BJH desorption pore size distribution curves (b) of the CuO_x-CeO_2 catalysts with different copper content.

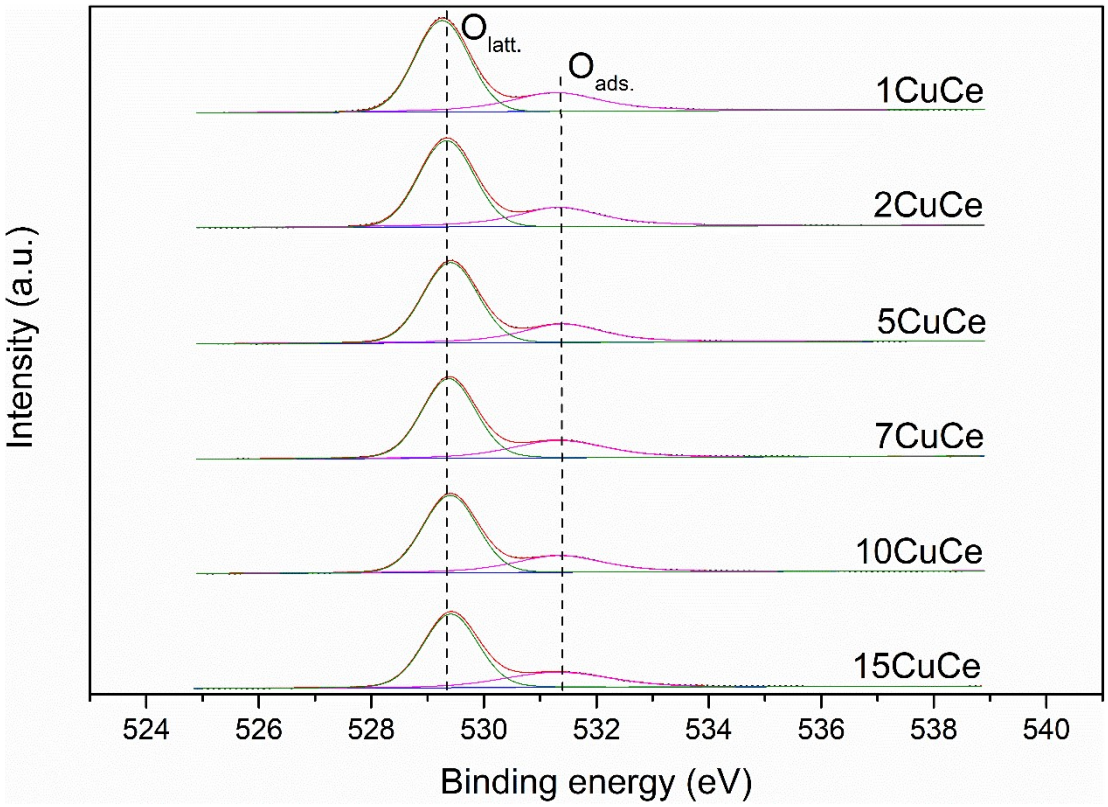

Fig. S4 O 1s XPS spectra of the CuO_x-CeO_2 catalysts.

Table S3 Reduction temperature and H_2 consumption of H_2-TPR peaks, $T_{50\%}$ and operation temperature window of the CuO_x-CeO_2 catalysts.

	Peak α		Peak β		Peak γ		Total H_2	Theoretical H_2
Catalyst	Tem. (^oC)	H_2 cons. ($\mu mol\ g^{-1}$)	Tem. (^oC)	H_2 cons. ($\mu mol\ g^{-1}$)	Tem. (^oC)	H_2 cons. ($\mu mol\ g^{-1}$)	cons. ($\mu mol\ g^{-1}$)	cons. by Cu^{2+} ($\mu mol\ g^{-1}$)
1CuCe	148	105	176	185	-	-	290	157
2CuCe	148	178	172	255	-	-	433	315
5CuCe	141	238	164	608	-	-	846	787
7CuCe	142	192	161	315	170	468	975	1102
10CuCe	142	157	164	352	178	948	1457	1574
15CuCe	146	114	177	760	199	1149	2023	2360

