Electronic Supplementary Information

Investigation of the Deactivation of a Washcoated Monolith Using a Spatially Resolved Technique

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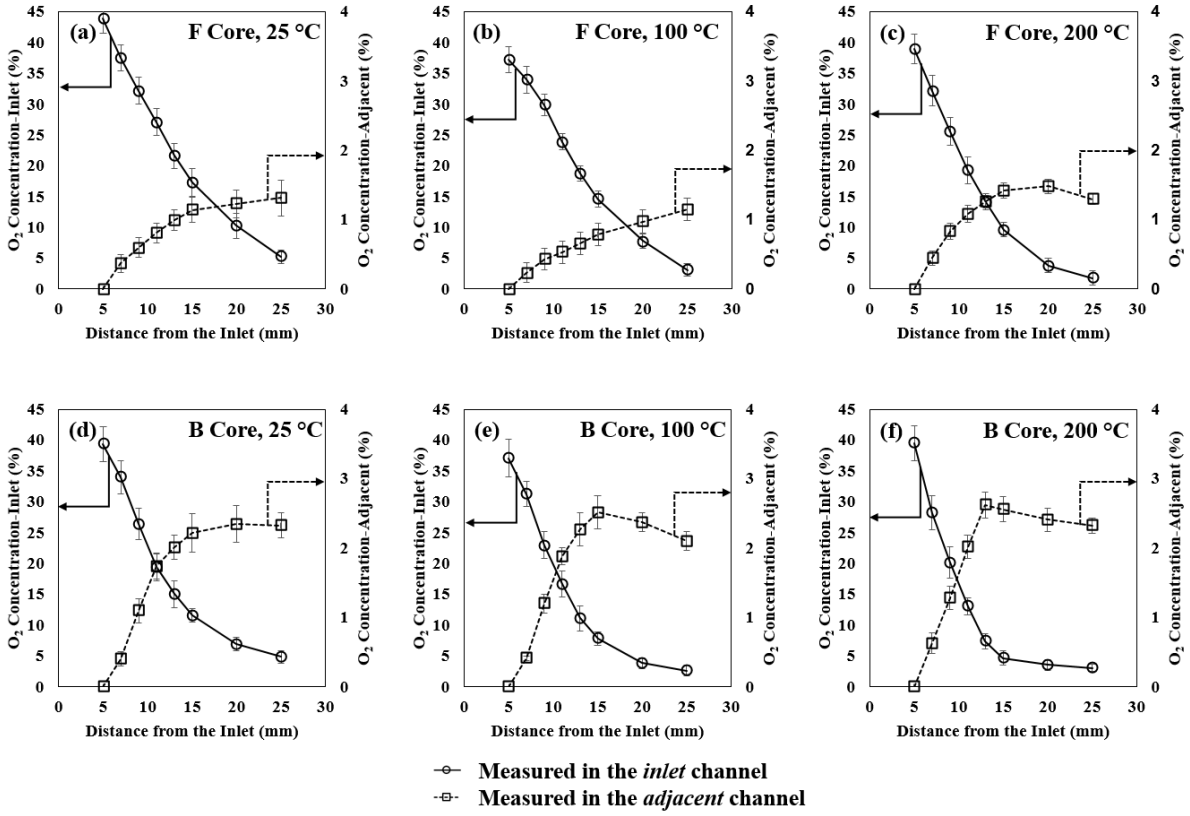
Experiment Description:

The monolith core was placed inside a sealed stainless-steel reactor (internal diameter ca. 20 mm, length 200 mm) and heated by a 1 m long tubular split-furnace, manufactured by Carbolite. The temperature data was recorded continuously with type K Omega thermocouples with an outer diameter of 250 µm. The thermocouples were connected to a Pico technology 8-port interface which logged the temperature readings. Open-ended fused silica capillaries (Polymicro Technologies), of outer diameter 220 µm, were used to sample the gaseous species and were axially inserted inside the monolith channels. A Hiden HPR20 quartz inlet capillary quadrupole MS was connected to the sampling unit using a heated capillary. To gain information at various axial positions within the monolith, the capillaries and thermocouples are moved along the length of the monolith during the experiment. This motion was provided by a z-motion drive unit consisting of a stepper motor and bellows coupled to a Thorlabs APT Microstepping Controller (BSC101) toolbox. The smallest movement of the probes is steps of 0.1 mm with an accuracy of ±5%. To ensure that no gaseous species fed via the inlet capillary leaked to neighbouring channels from the upstream face of the monolith core, the inlet capillary was positioned at a distance of 3 mm into the central channel (Fig. 4(b)). To minimise the impact of unsteady flow at the exit of the inlet capillary, which may lead to fluctuation artefacts in the MS detection, a gap of 2 mm between the sampling capillary and the inlet capillary was set up at the starting position.



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2 Fig. S.1. Concentrations profiles for O_2 in the inlet and adjacent channels: (a) F core 25 °C; (b) F core
3 100 °C; (c) F core 200 °C; (d) B core 25 °C; (e) B core 100 °C; (f) B core 200 °C. Concentrations inside
4 the inlet channel - left axis; Concentrations inside the adjacent channel - right axis.

