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Supporting Information

Tab. S1: Characteristic temperatures and CO conversion of a cooled multi-tubular fixed bed FT reactor for a uniform axial activity (C_a). Assumptions: 1) $T_{max,ax}$ < 240°C to avoid excessive methane formation; 2) $T_{cool,max} = T_{cool,\ ignition}$ - 5 K to ensure thermal stability of reactor; 3) C_a < 4, corresponding to a realistic value of the max. Co content of 40 wt.-%.

C_a	X_{CO}[a] in %	T_{cool} in °C	T_{ig} in °C	$T_{max,ax}$ in °C	$r_{m,eff,CO}$ (η_{pore} in %) at $T_{max,ax}$ for X_{CO} = 0 in $mol_{CO}\ kg_{cat}^{-1}\ s^{-1}$
0.25	21.2	231.0	249.0	240.0	0.00262 (70%)
0.5	29.8	226.1	237.7	240.0	0.00417 (55%)
1	38.4	220.1	226.6	240.0	0.00621 (42%)
1.125	39.8	219.0	224.8	240.0	0.00662 (39%)
1.25 (best case)	**40.9**	**218.0**	**223.1**	**240.0**	**0.00700 (37%)**
1.5	40.6	215.3	220.3	237.1	0.00696 (38%)
2	39.8	211.0	216.0	232.2	0.00679 (39%)
3	38.5	205.0	210.0	225.1	0.00645 (41%)
4	37.4	200.8	205.8	220.1	0.00621 (43%)

[a] It may be interesting to know X_{CO} reached at the maximum axial temperature ($z \approx$ about 2 m, see Fig.3): 4% (C_a = 0.25), 5% for C_a = 0.5, 8% (C_a = 1.25), 8% (C_a = 1.5), and 1% (C_a = 3 and 4).

A good approximation for the maximum temperature difference between the maximum axial temperature and the cooling temperature to avoid a temperature runaway of a cooled fixed bed reactor is given by:[1]

$$\Delta T_{max} = T^*_{max,ax} - T_{max,cool} = \frac{R\, T^*_{max,ax}\, T_{max,cool}}{E_{A,eff}} \quad \text{(S1)}$$

The temperatures $T^*_{max,ax}$ and $T_{max,cool}$ are the highest values of the axial temperature (center of bed) and the cooling temperature, respectively, to avoid a thermal runaway.

The effective activation energy $E_{A,eff}$ valid for the axial position, where $T_{max,ax}$ is just reached, is calculated based on the mean radial temperature $T_{mean} = 0.5\ (T_{max,ax} - T_{cool})$ by:

$$E_{A,eff} = \frac{R\ ln\left(\frac{r_{CO,eff,T_{mean}}}{r_{CO,eff,T_{mean}+1\,K}}\right)}{\left[\frac{1}{(T_{mean}+1\,K)} - \frac{1}{T_{mean}}\right]} \quad \text{(S2)}$$

Tab. S2 shows the values of ΔT_{max} calculated by the reactor model and by the approximation based on Eq. (S1) and Eq. (S2). The deviation of only about 2 K is small, and hence, the agreement is quite well, which is also a good proof, that the calculations by the reactor model are reliable.

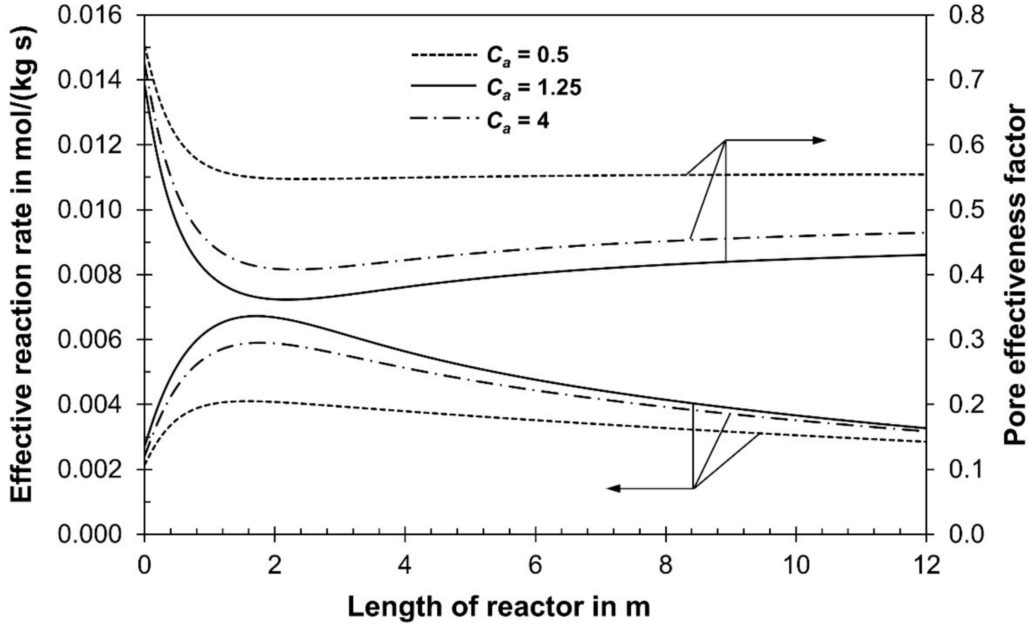

Fig. S1: Axial profiles of effective rate of conversion of CO and pore effectiveness factor in a cooled fixed bed FT reactor for three different but uniform axial activities (value of C_a) (conditions/assumptions see Fig. 3 - 5).

