Supplementary information for

Hydrogenation of CO/CO_2 Mixtures on Nickel Catalysts: Kinetics and Flexibility for Nickel Catalysts

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Criteria for absence of transfer limitations

Table S1: Criteria for the exclusion of transfer limitations (symbols see Table S2).

	mass-transfer	heat-transfer
internal transfer limitations	Mears criterion[1]: $\frac{r_{\mathrm{CH_4}}\, r_{\mathrm{P}}}{c_{\mathrm{i}}\, D_{\mathrm{i,eff}}} \leq \frac{1}{\lvert n \rvert}\; i\; \in \mathrm{CO}, \mathrm{CO_2}$	Anderson criterion[2]: $\frac{r_{\mathrm{CH_4}}\, \lvert \Delta \mathrm{H} \rvert\, \rho_{\mathrm{cat}}\, d_{\mathrm{cat}}^2}{4\, \lambda_{\mathrm{eff}}\, T} \leq \frac{0.75\, R\, T}{E_{\mathrm{A}}}$
external transfer limitations	Carberry criterion[3]: $\mathrm{Ca} = \frac{r_{\mathrm{CH_4}}\, \rho_{\mathrm{cat}}}{k_{\mathrm{g}} a\, c_i} \leq 0.05$	Mears criterion[1]: $\frac{r_{\mathrm{CH_4}} \lvert \Delta \mathrm{H} \rvert\, \rho_{\mathrm{cat}} d_{\mathrm{cat}}}{h_{\mathrm{t}}\, T} \leq \frac{0.3\, R\, T}{E_{\mathrm{A}}}$

Table S2: Symbols used in equations in Table S1.

Latin symbols		
Carberry Number	Ca	1
Concentration of component *i*	c_i	mol m-^{3}
Effective diffusion coefficient of component *i*	$D_{i,\mathrm{eff}}$	m² s^{-1}
Catalyst particle diameter	d_{cat}	m
Activation energy	E_{A}	J mol^{-1}
Enthalpy of reaction	ΔH	J mol^{-1}
Heat transfer coefficient between gas and particle	h_{t}	W m^{-2} K^{-1}
Mass transfer coefficient	$k_{\mathrm{g}}a$	m s^{-1}
Reaction order	n	1
Universal gas constant	R	J mol^{-1} K^{-1}
Observed reaction rate	$r_{\mathrm{CH_4}}$	mol s^{-1}
Catalyst particle radius	r_{P}	m
Reaction temperature	T	K
Greek symbols		
Effective heat conductivity	λ_{eff}	W m^{-1} K^{-1}
Catalyst particle density	ρ_{cat}	kg m^{-3}

Additional Figures

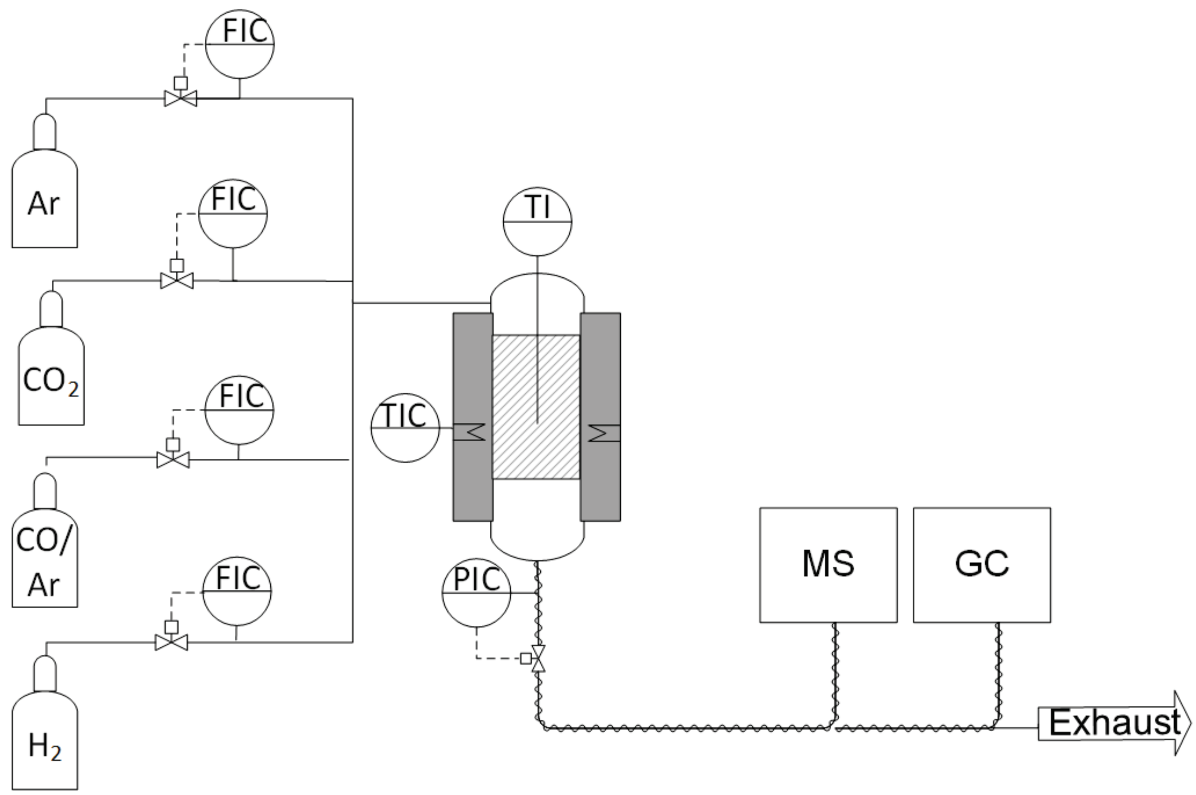

Figure S1: Flowsheet of the fixed bed reactor setup.

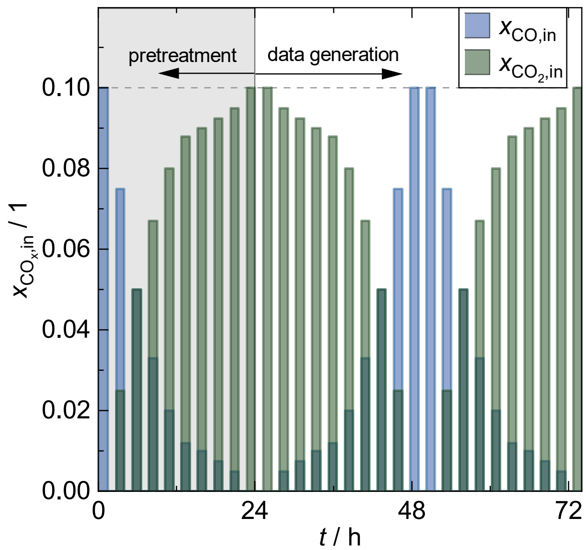

Figure S2: Typical variation of the specific inlet carbon oxide composition in one experimental run.

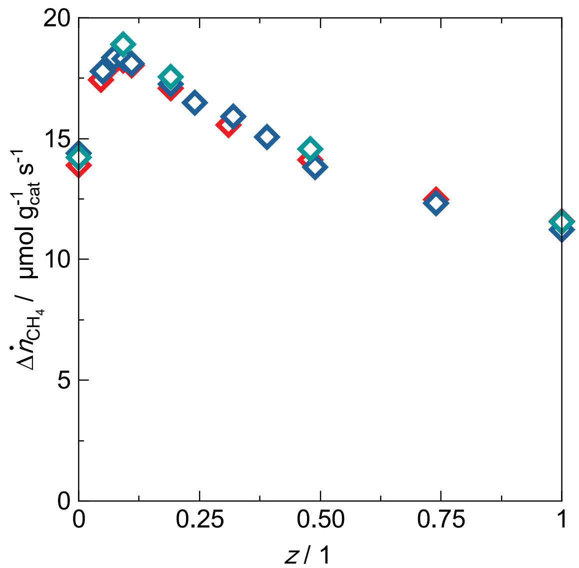

Figure S3: CH_4 formation rates of three different campaigns indicated with different colors; for sake of clarity average values of single experiments within one run are shown as symbols; reaction conditions: 556 K, 2 bar, 250 mL_{STP} min^{-1} total flow rate, 800 mbar H_2 inlet partial pressure.

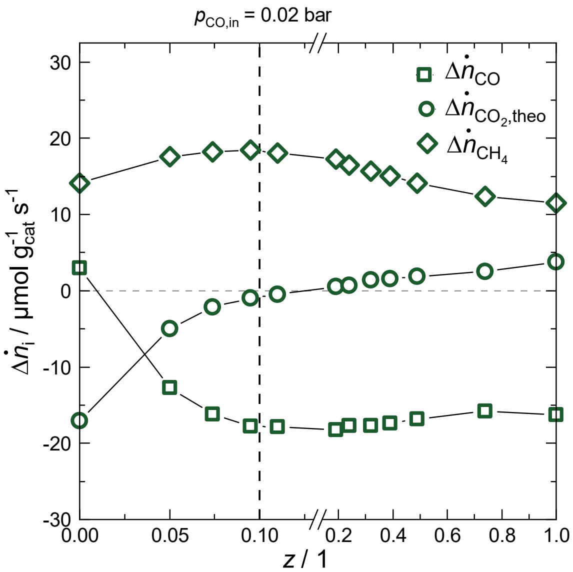

Figure S4: Measured conversion rates $\Delta\dot{n}_i$ for CO and CH_4, as well as the theoretical CO_2 conversion rate during CO_x methanation; shaded background indicates 95 % confidence interval; reaction conditions: 556 K, 2 bar(a), total flow rate 250 mL_{STP} min^{-1}, 800 mbar H_2 inlet partial pressure.