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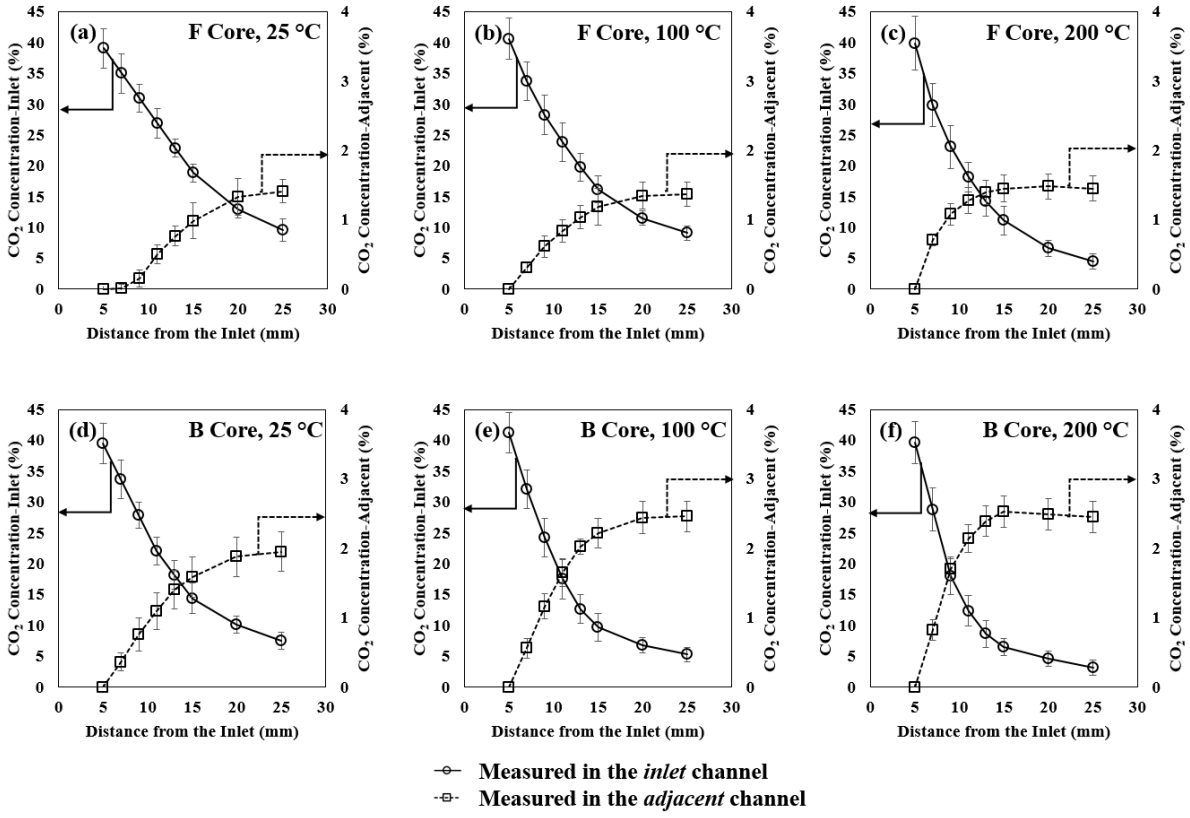

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2 Fig. S.2. Concentrations profiles for CO_2 in the inlet and adjacent channels: (a) F core 25 °C; (b) F core
3 100 °C; (c) F core 200 °C; (d) B core 25 °C; (e) B core 100 °C; (f) B core 200 °C. Concentrations inside
4 the inlet channel - left axis; Concentrations inside the adjacent channel - right axis.

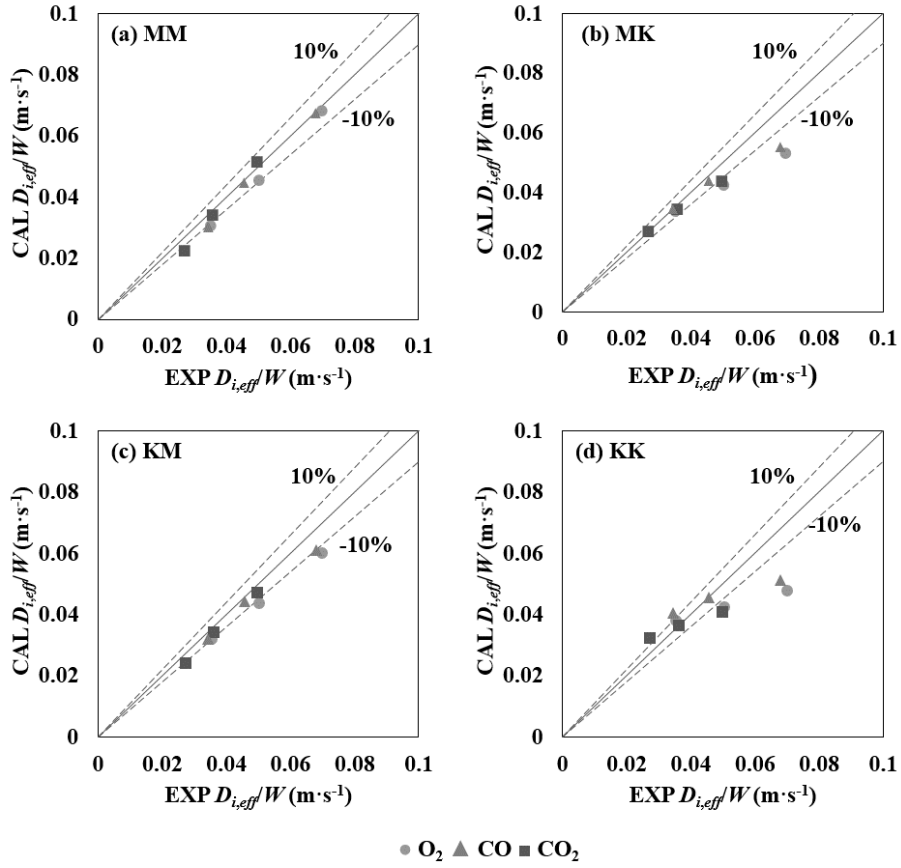

Fig. S.3. Parity plots of assumptions of O_2, CO and CO_2 diffusion in the B core: (a) substrate: molecular diffusion, washcoat: molecular diffusion; (b) substrate: molecular diffusion, washcoat: Knudsen diffusion; (c) substrate: Knudsen diffusion, washcoat: molecular diffusion; (d) substrate: Knudsen diffusion, washcoat: Knudsen diffusion.