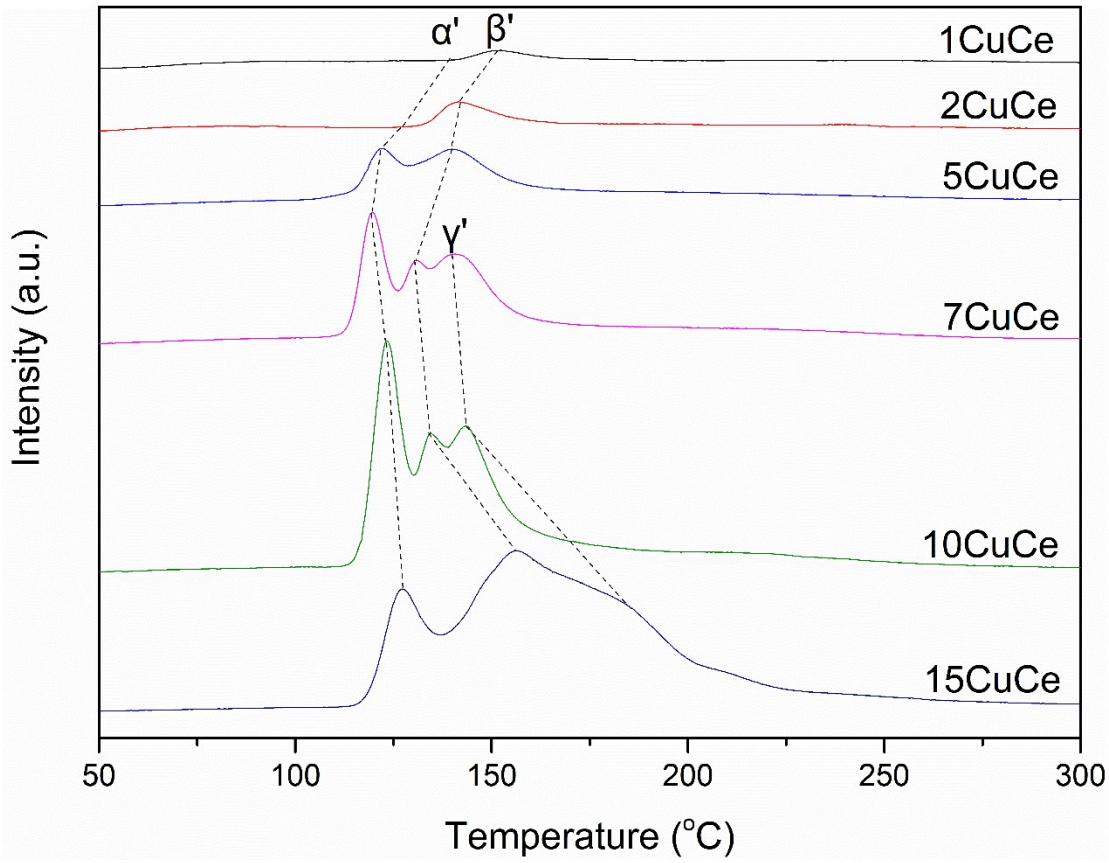

Fig. S5 CO-TPR profiles of the CuO_x-CeO_2 catalysts with different copper content.