The theoretical CO_2 conversion rate is calculated as follows:

$$\Delta\dot{n}_{CO_2,theo} = \dot{n}_{CO,in} - (\dot{n}_{CO,out} + \dot{n}_{CH_4,out} + 2\,\dot{n}_{C_2H_6,out} + 3\,\dot{n}_{C_3H_8,out}).$$

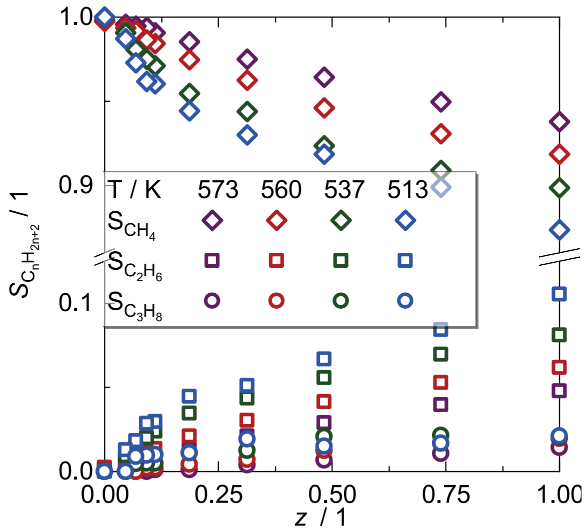

Figure S5: Hydrocarbon selectivity at different temperatures; reaction conditions: 2 bar, total flow rate 250 mL_{STP} min^{-1}, 800 mbar H_2 inlet partial pressure.

The selectivity $S_{C_nH_{2n+2}}$ is calculated as follows: $S_{C_nH_{2n+2}} = \frac{\dot{n}_{C_nH_{2n+2}}}{\dot{n}_{CH_4}+\dot{n}_{C_2H_4}+\dot{n}_{C_3H_6}}$.

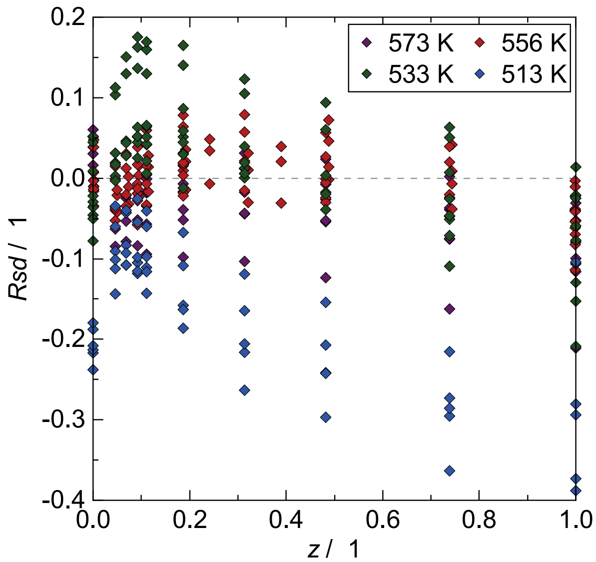

Figure S6: Residuals Rsd for the simulated methane formation rate over the complete range of CO_x inlet compositions between pure CO and pure CO_2 methanation at different temperatures; residuals at 556 K for parameter estimation; residuals at 513, 533, and 573 K for model validation; reaction conditions: 2 bar, total flow rate 250 mL_{STP} min^{-1}, 800 mbar H_2 inlet partial pressure.

Residuals are calculated as follows:

$$RSD = \frac{r_{\mathrm{CH_4,sim}} - r_{\mathrm{CH_4,obs}}}{r_{\mathrm{CH_4,obs}}}$$

with $r_{\mathrm{CH_4,sim}}$ as the simulated methane formation rate and $r_{\mathrm{CH_4,obs}}$ as the observed methane formation rate.

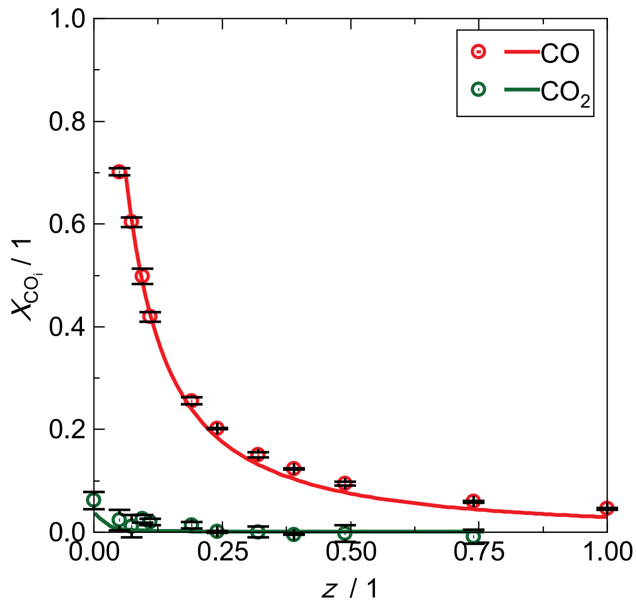

Figure S7: Comparison between simulated (lines) and experimental (symbols) CO and CO_2 conversion X_{CO_i} observed during CO_x methanation; reaction conditions: 556 K, 2 bar, total flow rate 250 mL_{STP} min^{-1}, 800 mbar H_2 inlet partial pressure.

The individual conversion X_{CO_i} for CO and CO_2 is calculated as follows: $X_{CO_i} = 1 - \frac{\dot{n}_{CO_i,out}}{\dot{n}_{CO_i,in}}$.

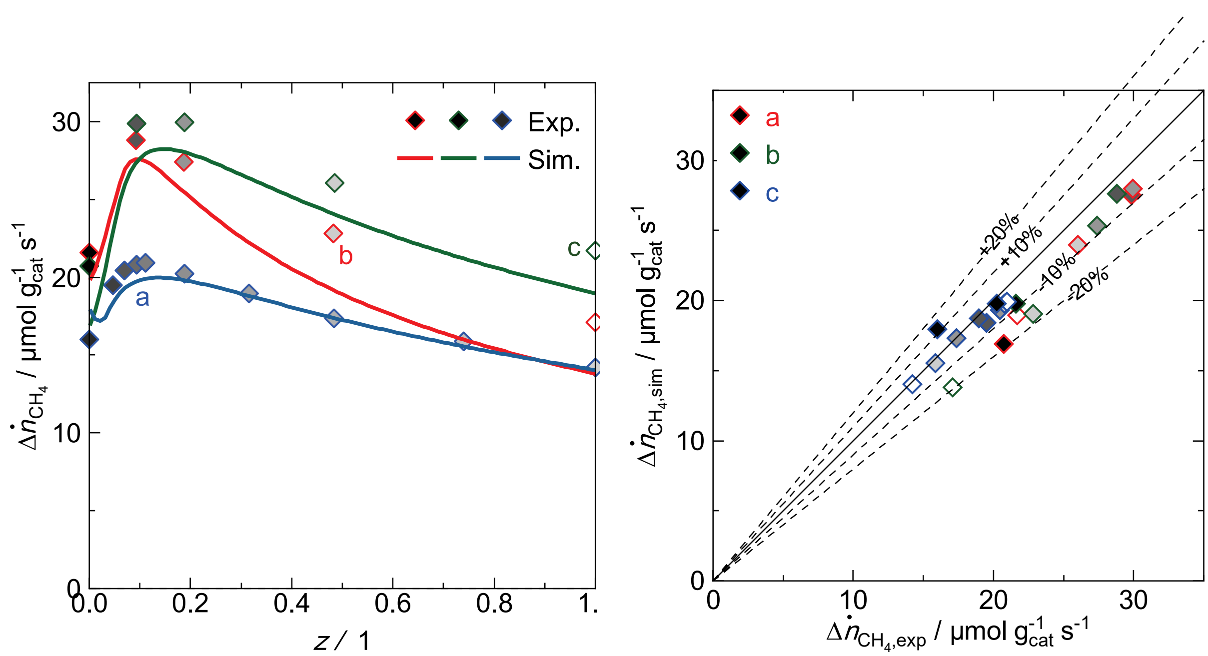

Figure S8: Comparison between experimental (symbols) and simulated (lines) results under different reaction conditions in dependency on the carbon oxide composition (left) and corresponding parity plot (right); for these experiments only two hysteresis are conducted with respect to the carbon oxide composition and the second one is shown; reaction conditions:

a) 570 K, 2 bar, 500 mbar H_2 and 166 mbar CO_x inlet partial pressure, total flow rate 300 mL_{STP} min^{-1}

b) 556 K, 3.85 bar, 1540 mbar H_2 and 385 mbar CO_x inlet partial pressure, total flow rate 250 mL_{STP} min^{-1}

c) 556 K, 2 bar, 1600 mbar H_2 and 200 mbar CO_x inlet partial pressure, total flow rate 250 mL_{STP} min^{-1}.

Data used for optimization of f_{CO}, f_{CO2} and f_{KC}

Table S3: Experimental data sets with z and r_{CH_4} used for estimation of f_{CO}, f_{CO_2}, and f_{K_C}; reaction conditions: 556 K, 2 bar, 250 mL_{STP} min^{-1} total flow rate, 800 mbar H_2 inlet partial pressure.