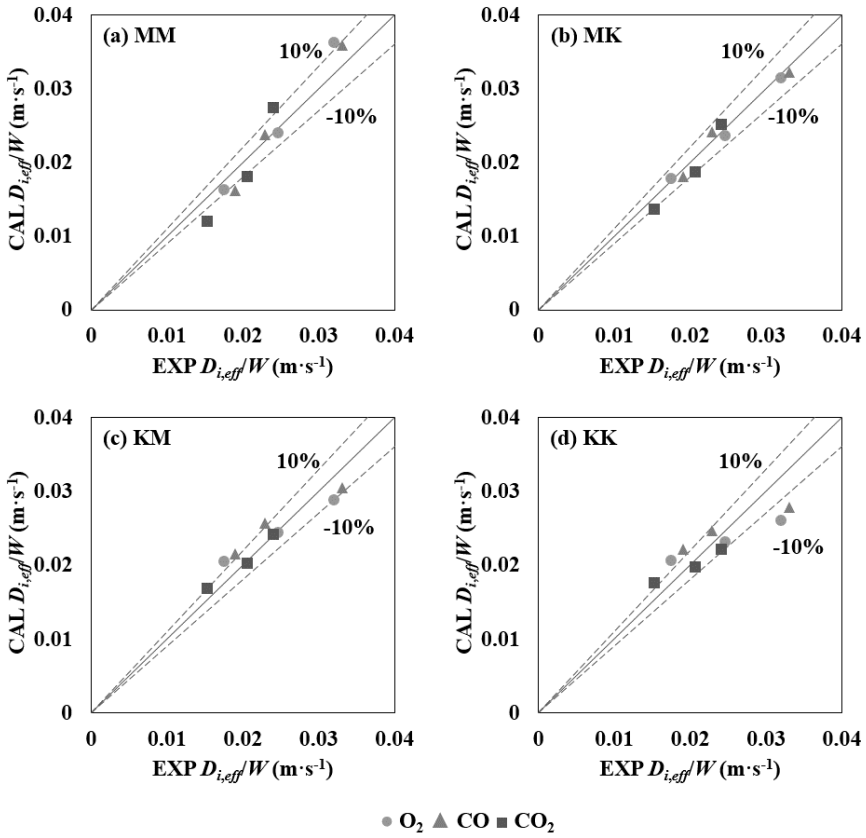

Fig. S.4. Parity plots of assumptions of O_2, CO and CO_2 diffusion at 9 mm from the entrance of the F core: (a) substrate: molecular diffusion, washcoat: molecular diffusion; (b) substrate: molecular diffusion, washcoat: Knudsen diffusion; (c) substrate: Knudsen diffusion, washcoat: molecular diffusion; (d) substrate: Knudsen diffusion, washcoat: Knudsen diffusion.

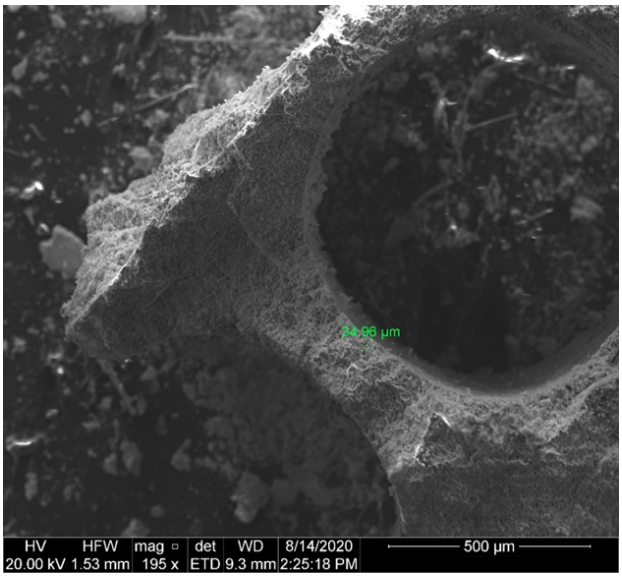

Fig. S.5. Cross sectional SEM image of the washcoat of the B core.

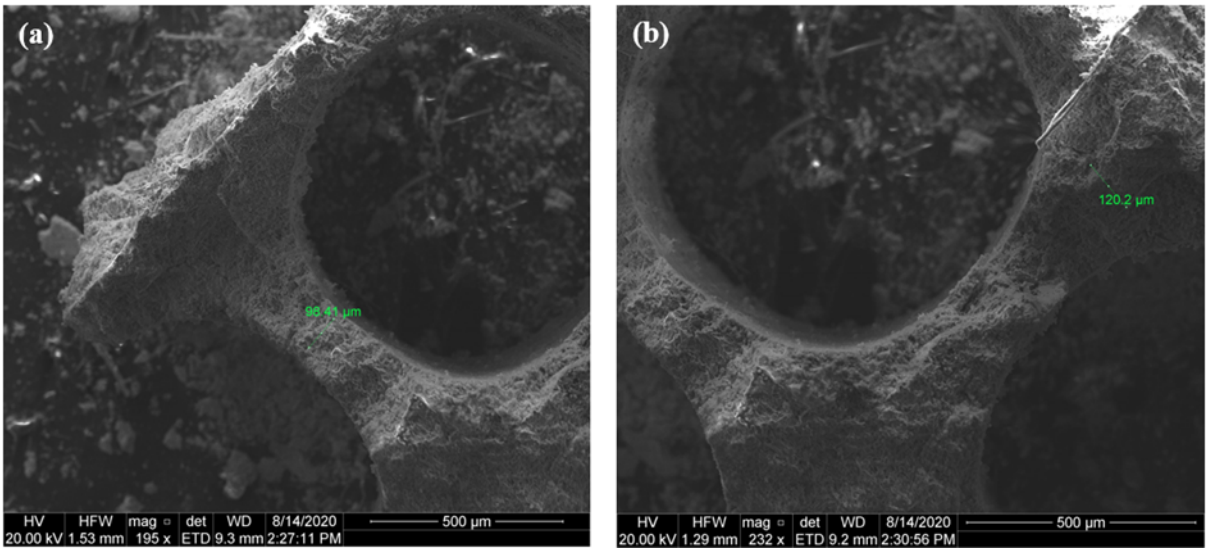

Fig. S.6. Cross sectional SEM image of the substrate of the B core.

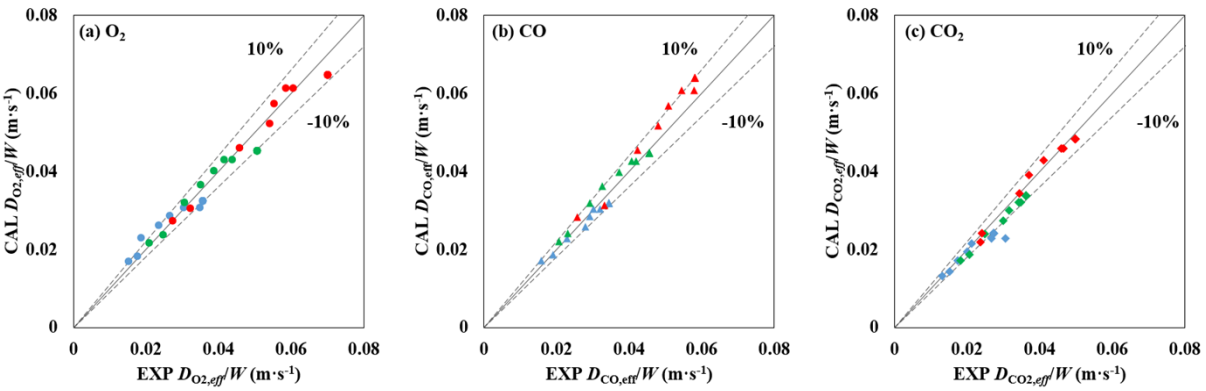

Fig. S.7. Parity plots between the experimentally measured and calculated internal mass transfer coefficients in the F and B core for (a) O_2, (b) CO and (c) CO_2 at 25 °C (blue), 100 °C (green) and 200 °C (red).