Tab. S2: Temperature difference between highest axial temperature (center of tube) and cooling temperature: Comparison of selected modelled values and estimations based on equations (S1) and (S2). Case of cooled fixed bed FT reactor for different but uniform axial activities (value of C_a) (conditions/assumptions see Figs. 3 to 5).

C_a	**Values of reactor model**				**Calculations by Eq. (S1) and Eq. (S2)**	
	$T^*_{max,ax}$ in °C	$T_{max,cool}$ in °C	T_{mean} in °C	$T^*_{max,ax} - T_{cool}$ in K	$E_{a,eff}$ (T_{mean}) in kJ/mol	$\Delta T_{max} = R\, T_{max,ax}\, T_{cool} / E_{a,eff}$ in K
Cases for $T_{cool,max} = T_{ig}$ - 5 K (only limited by runaway)						
0.25	265.5	244.3	257.4	26.1	82	28.5
0.5	257.7	232.7	245.2	25.0	84	26.6
1	244.6	221.6	233.1	23.0	87	24.5
1.5	237.1	215.3	226.2	21.8	89	23.3
2	232.2	211.0	221.6	21.1	90	22.6
3	225.1	205.0	215.1	19.3	92	21.5

4	220.1	200.8	210.5	18.9	94	20.7

Tab. S3: Characteristic temperatures and CO conversion of a two-zone FT reactor for different activities in both zones but constant mean activity of $C_{a,mean}$ of 1.25 = 0.5 ($C_{a,1}$ + $C_{a,2}$). Assumptions: 1) $T_{max,ax}$ < 240°C to avoid excessive formation of CH_4; 2) $T_{cool,max}$ = $T_{cool,\ ignition}$ - 5 K to ensure thermal stability of reactor.

Activity in zone 1 (z < 6 m) **and zone 2** (6 m < z < 12 m)		X_{CO} in %	T_{cool} in °C	T_{ig} in °C	$T_{max,ax,1}$ in °C	$T_{max,ax,2}$ in °C
$C_{a,1}$	$C_{a,2}$					
0.5	2	30.4	213.0	218.0	217.6	236.6
0.75	1.75	36.5	216.1	231.1	225.8	240.0
0.9	1.6	39.7	217.7	228.2	231.6	240.0
0.95	1.55	40.8	218.2	227.4	233.7	240.0
1	1.5	42.1	218.7	226.6	236.1	240.0
1.05	1.45	43.6	219.3	225.8	238.9	240.0
1.067 (best case)	**1.433**	**44.1**	**219.5**	**225.5**	**240.0**	**240.0**
1.1	1.4	43.4	219.2	225.1	240.0	238.5
1.175	1.325	42.1	219.3	224.1	240.0	236.0
1.25	1.25	40.9	218.0	223.1	240.0	234.6[a]
1.5	1	35.4	215.3	220.3	237.1	231.8

[a] In this case, there is no local maximum in axial temperature in the rear part of the bed. The given temperature is just the value reached at *z* = 6, i.e. at the entrance in zone 2.

Tab. S4: Characteristic temperatures and CO conversion of a cooled fixed bed two-zone FT reactor for different activities in the two zones of equal length (6 m). Assumptions: 1) $T_{max,ax}$ < 240°C to avoid excessive CH_4 formation; 2) $T_{cool,max}$ = $T_{cool,\ ignition}$ - 5 K to ensure thermal stability of reactor; 3) C_a < 4, which corresponds to a realistic value of maximum Co content of about 40 wt.-%.

Activity in zone 1 (z < 6 m) **and zone 2** (6 m < z < 12 m)		**Mean activity**	X_{CO} in %	T_{cool} in °C	$T_{cool,\ ig}$ in °C	$T_{max,ax,1}$ in °C	$T_{max,ax,2}$ in °C
$C_{a,1}$	$C_{a,2}$	$C_{a,mean}$					
0.5	0.59	0.545	32.1	226	237.7	239.9	240.0
0.75	0.95	0.85	38.5	222.6	231.1	239.8	240.0
1	1.35	1.175	43.1	220.0	226.6	239.7	239.9
1.25	2.75	2	41.7	211.7	216.7[a]	223.8	239.5
1.5	2.2	1.85	47.5	215.3	220.3	237.1	238.7
1.62	2.38	2	47.2	214.1	219.1	235.7	237.3
2	3.45	2.725	50.4	210.9	216.0	231.8	240
2	4	3	47.8	208.3	216.0	224.4	240.0
2.25	4	3.125	51.2	209.2	214.2	230.0	240
2.26 (best case)	**4**	**3.13**	**51.3**	**209.2**	**214.2**	**230.1**	**240**
2.27	4	3.135	51.0	209.1	214.1	229.9	239.5
2.28	4	3.14	50.7	209.0	214.0	229.7	239.1
2.3	4	3.15	50.7	208.9	213.9	230.0	239.0
2.5	4	3.25	48.1	207.7	212.7	228.3	233.5
2.75	4	3.375	45.6	206.3	211.3	226.7	228.9
3.5	4	3.75	40.2	202.8	207.8	222.6	219.7
4	4	4	37.4	200.8	205.8	220.1	216.1