z / 1	r_{CH_4} / mol/g_{cat} s^{-1}	z / 1	r_{CH_4} / mol/g_{cat} s^{-1}	z / 1	r_{CH_4} / mol/g_{cat} s^{-1}
0.00	$1.46\cdot10^{-5}$	0.11	$1.86\cdot10^{-5}$	0.49	$1.43\cdot10^{-5}$
0.00	$1.43\cdot10^{-5}$	0.11	$1.80\cdot10^{-5}$	0.49	$1.41\cdot10^{-5}$
0.00	$1.42\cdot10^{-5}$	0.11	$1.78\cdot10^{-5}$	0.49	$1.36\cdot10^{-5}$
0.00	$1.43\cdot10^{-5}$	0.11	$1.89\cdot10^{-5}$	0.49	$1.33\cdot10^{-5}$
0.00	$1.41\cdot10^{-5}$	0.11	$1.84\cdot10^{-5}$	0.49	$1.47\cdot10^{-5}$
0.00	$1.40\cdot10^{-5}$	0.11	$1.82\cdot10^{-5}$	0.49	$1.43\cdot10^{-5}$
0.00	$1.36\cdot10^{-5}$	0.11	$1.80\cdot10^{-5}$	0.49	$1.40\cdot10^{-5}$
0.00	$1.35\cdot10^{-5}$	0.11	$1.75\cdot10^{-5}$	0.49	$1.36\cdot10^{-5}$
0.00	$1.43\cdot10^{-5}$	0.11	$1.72\cdot10^{-5}$	0.49	$1.48\cdot10^{-5}$
0.00	$1.41\cdot10^{-5}$	0.19	$1.78\cdot10^{-5}$	0.49	$1.44\cdot10^{-5}$
0.05	$1.81\cdot10^{-5}$	0.19	$1.71\cdot10^{-5}$	0.74	$1.28\cdot10^{-5}$
0.05	$1.77\cdot10^{-5}$	0.19	$1.69\cdot10^{-5}$	0.74	$1.24\cdot10^{-5}$
0.05	$1.76\cdot10^{-5}$	0.19	$1.79\cdot10^{-5}$	0.74	$1.22\cdot10^{-5}$
0.05	$1.80\cdot10^{-5}$	0.19	$1.74\cdot10^{-5}$	0.74	$1.19\cdot10^{-5}$
0.05	$1.78\cdot10^{-5}$	0.19	$1.72\cdot10^{-5}$	0.74	$1.30\cdot10^{-5}$
0.05	$1.71\cdot10^{-5}$	0.19	$1.73\cdot10^{-5}$	0.74	$1.27\cdot10^{-5}$
0.05	$1.69\cdot10^{-5}$	0.19	$1.65\cdot10^{-5}$	0.74	$1.26\cdot10^{-5}$
0.07	$1.87\cdot10^{-5}$	0.19	$1.63\cdot10^{-5}$	0.74	$1.21\cdot10^{-5}$
0.07	$1.83\cdot10^{-5}$	0.19	$1.80\cdot10^{-5}$	0.74	$1.19\cdot10^{-5}$
0.07	$1.81\cdot10^{-5}$	0.19	$1.75\cdot10^{-5}$	1.00	$1.15\cdot10^{-5}$
0.07	$1.87\cdot10^{-5}$	0.19	$1.72\cdot10^{-5}$	1.00	$1.12\cdot10^{-5}$
0.07	$1.84\cdot10^{-5}$	0.24	$1.70\cdot10^{-5}$	1.00	$1.14\cdot10^{-5}$
0.07	$1.78\cdot10^{-5}$	0.24	$1.63\cdot10^{-5}$	1.00	$1.09\cdot10^{-5}$
0.07	$1.75\cdot10^{-5}$	0.24	$1.61\cdot10^{-5}$	1.00	$1.23\cdot10^{-5}$
0.10	$1.87\cdot10^{-5}$	0.32	$1.65\cdot10^{-5}$	1.00	$1.16\cdot10^{-5}$
0.10	$1.82\cdot10^{-5}$	0.32	$1.58\cdot10^{-5}$	1.00	$1.13\cdot10^{-5}$
0.10	$1.80\cdot10^{-5}$	0.32	$1.55\cdot10^{-5}$	1.00	$1.19\cdot10^{-5}$
0.10	$1.94\cdot10^{-5}$	0.32	$1.63\cdot10^{-5}$	1.00	$1.14\cdot10^{-5}$
0.10	$1.86\cdot10^{-5}$	0.32	$1.59\cdot10^{-5}$	1.00	$1.10\cdot10^{-5}$
0.10	$1.84\cdot10^{-5}$	0.32	$1.57\cdot10^{-5}$	1.00	$1.17\cdot10^{-5}$
0.10	$1.80\cdot10^{-5}$	0.32	$1.52\cdot10^{-5}$	1.00	$1.14\cdot10^{-5}$
0.10	$1.76\cdot10^{-5}$	0.32	$1.49\cdot10^{-5}$		
0.10	$1.74\cdot10^{-5}$	0.39	$1.57\cdot10^{-5}$		
0.10	$1.94\cdot10^{-5}$	0.39	$1.49\cdot10^{-5}$		
0.10	$1.88\cdot10^{-5}$	0.39	$1.46\cdot10^{-5}$		
0.10	$1.85\cdot10^{-5}$				

CO_x methanation @556 K for kinetic parameter estimation

Parameter			
	catalyst mass	5,000E-02	g
	reaction temperature	556	K
	reaction pressure	2,000E+05	Pa
	volumetric inlet flow rate	2,500E+02	mL_{STP} min^{-1}