All the data points in the diffusion experiments were provided as follow:

Fig. 5(a): CO, F core, 25 °C

Center	Adjacent

Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	5.23	5	0.00
7	4.64	7	0.08
9	4.26	9	0.17
11	3.90	11	0.24
13	3.53	13	0.29
15	3.21	15	0.32
20	2.60	20	0.39
25	2.01	25	0.45

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4 Fig. 5(b): CO, F core, 100 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	4.99	5	0.00
7	4.36	7	0.13
9	3.75	9	0.24
11	3.23	11	0.32
13	2.72	13	0.39
15	2.28	15	0.42
20	1.59	20	0.46
25	1.08	25	0.51

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6 Fig. 5(c): CO, F core, 200 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	4.78	5	0.00
7	3.99	7	0.21
9	3.10	9	0.36
11	2.43	11	0.44
13	1.86	13	0.48
15	1.50	15	0.51
20	1.00	20	0.54
25	0.70	25	0.55

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3 Fig. 5(d): CO, B core, 25 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	4.73	5	0.00
7	4.30	7	0.12
9	3.83	9	0.22
11	3.30	11	0.31
13	2.79	13	0.39
15	2.37	15	0.45
20	1.74	20	0.52
25	1.32	25	0.55

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5 Fig. 5(e): CO, B core, 100 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	5.39	5	0.00
7	4.06	7	0.18
9	3.22	9	0.33
11	2.57	11	0.42
13	2.05	13	0.49
15	1.70	15	0.54
20	1.16	20	0.57
25	0.87	25	0.58

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3 Fig. 5(f): CO, B core, 200 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	4.88	5	0.00
7	3.68	7	0.24
9	2.71	9	0.40
11	2.06	11	0.50
13	1.55	13	0.56
15	1.26	15	0.58
20	0.85	20	0.61
25	0.72	25	0.62

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5 Fig. S.1(a): O_2, F core, 25 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	43.86	5	0.00
7	37.51	7	0.37
9	32.17	9	0.60
11	27.09	11	0.81
13	21.61	13	0.99
15	17.33	15	1.14
20	10.29	20	1.23
25	5.27	25	1.32

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3 Fig. S.1(b): O_2, F core, 100 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	37.16	5	0.00
7	33.96	7	0.24
9	29.88	9	0.43
11	23.91	11	0.53
13	18.79	13	0.66
15	14.60	15	0.79
20	7.81	20	0.97
25	3.12	25	1.15

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5 Fig. S.1(c): O_2, F core, 200 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	38.99	5	0.00
7	32.19	7	0.45
9	25.61	9	0.83
11	19.26	11	1.08
13	14.04	13	1.27
15	9.61	15	1.42
20	3.83	20	1.48
25	1.80	25	1.30

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3 Fig. S.1(d): O_2, B core, 25 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	39.40	5	0.00
7	34.02	7	0.40
9	26.40	9	1.09
11	19.43	11	1.74
13	15.06	13	2.01
15	11.57	15	2.22
20	6.93	20	2.35
25	4.85	25	2.32

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5 Fig. S.1(e): O_2, B core, 100 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	37.10	5	0.00
7	31.29	7	0.41
9	22.98	9	1.20
11	16.65	11	1.88
13	11.12	13	2.27
15	7.84	15	2.51
20	3.83	20	2.37
25	2.64	25	2.10

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3 Fig. S.1(f): O_2, B core, 200 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	39.50	5	0.00
7	28.24	7	0.63
9	20.17	9	1.28
11	13.03	11	2.01
13	7.44	13	2.62
15	4.66	15	2.56
20	3.53	20	2.41
25	3.07	25	2.32

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5 Fig. S.2(a): CO_2, F core, 25 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	39.05	5	0.00
7	35.01	7	0.01
9	30.97	9	0.16
11	26.93	11	0.50
13	22.89	13	0.77
15	18.85	15	0.99
20	12.93	20	1.33
25	9.58	25	1.41

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3 Fig. S.2(b): CO_2, F core, 100 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	40.63	5	0.00
7	33.72	7	0.31
9	28.28	9	0.61
11	23.89	11	0.84
13	19.74	13	1.04
15	16.15	15	1.19
20	11.49	20	1.35
25	9.12	25	1.37

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5 Fig. S.2(c): CO_2, F core, 200 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	39.85	5	0.00
7	29.87	7	0.71
9	23.08	9	1.08
11	18.15	11	1.28
13	14.19	13	1.40
15	11.13	15	1.45
20	6.63	20	1.48
25	4.45	25	1.45

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3 Fig. S.2(d): CO_2, B core, 25 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	39.52	5	0.00
7	33.70	7	0.36
9	27.88	9	0.76
11	22.06	11	1.09
13	18.20	13	1.41
15	14.40	15	1.59
20	10.18	20	1.88
25	7.53	25	1.95

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5 Fig. S.2(e): CO_2, B core, 100 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	41.29	5	0.00
7	32.10	7	0.56
9	24.20	9	1.16
11	17.50	11	1.65
13	12.65	13	2.03
15	9.72	15	2.22
20	6.79	20	2.44
25	5.26	25	2.46

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3 Fig. S.2(f): CO_2, B core, 200 °C

Center		Adjacent	
Distance from the Inlet (mm)	Concentration (%)	Distance from the Inlet (mm)	Concentration (%)
5	39.66	5	0.00
7	28.79	7	0.82
9	17.92	9	1.70
11	12.33	11	2.14
13	8.66	13	2.39
15	6.52	15	2.53
20	4.60	20	2.49
25	3.17	25	2.45

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Fig. 6: Overall mass transfer coefficients for O_2

Core	Distance from F Core Inlet (mm)	$k_{overall}$ (m·s^{-1})		
		25 °C	100 °C	200 °C
F	7	0.00670475	0.016621291	0.024130207
	9	0.011435223	0.018519482	0.026735835
	11	0.013579553	0.020839015	0.028589323
	13	0.015818881	0.022319029	0.030211506
	15	0.017011043	0.023304455	0.031882079
	20	0.018299829	0.024571747	0.033890715
	25	0.019647872	0.026174015	0.035598542
B	37	0.019888998	0.029024759	0.03932411
	39	0.020328181	0.029809997	0.040301608
	41	0.020562064	0.030476806	0.041419011