[a] In contrast to all other cases, here the ignition (thermal runaway) takes place in the second zone.

Tab. S5: Optimal distribution of activity in a two-zone FT reactor for different mean activities (each zone has a length of 6 m). Assumptions: 1) $T_{max,ax}$ < 240°C to avoid excessive CH_4 formation; 2) $T_{cool,max} = T_{cool,\ ignition}$ - 5 K to ensure stability of reactor; 3) C_a < 4, which corresponds to a realistic value of maximum Co content of about 40 wt.-%.

Optimal activity in zone 1 (z < 6 m) **and zone 2** (6 m < z < 12 m)		**Mean activity**	X_{CO} in %	T_{cool} in °C	$T_{cool,\ ig}$ in °C	$T_{max,ax,1}$ in °C	$T_{max,ax,2}$ in °C
$C_{a,1}$	$C_{a,2}$	$C_{a,mean}$					
0.465	0.535	0.5	30.9	226.6	238.9	240.0	239.9
0.752	0.948	0.85	38.7	222.7	231.0	240.0	240.0
1.067	1.433	1.25	44.1	219.5	225.6	240.0	240.0
1.56	2.44	2	48.8	214.7	219.7	236.4	240.0
2.26	4	3.13	51.3	209.2	214.2	230.1	240.0
3	4	3.5	43.4	205.0	210.0	225.1	225.1
4	4	4	37.4	200.8	205.8	220.1	216.1

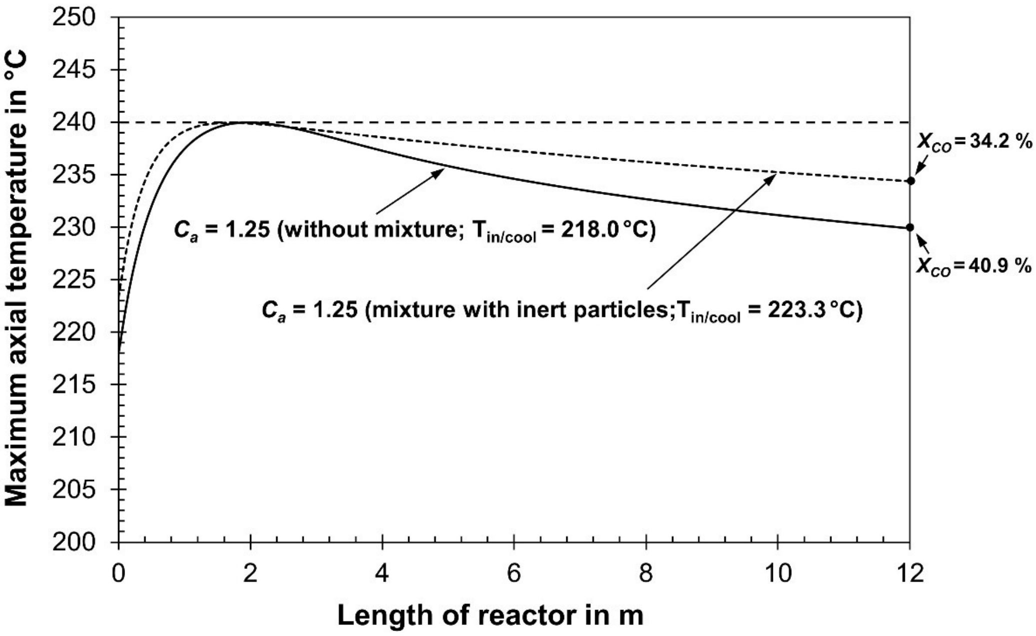

Fig. S2: Axial temperature profiles in the center of a single tube (r = 0) of a cooled fixed bed FT reactor and CO conversion for a constant (mean) value of activity coefficient C_a of 1.25. Case 1: C_a = 1.25 is realized by catalyst particles with C_a = 1.25 without dilution with inert particles. Case 2: C_a = 1.25 is realized by a 1-to-1 mixture of catalyst particles (C_a = 2.5) with inert particles (same density. C_a = 0). i.e. $m_{cat} = m_{inert}$. Other assumptions and conditions as given in Fig. 3.