feed ratio	consumption or formation rates for			conversion for		selectivity for		
CO/(CO+CO2)	CO	CO_2	CH_4	CO	CO_2	CH_4	C_2H_6	C_3H_8
z	$\Delta\dot{n}_{CO}$	$\Delta\dot{n}_{CO_2}$	$\Delta\dot{n}_{CH_4}$	X_{CO}	X_{CO2}	S_{CH4}	S_{C2H6}	S_{C3H8}
1	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	1	1	1	1	1
0,000E+00	-3,012E-06	1,482E-05	1,461E-05	-	3,974E-02	9,975E-01	2,538E-03	0,000E+00
0,000E+00	-3,090E-06	1,396E-05	1,433E-05	-	3,743E-02	9,974E-01	2,591E-03	0,000E+00
0,000E+00	-3,050E-06	1,364E-05	1,424E-05	-	3,658E-02	9,974E-01	2,604E-03	0,000E+00
0,000E+00	-2,968E-06	3,047E-05	1,426E-05	-	7,807E-02	9,974E-01	2,564E-03	0,000E+00
0,000E+00	-2,995E-06	2,950E-05	1,413E-05	-	7,560E-02	9,974E-01	2,577E-03	0,000E+00
0,000E+00	-2,844E-06	2,843E-05	1,400E-05	-	7,286E-02	9,974E-01	2,564E-03	0,000E+00
0,000E+00	-2,824E-06	2,776E-05	1,358E-05	-	7,114E-02	9,973E-01	2,660E-03	0,000E+00
0,000E+00	-2,831E-06	2,728E-05	1,346E-05	-	6,990E-02	9,973E-01	2,688E-03	0,000E+00
0,000E+00	-2,912E-06	2,740E-05	1,430E-05	-	7,022E-02	9,974E-01	2,571E-03	0,000E+00
0,000E+00	-2,955E-06	2,691E-05	1,415E-05	-	6,897E-02	9,974E-01	2,604E-03	0,000E+00
4,986E-02	1,309E-05	1,299E-06	1,809E-05	7,085E-01	3,688E-03	9,939E-01	6,122E-03	0,000E+00
4,986E-02	1,303E-05	1,062E-06	1,770E-05	7,055E-01	3,016E-03	9,937E-01	6,276E-03	0,000E+00
4,986E-02	1,298E-05	6,431E-07	1,758E-05	7,028E-01	1,827E-03	9,937E-01	6,289E-03	0,000E+00
4,986E-02	1,259E-05	1,428E-05	1,804E-05	7,064E-01	3,855E-02	9,940E-01	6,048E-03	0,000E+00
4,986E-02	1,255E-05	1,354E-05	1,776E-05	7,042E-01	3,654E-02	9,939E-01	6,148E-03	0,000E+00
4,986E-02	1,232E-05	1,519E-05	1,711E-05	6,909E-01	4,100E-02	9,937E-01	6,316E-03	0,000E+00
4,986E-02	1,235E-05	1,524E-05	1,685E-05	6,930E-01	4,113E-02	9,936E-01	6,410E-03	0,000E+00
7,371E-02	1,646E-05	-3,573E-06	1,871E-05	6,058E-01	-1,046E-02	9,921E-01	7,890E-03	0,000E+00
7,371E-02	1,638E-05	-4,030E-06	1,830E-05	6,027E-01	-1,180E-02	9,919E-01	8,097E-03	0,000E+00
7,371E-02	1,637E-05	-4,160E-06	1,807E-05	6,023E-01	-1,218E-02	9,918E-01	8,180E-03	0,000E+00
7,371E-02	1,641E-05	9,244E-06	1,866E-05	6,159E-01	2,569E-02	9,922E-01	7,797E-03	0,000E+00
7,371E-02	1,636E-05	8,536E-06	1,839E-05	6,142E-01	2,372E-02	9,921E-01	7,921E-03	0,000E+00
7,371E-02	1,582E-05	1,205E-05	1,779E-05	5,941E-01	3,350E-02	9,919E-01	8,065E-03	0,000E+00
7,371E-02	1,572E-05	1,154E-05	1,748E-05	5,902E-01	3,209E-02	9,918E-01	8,230E-03	0,000E+00
9,510E-02	1,769E-05	1,288E-05	1,872E-05	4,933E-01	3,776E-02	9,864E-01	1,170E-02	1,949E-03
9,510E-02	1,752E-05	1,211E-05	1,822E-05	4,887E-01	3,549E-02	9,859E-01	1,205E-02	2,008E-03
9,510E-02	1,748E-05	1,151E-05	1,801E-05	4,875E-01	3,375E-02	9,858E-01	1,217E-02	2,028E-03
9,510E-02	1,846E-05	6,417E-06	1,939E-05	5,192E-01	1,837E-02	9,870E-01	1,115E-02	1,859E-03
9,510E-02	1,791E-05	5,996E-06	1,863E-05	5,037E-01	1,716E-02	9,864E-01	1,165E-02	1,942E-03
9,510E-02	1,799E-05	5,521E-06	1,841E-05	5,061E-01	1,580E-02	9,881E-01	9,881E-03	1,976E-03
9,510E-02	1,707E-05	1,007E-05	1,797E-05	4,802E-01	2,882E-02	9,861E-01	1,193E-02	1,988E-03
9,510E-02	1,698E-05	9,691E-06	1,760E-05	4,775E-01	2,774E-02	9,858E-01	1,217E-02	2,028E-03
9,510E-02	1,705E-05	9,178E-06	1,739E-05	4,794E-01	2,627E-02	9,877E-01	1,029E-02	2,058E-03
9,510E-02	1,844E-05	8,522E-06	1,940E-05	5,186E-01	2,439E-02	9,869E-01	1,126E-02	1,876E-03
9,510E-02	1,815E-05	8,309E-06	1,880E-05	5,105E-01	2,378E-02	9,865E-01	1,158E-02	1,931E-03
9,510E-02	1,810E-05	8,225E-06	1,852E-05	5,092E-01	2,354E-02	9,863E-01	1,176E-02	1,961E-03
1,145E-01	1,793E-05	7,673E-06	1,857E-05	4,198E-01	2,324E-02	9,843E-01	1,373E-02	1,961E-03
1,145E-01	1,779E-05	7,544E-06	1,800E-05	4,164E-01	2,285E-02	9,838E-01	1,417E-02	2,024E-03
1,145E-01	1,774E-05	6,800E-06	1,776E-05	4,153E-01	2,059E-02	9,836E-01	1,434E-02	2,049E-03
1,145E-01	1,842E-05	4,671E-06	1,889E-05	4,328E-01	1,369E-02	9,847E-01	1,338E-02	1,912E-03
1,145E-01	1,829E-05	4,010E-06	1,840E-05	4,298E-01	1,175E-02	9,843E-01	1,375E-02	1,965E-03
1,145E-01	1,833E-05	3,588E-06	1,818E-05	4,306E-01	1,052E-02	9,841E-01	1,389E-02	1,984E-03
1,145E-01	1,746E-05	8,650E-06	1,799E-05	4,102E-01	2,536E-02	9,841E-01	1,389E-02	1,984E-03
1,145E-01	1,736E-05	8,399E-06	1,753E-05	4,080E-01	2,462E-02	9,838E-01	1,420E-02	2,028E-03
1,145E-01	1,741E-05	8,271E-06	1,724E-05	4,091E-01	2,424E-02	9,855E-01	1,245E-02	2,075E-03
1,921E-01	1,804E-05	3,691E-06	1,776E-05	2,545E-01	1,238E-02	9,756E-01	2,033E-02	4,065E-03
1,921E-01	1,799E-05	3,477E-06	1,715E-05	2,538E-01	1,166E-02	9,747E-01	2,110E-02	4,219E-03
1,921E-01	1,780E-05	3,300E-06	1,690E-05	2,511E-01	1,107E-02	9,744E-01	2,132E-02	4,264E-03
1,921E-01	1,850E-05	2,261E-06	1,789E-05	2,594E-01	7,296E-03	9,759E-01	2,008E-02	4,016E-03
1,921E-01	1,876E-05	1,642E-06	1,739E-05	2,631E-01	5,298E-03	9,752E-01	2,066E-02	4,132E-03
1,921E-01	1,849E-05	1,418E-06	1,723E-05	2,592E-01	4,576E-03	9,751E-01	2,079E-02	4,158E-03
1,921E-01	1,763E-05	6,854E-06	1,727E-05	2,472E-01	2,212E-02	9,754E-01	2,049E-02	4,098E-03
1,921E-01	1,757E-05	6,570E-06	1,651E-05	2,463E-01	2,120E-02	9,742E-01	2,146E-02	4,292E-03
1,921E-01	1,749E-05	6,416E-06	1,629E-05	2,452E-01	2,071E-02	9,740E-01	2,165E-02	4,329E-03
1,921E-01	1,880E-05	5,456E-06	1,796E-05	2,636E-01	1,761E-02	9,739E-01	2,204E-02	4,008E-03
1,921E-01	1,885E-05	5,375E-06	1,750E-05	2,643E-01	1,734E-02	9,754E-01	2,053E-02	4,107E-03
1,921E-01	1,858E-05	5,154E-06	1,723E-05	2,606E-01	1,663E-02	9,749E-01	2,092E-02	4,184E-03
2,416E-01	1,772E-05	7,542E-07	1,702E-05	2,019E-01	2,738E-03	9,687E-01	2,505E-02	6,263E-03
2,416E-01	1,785E-05	9,897E-08	1,634E-05	2,033E-01	3,593E-04	9,717E-01	2,397E-02	4,357E-03
2,416E-01	1,761E-05	-2,484E-07	1,612E-05	2,007E-01	-9,018E-04	9,712E-01	2,434E-02	4,425E-03
3,210E-01	1,725E-05	-1,764E-06	1,646E-05	1,476E-01	-7,138E-03	9,632E-01	3,030E-02	6,494E-03
3,210E-01	1,754E-05	-1,984E-06	1,580E-05	1,501E-01	-8,027E-03	9,639E-01	2,935E-02	6,772E-03
3,210E-01	1,718E-05	-2,350E-06	1,547E-05	1,470E-01	-9,507E-03	9,631E-01	2,995E-02	6,912E-03
3,210E-01	1,867E-05	2,293E-07	1,628E-05	1,585E-01	8,905E-04	9,610E-01	3,037E-02	8,677E-03
3,210E-01	1,834E-05	-3,894E-07	1,585E-05	1,557E-01	-1,512E-03	9,621E-01	3,118E-02	6,682E-03
3,210E-01	1,812E-05	-7,806E-07	1,570E-05	1,538E-01	-3,031E-03	9,639E-01	2,935E-02	6,772E-03
3,210E-01	1,739E-05	4,369E-06	1,516E-05	1,477E-01	1,697E-02	9,630E-01	3,002E-02	6,928E-03
3,210E-01	1,701E-05	4,070E-06	1,487E-05	1,444E-01	1,580E-02	9,624E-01	3,059E-02	7,059E-03
3,902E-01	1,720E-05	-8,206E-07	1,569E-05	1,223E-01	-3,735E-03	9,556E-01	3,556E-02	8,889E-03
3,902E-01	1,759E-05	-9,713E-07	1,490E-05	1,251E-01	-4,421E-03	9,554E-01	3,521E-02	9,390E-03
3,902E-01	1,722E-05	-1,102E-06	1,463E-05	1,225E-01	-5,017E-03	9,570E-01	3,341E-02	9,547E-03
4,886E-01	1,682E-05	-4,036E-07	1,429E-05	9,517E-02	-2,182E-03	9,463E-01	4,146E-02	1,220E-02
4,886E-01	1,643E-05	-5,766E-07	1,407E-05	9,296E-02	-3,117E-03	9,502E-01	3,980E-02	9,950E-03
4,886E-01	1,607E-05	-4,641E-06	1,363E-05	9,091E-02	-2,508E-02	9,487E-01	4,103E-02	1,026E-02
4,886E-01	1,556E-05	-5,976E-06	1,330E-05	8,803E-02	-3,230E-02	9,472E-01	4,222E-02	1,055E-02
4,886E-01	1,763E-05	-5,650E-07	1,467E-05	9,894E-02	-2,954E-03	9,480E-01	4,019E-02	1,182E-02
4,886E-01	1,716E-05	-9,714E-07	1,433E-05	9,632E-02	-5,078E-03	9,469E-01	4,106E-02	1,208E-02
4,886E-01	1,663E-05	3,234E-06	1,395E-05	9,331E-02	1,690E-02	9,457E-01	4,198E-02	1,235E-02
4,886E-01	1,608E-05	2,793E-06	1,355E-05	9,026E-02	1,460E-02	9,466E-01	4,071E-02	1,272E-02
4,886E-01	1,792E-05	1,949E-06	1,477E-05	1,006E-01	1,019E-02	9,480E-01	4,019E-02	1,182E-02
4,886E-01	1,752E-05	1,662E-06	1,440E-05	9,831E-02	8,690E-03	9,467E-01	4,116E-02	1,211E-02
7,439E-01	1,640E-05	3,949E-07	1,283E-05	6,190E-02	4,328E-03	9,307E-01	5,333E-02	1,600E-02
7,439E-01	1,575E-05	2,342E-07	1,243E-05	5,943E-02	2,567E-03	9,311E-01	5,234E-02	1,653E-02
7,439E-01	1,568E-05	-7,139E-07	1,224E-05	5,916E-02	-7,825E-03	9,302E-01	5,307E-02	1,676E-02
7,439E-01	1,513E-05	-1,004E-06	1,185E-05	5,710E-02	-1,100E-02	9,335E-01	5,202E-02	1,445E-02
7,439E-01	1,657E-05	-9,470E-07	1,299E-05	6,200E-02	-1,002E-02	9,295E-01	5,222E-02	1,828E-02
7,439E-01	1,610E-05	-1,091E-06	1,269E-05	6,023E-02	-1,155E-02	9,330E-01	5,094E-02	1,609E-02
7,439E-01	1,614E-05	-1,963E-06	1,263E-05	6,037E-02	-2,077E-02	9,303E-01	5,362E-02	1,609E-02
7,439E-01	1,545E-05	-3,227E-06	1,213E-05	5,781E-02	-3,415E-02	9,304E-01	5,292E-02	1,671E-02
7,439E-01	1,505E-05	9,772E-07	1,190E-05	5,629E-02	1,034E-02	9,316E-01	5,128E-02	1,709E-02

CO_x methanation @556 K for kinetic parameter estimation, continued								
feed ratio	consumption or formation rates for			conversion for		selectivity for		
CO/(CO+CO2)	CO	CO_2	CH_4	CO	CO_2	CH_4	C_2H_6	C_3H_8
z	$\Delta\dot{n}_{CO}$	$\Delta\dot{n}_{CO_2}$	$\Delta\dot{n}_{CH_4}$	X_{CO}	X_{CO2}	S_{CH4}	S_{C2H6}	S_{C3H8}
1	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	1	1	1	1	1
1,000E+00	1,606E-05	-1,836E-07	1,153E-05	4,544E-02	-	9,181E-01	6,433E-02	1,754E-02
1,000E+00	1,553E-05	-1,101E-07	1,116E-05	4,396E-02	-	9,184E-01	6,344E-02	1,813E-02
1,000E+00	1,592E-05	-1,103E-07	1,136E-05	4,506E-02	-	9,196E-01	6,250E-02	1,786E-02
1,000E+00	1,508E-05	-1,101E-07	1,094E-05	4,269E-02	-	9,198E-01	6,173E-02	1,852E-02
1,000E+00	1,745E-05	-1,825E-07	1,230E-05	4,865E-02	-	9,158E-01	6,250E-02	2,174E-02
1,000E+00	1,666E-05	-1,096E-07	1,162E-05	4,643E-02	-	9,191E-01	6,069E-02	2,023E-02
1,000E+00	1,616E-05	-7,295E-08	1,134E-05	4,504E-02	-	9,201E-01	5,917E-02	2,071E-02
1,000E+00	1,705E-05	-1,094E-07	1,189E-05	4,753E-02	-	9,183E-01	6,197E-02	1,972E-02
1,000E+00	1,599E-05	-1,097E-07	1,137E-05	4,456E-02	-	9,174E-01	6,195E-02	2,065E-02
1,000E+00	1,563E-05	-7,300E-08	1,102E-05	4,355E-02	-	9,207E-01	6,098E-02	1,829E-02
1,000E+00	1,722E-05	-1,107E-07	1,173E-05	4,801E-02	-	9,164E-01	6,340E-02	2,017E-02
1,000E+00	1,674E-05	-7,389E-08	1,138E-05	4,667E-02	-	9,167E-01	6,250E-02	2,083E-02