	43	0.020885758	0.030872363	0.042158568
	45	0.021118373	0.031048849	0.042601651
	50	0.021274356	0.031366675	0.042687855
	55	0.021040518	0.031597333	0.042817398

Overall mass transfer coefficients for CO

Core	Distance from F Core Inlet (mm)	$k_{overall}$ (m·s^{-1})		
		25 °C	100 °C	200 °C
F	7	0.00984938	0.017950116	0.030162562
	9	0.010629261	0.019294525	0.032580984
	11	0.011109324	0.019870852	0.033653377
	13	0.011743442	0.020845658	0.035105242
	15	0.01206508	0.021748378	0.036348954
	20	0.01371811	0.023692548	0.037853509
	25	0.015104562	0.025485341	0.03917486
B	37	0.017870312	0.027963122	0.041528341
	39	0.018203868	0.028910727	0.042647424
	41	0.018582503	0.029821763	0.042906785

	43	0.018906459	0.030068333	0.043052905
	45	0.019353902	0.030224271	0.04308983
	50	0.019700898	0.03058382	0.043323751
	55	0.01982811	0.030960736	0.04313049

Overall mass transfer coefficients for CO_2

Core	Distance from F Core Inlet (mm)	$k_{overall}$ (m·s^{-1})		
		25 °C	100 °C	200 °C
F	7	0.009959537	0.015344584	0.024673621
	9	0.010552628	0.016162655	0.025369346
	11	0.011188727	0.017599126	0.026112344
	13	0.012004503	0.018209081	0.026676133
	15	0.012213037	0.018786441	0.027318019
	20	0.013482134	0.020266474	0.029262834
	25	0.014189246	0.02146544	0.030571657
B	37	0.015254099	0.024187299	0.032646431
	39	0.015733886	0.024220622	0.03308341
	41	0.015809943	0.024611458	0.034244065

43	0.015989097	0.024520025	0.034687429
45	0.016356387	0.024547167	0.035192668
50	0.016429701	0.024565936	0.035025932
55	0.016411604	0.024294838	0.034721672

Fig. 7: Mass transfer coefficients for O_2 at 25 °C in the F core

Distance from the Inlet (mm)	k_{m1} (m·s^{-1})	k_{m2} (m·s^{-1})	$D_{O2,eff}/W$ (m·s^{-1})
7	0.141670048	0.114665681	0.014980316
9	0.117678537	0.101306368	0.017475901
11	0.10820752	0.096342913	0.018511994
13	0.10306848	0.093739863	0.023339679
15	0.09982867	0.092134699	0.026375128
20	0.095297804	0.089939767	0.030272441
25	0.092930448	0.088817351	0.034630477

Mass transfer coefficients for O_2 at 25 °C in the B core

Distance from the Inlet (mm)	k_{m1} (m·s^{-1})	k_{m2} (m·s^{-1})	$D_{O2,eff}/W$

			$(m \cdot s^{-1})$
7	0.141670048	0.114665681	0.028986017
9	0.117678537	0.101306368	0.032442232
11	0.10820752	0.096342913	0.034468309
13	0.10306848	0.093739863	0.036351197
15	0.09982867	0.092134699	0.037762503
20	0.095297804	0.089939767	0.039380971
25	0.092930448	0.088817351	0.03920408

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6 Mass transfer coefficients for O_2 at 100 °C in the F core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{O2,eff}/W$ $(m \cdot s^{-1})$
7	0.182870793	0.154329075	0.020740091
9	0.157443704	0.140863848	0.024662943
11	0.147759454	0.136009448	0.030527507
13	0.142613211	0.133500934	0.03500084
15	0.139413392	0.131967767	0.038511705
20	0.135001918	0.129889032	0.041390763
25	0.132728664	0.128834256	0.043649533

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8 Mass transfer coefficients for O_2 at 100 °C in the B core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{O2,eff}/W$

			$(m \cdot s^{-1})$
7	0.182870793	0.154329075	0.044433896
9	0.157443704	0.140863848	0.04676297
11	0.147759454	0.136009448	0.048499823
13	0.142613211	0.133500934	0.05190067
15	0.139413392	0.131967767	0.052284289
20	0.135001918	0.129889032	0.053613274
25	0.132728664	0.128834256	0.055153992

Mass transfer coefficients for O_2 at 200 °C in the F core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{O2,eff}/W$ $(m \cdot s^{-1})$
7	0.256561607	0.222428654	0.02723286
9	0.226085344	0.206767168	0.031978946
11	0.214734645	0.201212685	0.045501115
13	0.208774364	0.198363874	0.053867828
15	0.205096121	0.196630318	0.055204795
20	0.200062622	0.194289432	0.058464847
25	0.197486858	0.19310596	0.060423259

Mass transfer coefficients for O_2 at 200 °C in the B core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{O2,eff}/W$

			$(m \cdot s^{-1})$
7	0.256561607	0.222428654	0.058698643
9	0.226085344	0.206767168	0.06429446
11	0.214734645	0.201212685	0.068886054
13	0.208774364	0.198363874	0.072000098
15	0.205096121	0.196630318	0.074009274
20	0.200062622	0.194289432	0.075298532
25	0.197486858	0.19310596	0.076261014

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6 Mass transfer coefficients for CO at 25 °C in the F core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{CO,eff}/W$ $(m \cdot s^{-1})$
7	0.25282657	0.187418369	0.015841483
9	0.202990259	0.16182338	0.019051968
11	0.182600303	0.15210244	0.022826511
13	0.171276871	0.146944635	0.027911769
15	0.164019673	0.14374078	0.029143205
20	0.153684851	0.139328097	0.030168884
25	0.148184039	0.137056344	0.031917159

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8 Mass transfer coefficients for CO at 25 °C in the B core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{CO,eff}/W$

			$(m \cdot s^{-1})$
7	0.25282657	0.187418369	0.032142805
9	0.202990259	0.16182338	0.032281675
11	0.182600303	0.15210244	0.032394458
13	0.171276871	0.146944635	0.033484584
15	0.164019673	0.14374078	0.035896424
20	0.153684851	0.139328097	0.036697237
25	0.148184039	0.137056344	0.037480971