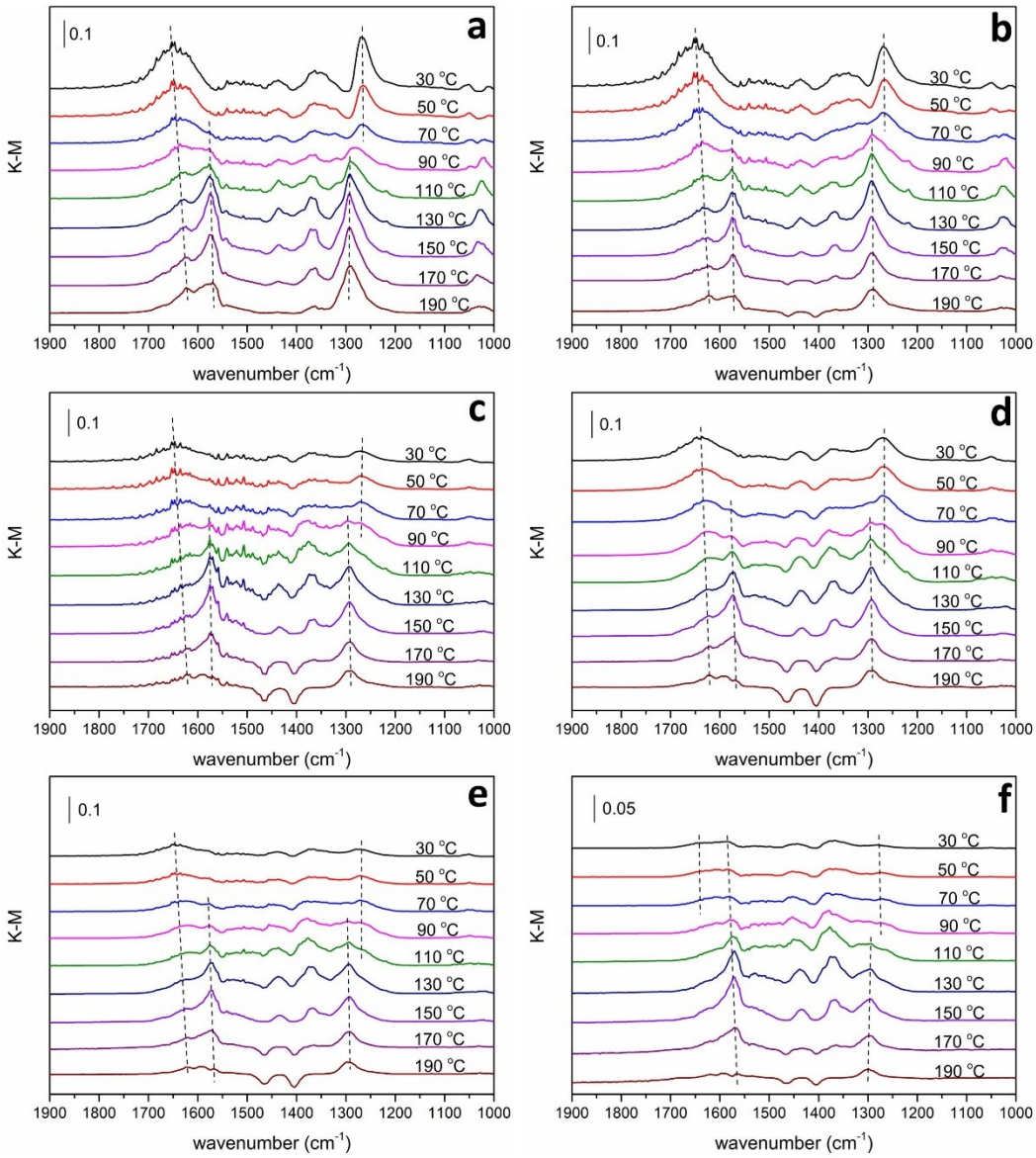

Fig. S6 *In situ* DRIFTs spectra at 1000-1900 cm^{-1} region of (a) 1CuCe, (b) 2CuCe, (c) 5CuCe, (d) 7CuCe, (e) 10CuCe and (f) 15CuCe under the H_2+CO+O_2+Ar reaction stream.