CO_x methanation @573 K

parameter			
	catalyst mass	5,000E-02	g
	reaction temperature	573	K
	reaction pressure	2,000E+05	Pa
	volumetric inlet flow rate	2,500E+02	mL_{STP} min^{-1}

feed ratio	consumption or formation rates for			conversion for		selectivity for		
CO/(CO+CO2)	CO	CO_2	CH_4	CO	CO_2	CH_4	C_2H_6	C_3H_8
z	$\Delta\dot{n}_{CO}$	$\Delta\dot{n}_{CO_2}$	$\Delta\dot{n}_{CH_4}$	X_{CO}	X_{CO2}	S_{CH4}	S_{C2H6}	S_{C3H8}
1	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	1	1	1	1	1
0,000E+00	-5,154E-06	3,030E-05	2,308E-05	-	7,766E-02	9,968E-01	3,226E-03	0,000E+00
0,000E+00	-4,995E-06	4,279E-05	2,326E-05	-	1,097E-01	9,968E-01	3,195E-03	0,000E+00
0,000E+00	-5,113E-06	4,045E-05	2,281E-05	-	1,037E-01	9,967E-01	3,263E-03	0,000E+00
0,000E+00	-5,052E-06	4,108E-05	2,260E-05	-	1,053E-01	9,983E-01	1,653E-03	0,000E+00
4,590E-02	1,187E-05	2,796E-05	2,696E-05	6,657E-01	7,547E-02	9,959E-01	4,127E-03	0,000E+00
4,590E-02	1,190E-05	2,741E-05	2,684E-05	6,675E-01	7,399E-02	9,959E-01	4,149E-03	0,000E+00
6,892E-02	1,880E-05	1,649E-05	2,918E-05	7,058E-01	4,582E-02	9,949E-01	5,089E-03	0,000E+00
6,892E-02	1,866E-05	1,437E-05	2,864E-05	7,007E-01	3,993E-02	9,948E-01	5,175E-03	0,000E+00
6,892E-02	1,866E-05	1,195E-05	2,853E-05	7,008E-01	3,322E-02	9,948E-01	5,242E-03	0,000E+00
9,237E-02	2,398E-05	1,727E-05	2,984E-05	6,745E-01	4,943E-02	9,926E-01	7,426E-03	0,000E+00
9,237E-02	2,394E-05	1,673E-05	2,984E-05	6,734E-01	4,788E-02	9,938E-01	6,219E-03	0,000E+00
1,109E-01	2,688E-05	9,081E-06	3,096E-05	6,315E-01	2,662E-02	9,905E-01	8,323E-03	1,189E-03
1,109E-01	2,662E-05	7,499E-06	3,044E-05	6,254E-01	2,198E-02	9,903E-01	8,464E-03	1,209E-03
1,109E-01	2,649E-05	3,871E-06	3,039E-05	6,223E-01	1,135E-02	9,902E-01	8,547E-03	1,221E-03
1,109E-01	2,623E-05	1,490E-07	2,992E-05	6,162E-01	4,367E-04	9,913E-01	7,500E-03	1,250E-03
1,871E-01	3,149E-05	1,307E-06	3,156E-05	4,416E-01	4,216E-03	9,838E-01	1,392E-02	2,320E-03
1,871E-01	3,107E-05	-1,072E-06	3,082E-05	4,357E-01	-3,461E-03	9,845E-01	1,310E-02	2,381E-03
1,871E-01	3,077E-05	9,402E-06	3,053E-05	4,314E-01	3,034E-02	9,855E-01	1,332E-02	1,211E-03
1,871E-01	3,013E-05	7,102E-06	2,986E-05	4,224E-01	2,292E-02	9,851E-01	1,361E-02	1,238E-03
3,139E-01	3,277E-05	6,184E-06	3,037E-05	2,782E-01	2,402E-02	9,750E-01	2,143E-02	3,571E-03
3,139E-01	3,204E-05	4,418E-06	2,955E-05	2,720E-01	1,716E-02	9,755E-01	2,083E-02	3,676E-03
3,139E-01	3,130E-05	-2,707E-06	2,888E-05	2,657E-01	-1,051E-02	9,747E-01	2,146E-02	3,788E-03
3,139E-01	3,038E-05	-5,483E-06	2,818E-05	2,579E-01	-2,129E-02	9,753E-01	2,078E-02	3,896E-03
4,823E-01	3,203E-05	-1,108E-07	2,844E-05	1,797E-01	-5,794E-04	9,622E-01	3,023E-02	7,557E-03
4,823E-01	3,101E-05	-1,036E-06	2,768E-05	1,740E-01	-5,415E-03	9,637E-01	2,979E-02	6,477E-03
4,823E-01	3,056E-05	2,391E-07	2,715E-05	1,715E-01	1,250E-03	9,642E-01	2,918E-02	6,631E-03
4,823E-01	2,936E-05	-4,906E-07	2,633E-05	1,647E-01	-2,565E-03	9,644E-01	2,877E-02	6,849E-03
7,388E-01	3,108E-05	1,235E-06	2,611E-05	1,163E-01	1,307E-02	9,475E-01	4,038E-02	1,211E-02
7,388E-01	2,949E-05	5,298E-07	2,513E-05	1,103E-01	5,607E-03	9,495E-01	3,927E-02	1,122E-02
7,388E-01	2,967E-05	1,231E-06	2,507E-05	1,110E-01	1,303E-02	9,493E-01	3,944E-02	1,127E-02
7,388E-01	2,812E-05	5,201E-07	2,411E-05	1,052E-01	5,504E-03	9,500E-01	3,971E-02	1,029E-02
1,000E+00	3,066E-05	-2,610E-07	2,423E-05	8,545E-02	-	9,366E-01	4,899E-02	1,441E-02
1,000E+00	2,885E-05	-1,866E-07	2,303E-05	8,041E-02	-	9,391E-01	4,718E-02	1,370E-02
1,000E+00	3,005E-05	-2,240E-07	2,371E-05	8,375E-02	-	9,366E-01	4,867E-02	1,475E-02
1,000E+00	2,825E-05	-1,871E-07	2,252E-05	7,872E-02	-	9,392E-01	4,680E-02	1,404E-02

CO_x methanation @533 K

Parameter			
	catalyst mass	5,000E-02	g
	reaction temperature	533	K
	reaction pressure	2,000E+05	Pa
	volumetric inlet flow rate	2,500E+02	mL_{STP} min^{-1}