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6 Mass transfer coefficients for CO at 100 °C in the F core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{CO,eff}/W$ $(m \cdot s^{-1})$
7	0.328784289	0.253157896	0.020526153
9	0.270833312	0.22480641	0.022889793
11	0.247758181	0.214323215	0.029025222
13	0.235170127	0.208838775	0.032568647
15	0.227204807	0.205461868	0.037239018
20	0.216021083	0.200850915	0.04067544
25	0.210154466	0.198496184	0.041965132

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8 Mass transfer coefficients for CO at 100 °C in the B core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{CO,eff}/W$

			($m \cdot s^{-1}$)
7	0.328784289	0.253157896	0.04347587
9	0.270833312	0.22480641	0.04378091
11	0.247758181	0.214323215	0.044273028
13	0.235170127	0.208838775	0.045293381
15	0.227204807	0.205461868	0.046985768
20	0.216021083	0.200850915	0.047310608
25	0.210154466	0.198496184	0.048439133

Mass transfer coefficients for CO at 200 °C in the F core

Distance from the Inlet (mm)	k_{m1} ($m \cdot s^{-1}$)	k_{m2} ($m \cdot s^{-1}$)	$D_{CO,eff}/W$ ($m \cdot s^{-1}$)
7	0.439218812	0.35351833	0.025652906
9	0.373124371	0.322871136	0.03313571
11	0.347617594	0.311828515	0.042317144
13	0.333962426	0.306123714	0.047994837
15	0.325431054	0.302637557	0.050731717
20	0.31361168	0.297911551	0.054321372
25	0.307492651	0.295513826	0.057936582

Mass transfer coefficients for CO at 200 °C in the B core

Distance from the Inlet (mm)	k_{m1} ($m \cdot s^{-1}$)	k_{m2} ($m \cdot s^{-1}$)	$D_{CO,eff}/W$

			$(m \cdot s^{-1})$
7	0.439218812	0.35351833	0.052702412
9	0.373124371	0.322871136	0.056590557
11	0.347617594	0.311828515	0.058062832
13	0.333962426	0.306123714	0.058940597
15	0.325431054	0.302637557	0.059416993
20	0.31361168	0.297911551	0.060471669
25	0.307492651	0.295513826	0.060425125

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6 Mass transfer coefficients for CO_2 at 25 °C in the F core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{CO2,eff}/W$ $(m \cdot s^{-1})$
7	0.093998884	0.073021739	0.013145216
9	0.075420298	0.062117786	0.015289199
11	0.06781366	0.05791548	0.017432889
13	0.063587295	0.055667497	0.020156473
15	0.060877637	0.05426373	0.021265373
20	0.057017283	0.052319959	0.026652079
25	0.054961682	0.051314148	0.030493746

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8 Mass transfer coefficients for CO_2 at 25 °C in the B core

Distance from the Inlet (mm)	k_{m1} $(m \cdot s^{-1})$	k_{m2} $(m \cdot s^{-1})$	$D_{CO2,eff}/W$

			($m \cdot s^{-1}$)
7	0.093998884	0.073021739	0.0242582
9	0.075420298	0.062117786	0.025240099
11	0.06781366	0.05791548	0.026011776
13	0.063587295	0.055667497	0.027659157
15	0.060877637	0.05426373	0.028046992
20	0.057017283	0.052319959	0.029298976
25	0.054961682	0.051314148	0.030010386

Mass transfer coefficients for CO_2 at 100 °C in the F core

Distance from the Inlet (mm)	k_{m1} ($m \cdot s^{-1}$)	k_{m2} ($m \cdot s^{-1}$)	$D_{CO2,eff}/W$ ($m \cdot s^{-1}$)
7	0.123526235	0.099326851	0.018273718
9	0.102041219	0.087267925	0.020623205
11	0.093511213	0.082763953	0.024937328
13	0.088866411	0.080395441	0.030024296
15	0.085931067	0.078932446	0.031457386
20	0.081815334	0.076928632	0.034145788
25	0.079659319	0.075902388	0.034794269

Mass transfer coefficients for CO_2 at 100 °C in the B core

Distance from the Inlet (mm)	k_{m1} ($m \cdot s^{-1}$)	k_{m2} ($m \cdot s^{-1}$)	$D_{CO2,eff}/W$

			(m·s^{-1})
7	0.123526235	0.099326851	0.034313916
9	0.102041219	0.087267925	0.034992958
11	0.093511213	0.082763953	0.035600665
13	0.088866411	0.080395441	0.035850817
15	0.085931067	0.078932446	0.036085833
20	0.081815334	0.076928632	0.037645784
25	0.079659319	0.075902388	0.038647973

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6 Mass transfer coefficients for CO_2 at 200 °C in the F core

Distance from the Inlet (mm)	k_{m1} (m·s^{-1})	k_{m2} (m·s^{-1})	$D_{CO2,eff}/W$ (m·s^{-1})
7	0.168661726	0.139908154	0.02364265
9	0.143072111	0.126077763	0.024082207
11	0.133182358	0.121033142	0.03443944
13	0.12788341	0.118411748	0.037120997
15	0.124570957	0.116804277	0.040995756
20	0.119979298	0.114617964	0.045843295
25	0.117600853	0.113505453	0.046494963

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8 Mass transfer coefficients for CO_2 at 200 °C in the B core

Distance from the Inlet (mm)	k_{m1} (m·s^{-1})	k_{m2} (m·s^{-1})	$D_{CO2,eff}/W$

			($m \cdot s^{-1}$)
	7	0.168661726	0.139908154	0.046964976
	9	0.143072111	0.126077763	0.047533584
	11	0.133182358	0.121033142	0.048452186
	13	0.12788341	0.118411748	0.049591493
	15	0.124570957	0.116804277	0.050558547
	20	0.119979298	0.114617964	0.052025628
	25	0.117600853	0.113505453	0.053055179

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2 Fig. 8: Validation of MM assumption of O_2 in the B core

Temp. (°C)	$D_{O2,eff}/W_{,EXP}$ ($m \cdot s^{-1}$)	$D_{O2,eff}/W_{,CAL}$ ($m \cdot s^{-1}$)
25	0.035513616	0.030660377
100	0.050378416	0.045125786
200	0.069921154	0.068081761

3 Validation of MM assumption of CO in the B core

Temp. (°C)	$D_{CO,eff}/W_{,EXP}$ ($m \cdot s^{-1}$)	$D_{CO,eff}/W_{,CAL}$ ($m \cdot s^{-1}$)
25	0.034339736	0.030345912
100	0.045651243	0.044654088
200	0.068087169	0.067295597