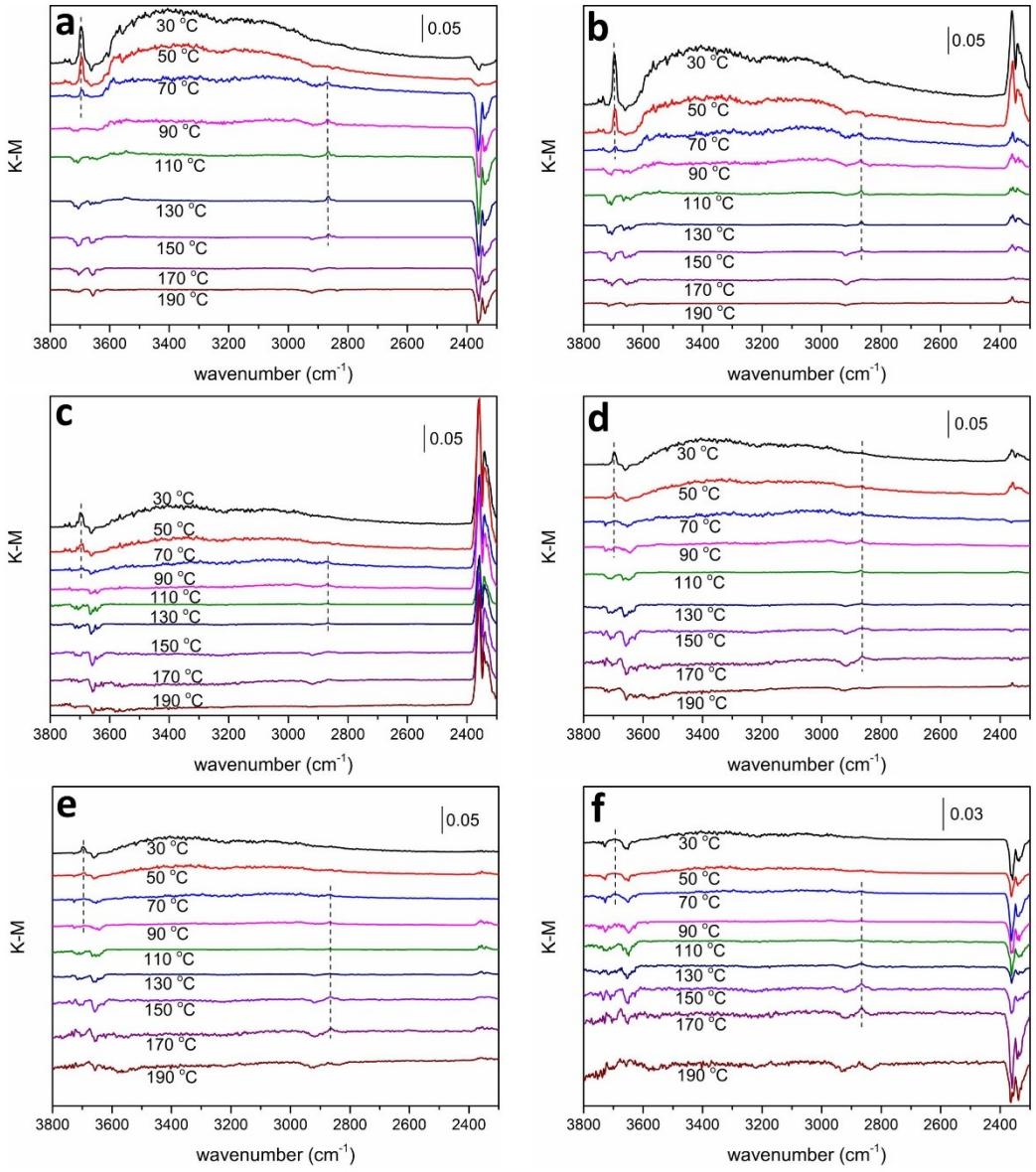

Fig. S7 *In situ* DRIFTs spectra at 2300-3800 cm^{-1} region of (a) 1CuCe, (b) 2CuCe, (c) 5CuCe, (d) 7CuCe, (e) 10CuCe and (f) 15CuCe under the H_2+CO+O_2+Ar reaction stream.