feed ratio	consumption or formation rates for			conversion for		selectivity for		
CO/(CO+CO2)	CO	CO_2	CH_4	CO	CO_2	CH_4	C_2H_6	C_3H_8
z	$\Delta\dot{n}_{CO}$	$\Delta\dot{n}_{CO_2}$	$\Delta\dot{n}_{CH_4}$	X_{CO}	X_{CO2}	S_{CH4}	S_{C2H6}	S_{C3H8}
1	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	1	1	1	1	1
0,000E+00	-1,386E-06	1,896E-05	6,675E-06	-	4,858E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-1,421E-06	1,956E-05	6,776E-06	-	5,012E-02	9,947E-01	5,348E-03	0,000E+00
0,000E+00	-1,457E-06	1,913E-05	6,628E-06	-	4,902E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-1,425E-06	1,895E-05	6,577E-06	-	4,857E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-1,357E-06	1,933E-05	6,379E-06	-	4,955E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-1,357E-06	1,856E-05	6,160E-06	-	4,757E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-1,355E-06	1,854E-05	6,115E-06	-	4,751E-02	1,000E+00	0,000E+00	0,000E+00
4,590E-02	8,168E-06	1,112E-05	8,599E-06	4,583E-01	3,002E-02	9,874E-01	1,255E-02	0,000E+00
4,590E-02	8,156E-06	1,091E-05	8,427E-06	4,576E-01	2,946E-02	9,872E-01	1,282E-02	0,000E+00
4,590E-02	8,128E-06	1,079E-05	8,311E-06	4,560E-01	2,911E-02	9,870E-01	1,299E-02	0,000E+00
4,590E-02	7,566E-06	1,083E-05	7,767E-06	4,245E-01	2,923E-02	9,907E-01	9,346E-03	0,000E+00
4,590E-02	7,637E-06	1,072E-05	7,704E-06	4,285E-01	2,892E-02	9,906E-01	9,390E-03	0,000E+00
6,892E-02	8,272E-06	9,517E-06	8,270E-06	3,106E-01	2,645E-02	9,784E-01	1,724E-02	4,310E-03
6,892E-02	8,270E-06	9,261E-06	8,141E-06	3,105E-01	2,574E-02	9,781E-01	1,754E-02	4,386E-03
6,892E-02	7,638E-06	9,334E-06	7,525E-06	2,868E-01	2,594E-02	9,810E-01	1,429E-02	4,762E-03
6,892E-02	7,696E-06	9,133E-06	7,385E-06	2,890E-01	2,538E-02	9,806E-01	1,456E-02	4,854E-03
9,237E-02	8,245E-06	8,151E-06	7,923E-06	2,319E-01	2,333E-02	9,775E-01	1,802E-02	4,505E-03
9,237E-02	8,454E-06	8,040E-06	7,863E-06	2,378E-01	2,301E-02	9,773E-01	1,818E-02	4,545E-03
9,237E-02	7,424E-06	8,149E-06	7,280E-06	2,088E-01	2,333E-02	9,755E-01	1,961E-02	4,902E-03
9,237E-02	7,595E-06	8,140E-06	7,118E-06	2,136E-01	2,330E-02	9,749E-01	2,010E-02	5,025E-03
9,237E-02	7,679E-06	7,974E-06	7,042E-06	2,160E-01	2,282E-02	9,746E-01	2,030E-02	5,076E-03
1,109E-01	8,109E-06	7,806E-06	8,021E-06	1,905E-01	2,288E-02	9,735E-01	2,212E-02	4,425E-03
1,109E-01	8,069E-06	7,620E-06	7,673E-06	1,896E-01	2,234E-02	9,722E-01	2,315E-02	4,630E-03
1,109E-01	8,349E-06	7,321E-06	7,574E-06	1,962E-01	2,146E-02	9,718E-01	2,347E-02	4,695E-03
1,109E-01	7,409E-06	7,555E-06	7,141E-06	1,741E-01	2,215E-02	9,701E-01	2,488E-02	4,975E-03
1,109E-01	7,395E-06	7,425E-06	6,960E-06	1,737E-01	2,176E-02	9,694E-01	2,551E-02	5,102E-03
1,109E-01	7,664E-06	7,063E-06	6,899E-06	1,801E-01	2,070E-02	9,741E-01	2,073E-02	5,181E-03
1,871E-01	7,537E-06	6,251E-06	7,045E-06	1,057E-01	2,017E-02	9,550E-01	3,500E-02	1,000E-02
1,871E-01	8,095E-06	6,009E-06	6,943E-06	1,135E-01	1,939E-02	9,596E-01	3,030E-02	1,010E-02
1,871E-01	8,022E-06	5,773E-06	6,848E-06	1,125E-01	1,863E-02	9,588E-01	3,093E-02	1,031E-02
1,871E-01	6,972E-06	6,247E-06	6,675E-06	9,777E-02	2,016E-02	9,531E-01	3,646E-02	1,042E-02
1,871E-01	7,261E-06	6,147E-06	6,361E-06	1,018E-01	1,984E-02	9,558E-01	3,315E-02	1,105E-02
1,871E-01	7,414E-06	5,758E-06	6,224E-06	1,040E-01	1,858E-02	9,548E-01	3,390E-02	1,130E-02
3,139E-01	7,734E-06	4,086E-06	6,174E-06	6,566E-02	1,587E-02	9,385E-01	4,469E-02	1,676E-02
3,139E-01	7,922E-06	3,663E-06	6,092E-06	6,725E-02	1,422E-02	9,379E-01	4,520E-02	1,695E-02
3,139E-01	7,904E-06	3,546E-06	5,977E-06	6,710E-02	1,377E-02	9,422E-01	4,624E-02	1,156E-02
3,139E-01	7,349E-06	3,969E-06	5,618E-06	6,239E-02	1,541E-02	9,444E-01	4,321E-02	1,235E-02
3,139E-01	7,168E-06	3,574E-06	5,531E-06	6,085E-02	1,388E-02	9,438E-01	4,375E-02	1,250E-02
4,823E-01	7,309E-06	2,734E-06	5,371E-06	4,102E-02	1,429E-02	9,241E-01	5,696E-02	1,899E-02
4,823E-01	7,103E-06	2,388E-06	5,248E-06	3,986E-02	1,248E-02	9,226E-01	5,806E-02	1,935E-02
4,823E-01	6,751E-06	2,588E-06	4,965E-06	3,788E-02	1,353E-02	9,247E-01	5,479E-02	2,055E-02
4,823E-01	6,575E-06	2,349E-06	4,814E-06	3,689E-02	1,228E-02	9,225E-01	5,634E-02	2,113E-02
7,388E-01	6,839E-06	9,318E-07	4,541E-06	2,558E-02	9,861E-03	9,118E-01	6,618E-02	2,206E-02
7,388E-01	6,376E-06	8,096E-07	4,442E-06	2,385E-02	8,568E-03	9,098E-01	6,767E-02	2,256E-02
7,388E-01	6,393E-06	9,439E-07	4,299E-06	2,392E-02	9,990E-03	9,070E-01	6,977E-02	2,326E-02
7,388E-01	6,014E-06	7,843E-07	4,121E-06	2,250E-02	8,301E-03	9,032E-01	7,258E-02	2,419E-02
7,388E-01	5,859E-06	8,481E-07	4,073E-06	2,192E-02	8,975E-03	9,174E-01	6,612E-02	1,653E-02
1,000E+00	5,623E-06	-1,098E-07	4,244E-06	1,567E-02	-	8,992E-01	7,752E-02	2,326E-02
1,000E+00	7,008E-06	-1,101E-07	3,927E-06	1,953E-02	-	9,068E-01	7,627E-02	1,695E-02
1,000E+00	6,768E-06	-7,400E-08	3,774E-06	1,886E-02	-	9,027E-01	7,965E-02	1,770E-02
1,000E+00	7,333E-06	-3,673E-08	4,003E-06	2,044E-02	-	8,934E-01	8,197E-02	2,459E-02
1,000E+00	6,740E-06	-3,679E-08	3,789E-06	1,879E-02	-	9,035E-01	7,895E-02	1,754E-02
1,000E+00	6,494E-06	-3,678E-08	3,641E-06	1,810E-02	-	9,000E-01	8,182E-02	1,818E-02

CO_x methanation @513 K

Parameter			
Parameter	catalyst mass	5,000E-02	g
	reaction temperature	513	K
	reaction pressure	2,000E+05	Pa
	volumetric inlet flow rate	2,500E+02	mL_{STP} min^{-1}

feed ratio	consumption or formation rates for			conversion for		selectivity for		
CO/(CO+CO2)	CO	CO_2	CH_4	CO	CO_2	CH_4	C_2H_6	C_3H_8
z	$\Delta\dot{n}_{CO}$	$\Delta\dot{n}_{CO_2}$	$\Delta\dot{n}_{CH_4}$	X_{CO}	X_{CO2}	S_{CH4}	S_{C2H6}	S_{C3H8}
1	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	1	1	1	1	1
0,000E+00	-8,874E-07	1,227E-05	3,882E-06	-	3,145E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-8,529E-07	1,177E-05	3,857E-06	-	3,016E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-8,111E-07	6,252E-06	3,761E-06	-	1,602E-02	1,000E+00	0,000E+00	0,000E+00
0,000E+00	-8,482E-07	4,451E-06	3,725E-06	-	1,141E-02	1,000E+00	0,000E+00	0,000E+00
4,590E-02	4,468E-06	6,199E-06	4,489E-06	2,507E-01	1,673E-02	9,837E-01	1,626E-02	0,000E+00
4,590E-02	4,543E-06	4,975E-06	4,712E-06	2,549E-01	1,343E-02	9,845E-01	1,550E-02	0,000E+00
4,590E-02	4,248E-06	4,262E-06	4,291E-06	2,383E-01	1,150E-02	9,915E-01	8,547E-03	0,000E+00
4,590E-02	4,397E-06	3,188E-06	4,180E-06	2,467E-01	8,605E-03	9,826E-01	1,739E-02	0,000E+00
6,892E-02	4,324E-06	4,070E-06	4,262E-06	1,623E-01	1,131E-02	9,746E-01	1,695E-02	8,475E-03
6,892E-02	4,536E-06	3,122E-06	4,190E-06	1,703E-01	8,677E-03	9,741E-01	1,724E-02	8,621E-03
6,892E-02	4,143E-06	5,455E-06	3,971E-06	1,556E-01	1,516E-02	9,727E-01	1,818E-02	9,091E-03
6,892E-02	4,319E-06	4,627E-06	3,960E-06	1,622E-01	1,286E-02	9,727E-01	1,818E-02	9,091E-03
9,237E-02	4,262E-06	7,840E-07	4,037E-06	1,199E-01	2,244E-03	9,646E-01	2,655E-02	8,850E-03
9,237E-02	4,425E-06	3,083E-08	3,961E-06	1,245E-01	8,825E-05	9,640E-01	2,703E-02	9,009E-03
9,237E-02	4,010E-06	6,242E-06	3,781E-06	1,128E-01	1,787E-02	9,623E-01	2,830E-02	9,434E-03
9,237E-02	4,252E-06	5,163E-06	3,667E-06	1,196E-01	1,478E-02	9,612E-01	2,913E-02	9,709E-03
1,109E-01	4,147E-06	-1,581E-06	3,856E-06	9,744E-02	-4,636E-03	9,630E-01	2,778E-02	9,259E-03
1,109E-01	4,338E-06	-4,128E-06	3,778E-06	1,019E-01	-1,210E-02	9,623E-01	2,830E-02	9,434E-03
1,109E-01	3,886E-06	9,499E-06	3,627E-06	9,131E-02	2,784E-02	9,608E-01	2,941E-02	9,804E-03
1,109E-01	4,167E-06	8,442E-06	3,554E-06	9,791E-02	2,475E-02	9,600E-01	3,000E-02	1,000E-02
1,871E-01	4,192E-06	7,613E-06	3,447E-06	5,879E-02	2,457E-02	9,490E-01	4,082E-02	1,020E-02
1,871E-01	3,382E-06	6,533E-06	3,235E-06	4,743E-02	2,108E-02	9,457E-01	4,348E-02	1,087E-02
1,871E-01	3,964E-06	2,780E-06	3,094E-06	5,558E-02	8,970E-03	9,432E-01	4,545E-02	1,136E-02
3,139E-01	4,163E-06	-5,571E-06	2,935E-06	3,534E-02	-2,163E-02	9,405E-01	4,762E-02	1,190E-02
3,139E-01	3,155E-06	-3,173E-06	2,790E-06	2,678E-02	-1,232E-02	9,259E-01	4,938E-02	2,469E-02
3,139E-01	3,885E-06	-6,736E-06	2,647E-06	3,298E-02	-2,616E-02	9,342E-01	5,263E-02	1,316E-02
4,823E-01	3,435E-06	1,467E-06	2,490E-06	1,928E-02	7,667E-03	9,178E-01	6,849E-02	1,370E-02
4,823E-01	2,754E-06	-1,714E-06	2,380E-06	1,545E-02	-8,960E-03	9,143E-01	7,143E-02	1,429E-02
4,823E-01	3,351E-06	-2,389E-06	2,232E-06	1,880E-02	-1,249E-02	9,231E-01	6,154E-02	1,538E-02
7,388E-01	3,129E-06	1,286E-08	2,045E-06	1,171E-02	1,361E-04	9,016E-01	8,197E-02	1,639E-02
7,388E-01	2,632E-06	-7,165E-07	2,080E-06	9,845E-03	-7,583E-03	9,032E-01	8,065E-02	1,613E-02
7,388E-01	2,954E-06	-1,065E-06	1,894E-06	1,105E-02	-1,127E-02	8,947E-01	8,772E-02	1,754E-02
1,000E+00	2,135E-06	-1,113E-07	1,966E-06	5,950E-03	-	8,833E-01	1,000E-01	1,667E-02
1,000E+00	4,670E-06	-3,714E-08	1,746E-06	1,302E-02	-	8,868E-01	9,434E-02	1,887E-02
1,000E+00	3,008E-06	-3,718E-08	1,376E-06	8,384E-03	-	8,605E-01	1,163E-01	2,326E-02
1,000E+00	3,540E-06	-3,724E-08	1,713E-06	9,867E-03	-	8,846E-01	9,615E-02	1,923E-02