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5 Validation of MM assumption of CO_2 in the B core

Temp. (°C)	$D_{CO2,eff}/W_{,EXP}$ ($m \cdot s^{-1}$)	$D_{CO2,eff}/W_{,CAL}$ ($m \cdot s^{-1}$)
25	0.027217941	0.022484277
100	0.036162564	0.033962264
200	0.049740227	0.051415094

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Fig. 9: Validation of MK assumption of O_2 at 9 mm from the entrance of the F core

Temp. (°C)	$D_{O2,eff}/W_{,EXP}$ (m·s^{-1})	$D_{O2,eff}/W_{,CAL}$ (m·s^{-1})
25	0.017475901	0.017800557
100	0.024662943	0.023682504
200	0.031978946	0.031450927

Validation of MK assumption of CO at 9 mm from the entrance of the F core

Temp. (°C)	$D_{CO,eff}/W_{,EXP}$ (m·s^{-1})	$D_{CO,eff}/W_{,CAL}$ (m·s^{-1})
25	0.019051968	0.01806924
100	0.022889793	0.024154096
200	0.03313571	0.032235223

Validation of MK assumption of CO_2 at 9 mm from the entrance of the F core

Temp. (°C)	$D_{CO2,eff}/W_{,EXP}$ (m·s^{-1})	$D_{CO2,eff}/W_{,CAL}$ (m·s^{-1})
25	0.015289199	0.013699873
100	0.020623205	0.018703523
200	0.024082207	0.02510858

Fig. S.7: Parity plots between the experimentally measured and calculated internal mass transfer coefficients in the F and B core for O_2

25 °C		100 °C		200 °C	
$D_{O2,eff}/W_{,EXP}$ (m·s^{-1})	$D_{O2,eff}/W_{,CAL}$ (m·s^{-1})	$D_{O2,eff}/W_{,EXP}$ (m·s^{-1})	$D_{O2,eff}/W_{,CAL}$ (m·s^{-1})	$D_{O2,eff}/W_{,EXP}$ (m·s^{-1})	$D_{O2,eff}/W_{,CAL}$ (m·s^{-1})
0.014980316	0.016949673	0.020740091	0.021558867	0.02723286	0.027432808

0.017475901	0.018426412	0.024662943	0.023720201	0.031978946	0.030581651
0.018511994	0.02296352	0.030527507	0.032152253	0.045501115	0.045907592
0.023339679	0.026148029	0.03500084	0.036611026	0.053867828	0.052273912
0.026375128	0.0287044	0.038511705	0.040190317	0.055204795	0.05738449
0.030272441	0.030705703	0.041390763	0.04299243	0.058464847	0.061385401
0.034630477	0.030705703	0.043649533	0.04299243	0.060423259	0.061385401
0.035513616	0.032315017	0.050378416	0.045245702	0.069921154	0.064602665
0.035513616	0.032315017	0.050378416	0.045245702	0.069921154	0.064602665
0.035513616	0.032315017	0.050378416	0.045245702	0.069921154	0.064602665
0.035513616	0.032315017	0.050378416	0.045245702	0.069921154	0.064602665
0.035513616	0.032315017	0.050378416	0.045245702	0.069921154	0.064602665
0.035513616	0.032315017	0.050378416	0.045245702	0.069921154	0.064602665
0.035513616	0.032315017	0.050378416	0.045245702	0.069921154	0.064602665

Parity plots between the experimentally measured and calculated internal mass transfer coefficients in the F and B core for CO

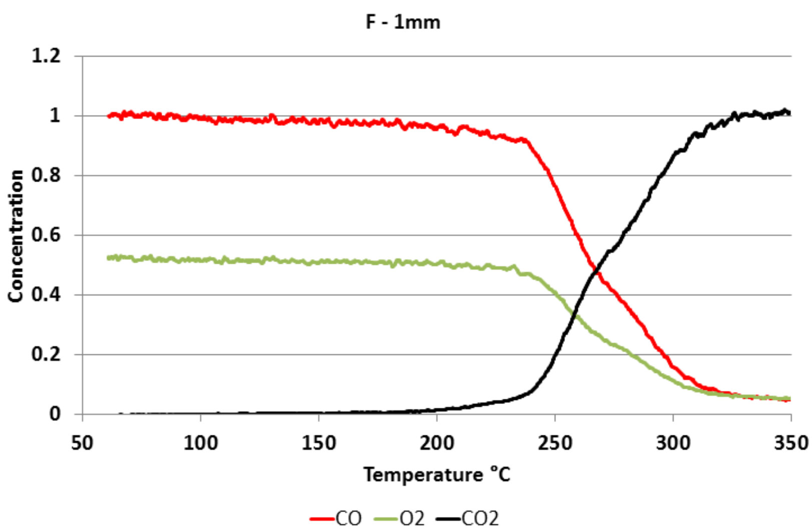
25 °C		100 °C		200 °C	
$D_{CO,eff}/W_{,EXP}$ (m·s^{-1})	$D_{CO,eff}/W_{,CAL}$ (m·s^{-1})	$D_{CO,eff}/W_{,EXP}$ (m·s^{-1})	$D_{CO,eff}/W_{,CAL}$ (m·s^{-1})	$D_{CO,eff}/W_{,EXP}$ (m·s^{-1})	$D_{CO,eff}/W_{,CAL}$ (m·s^{-1})
0.015841483	0.017284165	0.020526153	0.022077568	0.025652906	0.028222053
0.019051968	0.018714837	0.022889793	0.024188859	0.03313571	0.031326024
0.022826511	0.022716083	0.029025222	0.031805805	0.042317144	0.045412927
0.027911769	0.025866278	0.032568647	0.036216534	0.047994837	0.051710648
0.029143205	0.028395104	0.037239018	0.039757256	0.050731717	0.056766158
0.030168884	0.030374842	0.04067544	0.042529177	0.054321372	0.060723958
0.031917159	0.030374842	0.041965132	0.042529177	0.057936582	0.060723958
0.034339736	0.031966815	0.045651243	0.044758169	0.058087169	0.063906556

0.034339736	0.031966815	0.045651243	0.044758169	0.058087169	0.063906556
0.034339736	0.031966815	0.045651243	0.044758169	0.058087169	0.063906556
0.034339736	0.031966815	0.045651243	0.044758169	0.058087169	0.063906556
0.034339736	0.031966815	0.045651243	0.044758169	0.058087169	0.063906556
0.034339736	0.031966815	0.045651243	0.044758169	0.058087169	0.063906556
0.034339736	0.031966815	0.045651243	0.044758169	0.058087169	0.063906556