CO methanation @556 K

Parameter			
	catalyst mass	5,000E-02	g
	reaction temperature	556	K
	reaction pressure	2,000E+05	Pa
	volumetric inlet flow rate	2,500E+02	mL_{STP} min^{-1}

feed ratio	consumption or formation rates for			conversion for		selectivity for		
CO/(CO+CO2)	CO	CO_2	CH_4	CO	CO_2	CH_4	C_2H_6	C_3H_8
z	$\Delta\dot{n}_{CO}$	$\Delta\dot{n}_{CO_2}$	$\Delta\dot{n}_{CH_4}$	X_{CO}	X_{CO2}	S_{CH4}	S_{C2H6}	S_{C3H8}
1	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	1	1	1	1	1
5,216E-02	-3,304E-04	1,474E-06	1,599E-05	8,979E-01	-	9,931E-01	6,881E-03	0,000E+00
5,216E-02	-3,311E-04	1,475E-06	1,577E-05	8,961E-01	-	9,953E-01	4,651E-03	0,000E+00
5,216E-02	0,000E+00	0,000E+00	1,564E-05	8,980E-01	-	9,953E-01	4,695E-03	0,000E+00
7,646E-02	-3,783E-04	2,181E-06	1,838E-05	7,005E-01	-	9,902E-01	9,823E-03	0,000E+00
7,646E-02	-3,781E-04	2,195E-06	1,811E-05	7,000E-01	-	9,920E-01	7,968E-03	0,000E+00
7,646E-02	-3,769E-04	2,187E-06	1,796E-05	6,995E-01	-	9,919E-01	8,081E-03	0,000E+00
7,646E-02	-3,581E-04	1,471E-06	1,725E-05	6,651E-01	-	9,915E-01	8,493E-03	0,000E+00
7,646E-02	-3,569E-04	1,475E-06	1,692E-05	6,625E-01	-	9,914E-01	8,621E-03	0,000E+00
7,646E-02	-3,311E-04	1,477E-06	1,678E-05	6,603E-01	-	9,913E-01	8,715E-03	0,000E+00
1,015E-01	-4,478E-04	1,457E-06	2,130E-05	6,329E-01	-	9,882E-01	1,015E-02	1,692E-03
1,015E-01	-4,273E-04	1,457E-06	2,097E-05	6,295E-01	-	9,880E-01	1,029E-02	1,715E-03
1,015E-01	-3,781E-04	2,189E-06	1,816E-05	5,254E-01	-	9,861E-01	1,188E-02	1,980E-03
1,015E-01	-3,772E-04	2,200E-06	1,788E-05	5,270E-01	-	9,859E-01	1,207E-02	2,012E-03
1,015E-01	-3,710E-04	2,193E-06	1,771E-05	5,257E-01	-	9,857E-01	1,224E-02	2,041E-03
1,015E-01	-3,562E-04	1,480E-06	1,699E-05	4,977E-01	-	9,850E-01	1,282E-02	2,137E-03
1,015E-01	-3,555E-04	1,477E-06	1,665E-05	4,966E-01	-	9,847E-01	1,313E-02	2,188E-03
1,015E-01	-3,595E-04	1,477E-06	1,651E-05	4,955E-01	-	9,868E-01	1,104E-02	2,208E-03
1,207E-01	-3,721E-04	2,191E-06	1,773E-05	4,347E-01	-	9,838E-01	1,420E-02	2,028E-03
1,207E-01	-3,701E-04	2,194E-06	1,749E-05	4,360E-01	-	9,836E-01	1,437E-02	2,053E-03
1,207E-01	-3,554E-04	2,190E-06	1,733E-05	4,337E-01	-	9,834E-01	1,452E-02	2,075E-03
1,207E-01	-3,514E-04	1,472E-06	1,667E-05	4,132E-01	-	9,826E-01	1,522E-02	2,174E-03
1,207E-01	-3,496E-04	1,475E-06	1,634E-05	4,117E-01	-	9,823E-01	1,549E-02	2,212E-03
1,207E-01	-3,570E-04	1,474E-06	1,616E-05	4,096E-01	-	9,843E-01	1,348E-02	2,247E-03
2,000E-01	-4,277E-04	1,461E-06	2,010E-05	3,011E-01	-	9,753E-01	2,120E-02	3,534E-03
2,000E-01	-4,200E-04	1,460E-06	1,929E-05	3,014E-01	-	9,760E-01	2,033E-02	3,697E-03
2,000E-01	-3,936E-04	1,470E-06	1,898E-05	2,960E-01	-	9,756E-01	2,064E-02	3,752E-03
2,000E-01	-3,581E-04	2,195E-06	1,654E-05	2,514E-01	-	9,742E-01	2,151E-02	4,301E-03
2,000E-01	-3,526E-04	2,199E-06	1,624E-05	2,533E-01	-	9,737E-01	2,193E-02	4,386E-03
2,000E-01	-3,383E-04	1,468E-06	1,609E-05	2,493E-01	-	9,734E-01	2,217E-02	4,435E-03
2,000E-01	-3,356E-04	1,472E-06	1,545E-05	2,345E-01	-	9,722E-01	2,315E-02	4,630E-03
2,000E-01	-3,323E-04	1,473E-06	1,516E-05	2,373E-01	-	9,740E-01	2,128E-02	4,728E-03
2,000E-01	-3,527E-04	1,475E-06	1,495E-05	2,350E-01	-	9,736E-01	2,158E-02	4,796E-03
3,285E-01	-3,342E-04	1,473E-06	1,501E-05	1,457E-01	-	9,601E-01	3,286E-02	7,042E-03
3,285E-01	-3,325E-04	1,467E-06	1,469E-05	1,439E-01	-	9,614E-01	3,133E-02	7,229E-03
3,285E-01	-3,233E-04	1,471E-06	1,442E-05	1,432E-01	-	9,609E-01	3,178E-02	7,335E-03
3,285E-01	-3,171E-04	2,206E-06	1,398E-05	1,357E-01	-	9,596E-01	3,283E-02	7,576E-03
3,285E-01	-3,106E-04	1,474E-06	1,364E-05	1,366E-01	-	9,611E-01	3,109E-02	7,772E-03
3,285E-01	-3,315E-04	1,472E-06	1,349E-05	1,337E-01	-	9,606E-01	3,150E-02	7,874E-03
4,988E-01	-3,858E-04	1,467E-06	1,606E-05	1,104E-01	-	9,459E-01	4,113E-02	1,299E-02
4,988E-01	-3,786E-04	1,469E-06	1,558E-05	1,082E-01	-	9,465E-01	4,009E-02	1,336E-02
4,988E-01	-3,765E-04	2,209E-06	1,527E-05	1,062E-01	-	9,455E-01	4,091E-02	1,364E-02
4,988E-01	-3,183E-04	2,211E-06	1,349E-05	9,167E-02	-	9,483E-01	4,134E-02	1,034E-02
4,988E-01	-3,082E-04	2,217E-06	1,316E-05	9,027E-02	-	9,469E-01	4,244E-02	1,061E-02
4,988E-01	-3,085E-04	2,218E-06	1,293E-05	8,739E-02	-	9,485E-01	4,065E-02	1,084E-02
4,988E-01	-3,003E-04	1,478E-06	1,274E-05	8,716E-02	-	9,451E-01	4,396E-02	1,099E-02
4,988E-01	-2,941E-04	1,479E-06	1,231E-05	8,515E-02	-	9,460E-01	4,261E-02	1,136E-02
4,988E-01	-3,150E-04	1,472E-06	1,209E-05	8,341E-02	-	9,451E-01	4,335E-02	1,156E-02
7,480E-01	-2,960E-04	2,219E-06	1,187E-05	5,835E-02	-	9,304E-01	5,507E-02	1,449E-02
7,480E-01	-2,863E-04	2,214E-06	1,147E-05	5,598E-02	-	9,309E-01	5,405E-02	1,502E-02
7,480E-01	-3,090E-04	1,477E-06	1,122E-05	5,415E-02	-	9,325E-01	5,215E-02	1,534E-02
7,480E-01	-2,843E-04	1,480E-06	1,134E-05	5,601E-02	-	9,301E-01	5,471E-02	1,520E-02
7,480E-01	-2,800E-04	1,481E-06	1,091E-05	5,377E-02	-	9,306E-01	5,363E-02	1,577E-02
7,480E-01	-3,073E-04	1,482E-06	1,070E-05	5,295E-02	-	9,323E-01	5,484E-02	1,290E-02
1,000E+00	-3,587E-04	1,473E-06	1,266E-05	5,246E-02	-	9,173E-01	6,133E-02	2,133E-02
1,000E+00	-3,455E-04	1,476E-06	1,215E-05	4,997E-02	-	9,167E-01	6,111E-02	2,222E-02
1,000E+00	-3,786E-04	2,188E-06	1,181E-05	4,813E-02	-	9,195E-01	6,034E-02	2,011E-02
1,000E+00	-3,001E-04	2,218E-06	1,056E-05	4,371E-02	-	9,167E-01	6,410E-02	1,923E-02
1,000E+00	-2,870E-04	1,481E-06	1,024E-05	4,246E-02	-	9,203E-01	6,312E-02	1,661E-02
1,000E+00	-3,086E-04	2,223E-06	9,886E-06	4,061E-02	-	9,207E-01	6,207E-02	1,724E-02
1,000E+00	-2,944E-04	1,486E-06	1,041E-05	4,366E-02	-	9,183E-01	6,536E-02	1,634E-02
1,000E+00	-2,819E-04	1,485E-06	9,955E-06	4,165E-02	-	9,178E-01	6,507E-02	1,712E-02
1,000E+00	-2,962E-04	1,482E-06	9,801E-06	3,988E-02	-	9,199E-01	6,272E-02	1,742E-02

CO_2 methanation @556 K

Parameter			
	catalyst mass	5,000E-02	g
	reaction temperature	556	K
	reaction pressure	2,000E+05	Pa
	volumetric inlet flow rate	2,500E+02	mL_{STP} min^{-1}

feed ratio	consumption or formation rates for			conversion for		selectivity for		
CO/(CO+CO2)	CO	CO_2	CH_4	CO	CO_2	CH_4	C_2H_6	C_3H_8
z	$\Delta\dot{n}_{CO}$	$\Delta\dot{n}_{CO_2}$	$\Delta\dot{n}_{CH_4}$	X_{CO}	X_{CO2}	S_{CH4}	S_{C2H6}	S_{C3H8}
1	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	mol g^{-1} s^{-1}	1	1	1	1	1
0,000E+00	6,489E-05	-2,364E-04	1,486E-05	-	3,171E-02	9,975E-01	2,475E-03	0,000E+00
0,000E+00	6,567E-05	-2,233E-04	1,461E-05	-	2,995E-02	9,975E-01	2,519E-03	0,000E+00
0,000E+00	6,562E-05	-2,124E-04	1,452E-05	-	2,848E-02	9,975E-01	2,532E-03	0,000E+00
0,000E+00	6,583E-05	-3,981E-04	1,446E-05	-	5,339E-02	9,974E-01	2,551E-03	0,000E+00
0,000E+00	6,593E-05	-3,703E-04	1,430E-05	-	4,966E-02	9,974E-01	2,584E-03	0,000E+00
0,000E+00	6,758E-05	-3,497E-04	1,422E-05	-	4,689E-02	9,974E-01	2,604E-03	0,000E+00
0,000E+00	6,421E-05	-2,579E-04	1,509E-05	-	3,459E-02	9,976E-01	2,439E-03	0,000E+00
0,000E+00	6,484E-05	-2,324E-04	1,492E-05	-	3,116E-02	9,975E-01	2,463E-03	0,000E+00
0,000E+00	6,492E-05	-1,508E-04	1,509E-05	-	2,023E-02	9,976E-01	2,439E-03	0,000E+00
0,000E+00	6,536E-05	-1,218E-04	1,495E-05	-	1,633E-02	9,975E-01	2,451E-03	0,000E+00
0,000E+00	6,585E-05	-1,044E-04	1,487E-05	-	1,400E-02	9,975E-01	2,481E-03	0,000E+00
4,763E-02	6,202E-05	-2,441E-04	1,484E-05	-	3,447E-02	9,975E-01	2,481E-03	0,000E+00
4,763E-02	6,271E-05	-2,301E-04	1,453E-05	-	3,249E-02	9,975E-01	2,532E-03	0,000E+00
4,763E-02	6,263E-05	-2,239E-04	1,440E-05	-	3,163E-02	9,974E-01	2,551E-03	0,000E+00
4,763E-02	6,371E-05	-2,386E-04	1,437E-05	-	3,369E-02	9,974E-01	2,571E-03	0,000E+00
4,763E-02	6,442E-05	-2,232E-04	1,425E-05	-	3,152E-02	9,974E-01	2,591E-03	0,000E+00
4,763E-02	6,527E-05	-2,220E-04	1,413E-05	-	3,136E-02	9,974E-01	2,618E-03	0,000E+00
7,368E-02	6,063E-05	-2,398E-04	1,479E-05	-	3,482E-02	9,975E-01	2,494E-03	0,000E+00
7,368E-02	6,113E-05	-2,307E-04	1,451E-05	-	3,350E-02	9,975E-01	2,532E-03	0,000E+00
7,368E-02	6,116E-05	-2,280E-04	1,440E-05	-	3,311E-02	9,974E-01	2,551E-03	0,000E+00
7,368E-02	6,212E-05	-2,522E-04	1,435E-05	-	3,662E-02	9,974E-01	2,571E-03	0,000E+00
7,368E-02	6,295E-05	-2,376E-04	1,422E-05	-	3,450E-02	9,974E-01	2,597E-03	0,000E+00
7,368E-02	6,307E-05	-2,335E-04	1,413E-05	-	3,391E-02	9,974E-01	2,618E-03	0,000E+00
1,002E-01	5,898E-05	-2,370E-04	1,475E-05	-	3,542E-02	9,975E-01	2,494E-03	0,000E+00
1,002E-01	5,969E-05	-2,310E-04	1,444E-05	-	3,453E-02	9,975E-01	2,545E-03	0,000E+00
1,002E-01	6,048E-05	-2,171E-04	1,431E-05	-	3,246E-02	9,974E-01	2,571E-03	0,000E+00
1,002E-01	6,079E-05	-2,435E-04	1,435E-05	-	3,640E-02	9,974E-01	2,577E-03	0,000E+00
1,002E-01	6,067E-05	-2,287E-04	1,420E-05	-	3,419E-02	9,974E-01	2,597E-03	0,000E+00
1,002E-01	6,145E-05	-2,319E-04	1,403E-05	-	3,466E-02	9,974E-01	2,632E-03	0,000E+00
1,207E-01	5,588E-05	-3,939E-04	1,478E-05	-	6,026E-02	9,975E-01	2,481E-03	0,000E+00
1,207E-01	5,812E-05	-3,810E-04	1,438E-05	-	5,828E-02	9,974E-01	2,551E-03	0,000E+00
1,207E-01	5,893E-05	-3,623E-04	1,429E-05	-	5,543E-02	9,974E-01	2,571E-03	0,000E+00
1,207E-01	5,931E-05	-2,577E-04	1,427E-05	-	3,942E-02	9,974E-01	2,591E-03	0,000E+00
1,207E-01	6,017E-05	-2,465E-04	1,411E-05	-	3,771E-02	9,974E-01	2,625E-03	0,000E+00
1,207E-01	5,993E-05	-2,401E-04	1,410E-05	-	3,673E-02	9,974E-01	2,618E-03	0,000E+00
1,207E-01	5,714E-05	-2,172E-04	1,498E-05	-	3,323E-02	9,976E-01	2,439E-03	0,000E+00
1,207E-01	5,860E-05	-1,937E-04	1,483E-05	-	2,963E-02	9,975E-01	2,463E-03	0,000E+00
2,024E-01	5,290E-05	-3,307E-04	1,470E-05	-	5,577E-02	9,975E-01	2,494E-03	0,000E+00
2,024E-01	5,431E-05	-3,117E-04	1,431E-05	-	5,256E-02	9,974E-01	2,558E-03	0,000E+00
2,024E-01	5,366E-05	-3,055E-04	1,415E-05	-	5,152E-02	9,974E-01	2,591E-03	0,000E+00
2,024E-01	5,469E-05	-2,505E-04	1,415E-05	-	4,225E-02	9,974E-01	2,604E-03	0,000E+00
2,024E-01	5,484E-05	-2,414E-04	1,408E-05	-	4,071E-02	9,974E-01	2,625E-03	0,000E+00
3,344E-01	4,535E-05	-3,024E-04	1,452E-05	-	6,112E-02	9,975E-01	2,513E-03	0,000E+00
3,344E-01	4,554E-05	-2,843E-04	1,410E-05	-	5,746E-02	9,974E-01	2,597E-03	0,000E+00
3,344E-01	4,638E-05	-2,774E-04	1,402E-05	-	5,606E-02	9,974E-01	2,618E-03	0,000E+00
3,344E-01	4,645E-05	-2,550E-04	1,401E-05	-	5,153E-02	9,974E-01	2,625E-03	0,000E+00
3,344E-01	4,672E-05	-2,459E-04	1,390E-05	-	4,970E-02	9,973E-01	2,660E-03	0,000E+00
5,054E-01	3,688E-05	-2,402E-04	1,372E-05	-	6,532E-02	9,973E-01	2,681E-03	0,000E+00
5,054E-01	3,683E-05	-2,149E-04	1,363E-05	-	5,843E-02	9,973E-01	2,695E-03	0,000E+00
5,054E-01	3,608E-05	-2,564E-04	1,370E-05	-	6,972E-02	9,973E-01	2,681E-03	0,000E+00
5,054E-01	3,629E-05	-2,499E-04	1,359E-05	-	6,797E-02	9,973E-01	2,717E-03	0,000E+00
7,549E-01	1,987E-05	-2,601E-04	1,266E-05	-	1,427E-01	9,971E-01	2,899E-03	0,000E+00
7,549E-01	1,916E-05	-2,570E-04	1,257E-05	-	1,410E-01	9,971E-01	2,924E-03	0,000E+00
7,549E-01	1,992E-05	-2,450E-04	1,262E-05	-	1,344E-01	9,971E-01	2,915E-03	0,000E+00
7,549E-01	1,988E-05	-2,397E-04	1,252E-05	-	1,315E-01	9,971E-01	2,933E-03	0,000E+00

REFERENCES

(1) Mears, D. E. Tests for transport limitations in experimental catalytic reactors. *Ind. Eng. Chem. Process Des. Dev.* **1971**, *10*, 541–547.

(2) Anderson, J. B. A criterion for isothermal behaviour of a catalyst pellet. *Chem. Eng. Sci.* **1963**, *18*.

(3) Dekker, F. H.M.; Bliek, A.; Kapteijn, F.; Moulijn, J. A. Analysis of mass and heat transfer in transient experiments over heterogeneous catalysts. *Chem. Eng. Sci.* **1995**, *50*, 3573–3580.