Parity plots between the experimentally measured and calculated internal mass transfer coefficients in the F and B core for CO_2

25 °C		100 °C		200 °C	
$D_{CO2,eff}/W_{,EXP}$ ($m \cdot s^{-1}$)	$D_{CO2,eff}/W_{,CAL}$ ($m \cdot s^{-1}$)	$D_{CO2,eff}/W_{,EXP}$ ($m \cdot s^{-1}$)	$D_{CO2,eff}/W_{,CAL}$ ($m \cdot s^{-1}$)	$D_{CO2,eff}/W_{,EXP}$ ($m \cdot s^{-1}$)	$D_{CO2,eff}/W_{,CAL}$ ($m \cdot s^{-1}$)
0.013145216	0.013328547	0.018273718	0.01707485	0.02364265	0.021896915
0.015289199	0.014392103	0.020623205	0.018653343	0.024082207	0.024232242
0.017432889	0.017163465	0.024937328	0.024031336	0.03443944	0.034312393
0.020156473	0.01954364	0.030024296	0.027363925	0.037120997	0.039070727
0.021265373	0.021454331	0.031457386	0.03003917	0.040995756	0.042890491
0.026652079	0.022950151	0.034145788	0.032133534	0.045843295	0.045880864
0.030493746	0.022950151	0.034794269	0.032133534	0.046494963	0.045880864
0.027217941	0.024152989	0.036162564	0.033817681	0.049740227	0.048285521

0.027217941	0.024152989	0.036162564	0.033817681	0.049740227	0.048285521
0.027217941	0.024152989	0.036162564	0.033817681	0.049740227	0.048285521
0.027217941	0.024152989	0.036162564	0.033817681	0.049740227	0.048285521
0.027217941	0.024152989	0.036162564	0.033817681	0.049740227	0.048285521
0.027217941	0.024152989	0.036162564	0.033817681	0.049740227	0.048285521
0.027217941	0.024152989	0.036162564	0.033817681	0.049740227	0.048285521



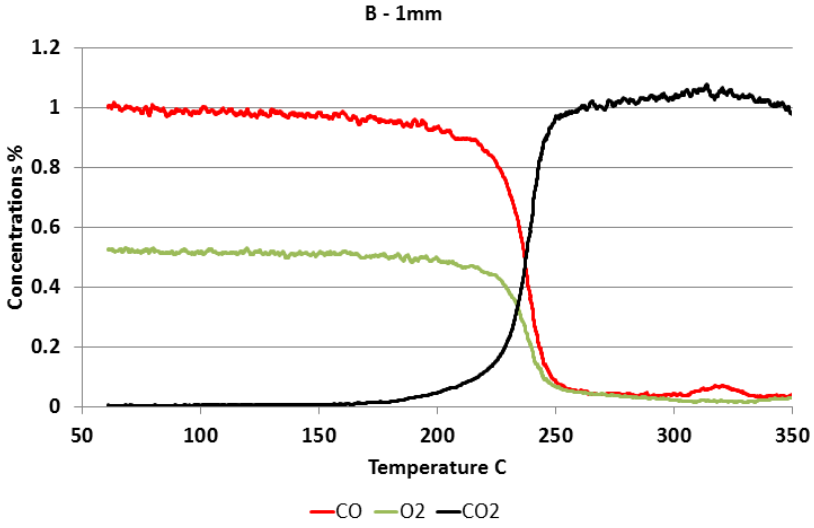


Fig. S.8. Light-off profiles for (up) F and (down) B core at 1 mm from inlet; Concentrations of CO, O_2 and CO_2.

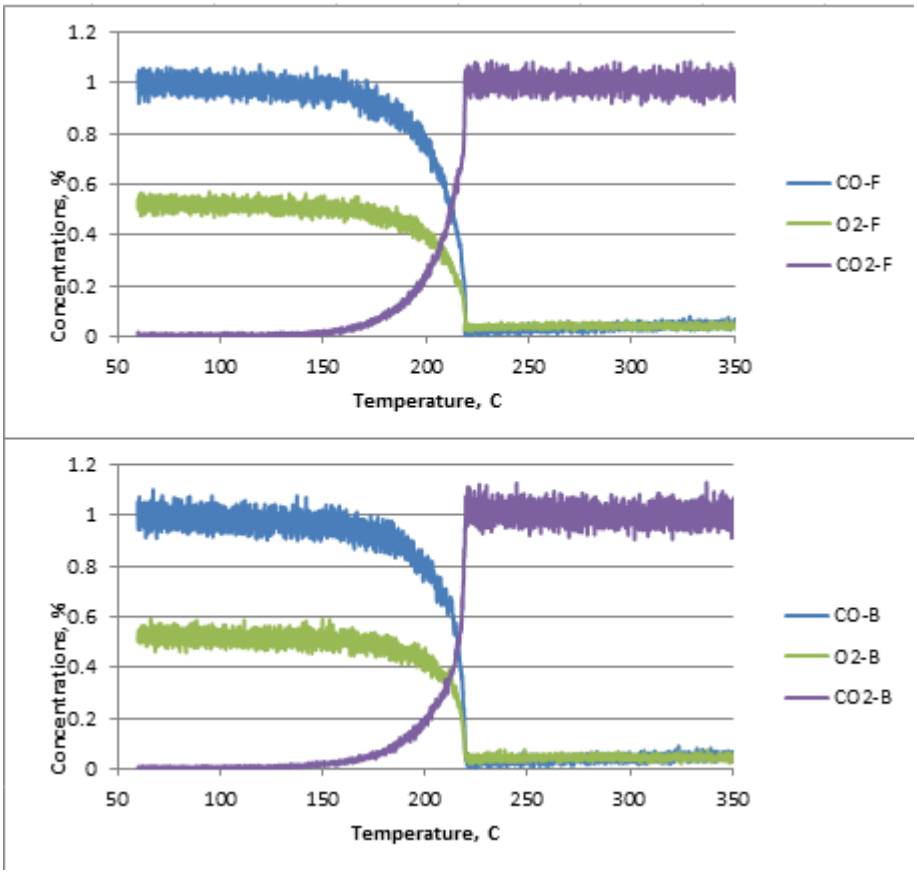


Fig. S.9. Light-off profiles for (up) F and (down) B core at 9 mm from inlet; Concentrations of CO, O_2 and CO_2.

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