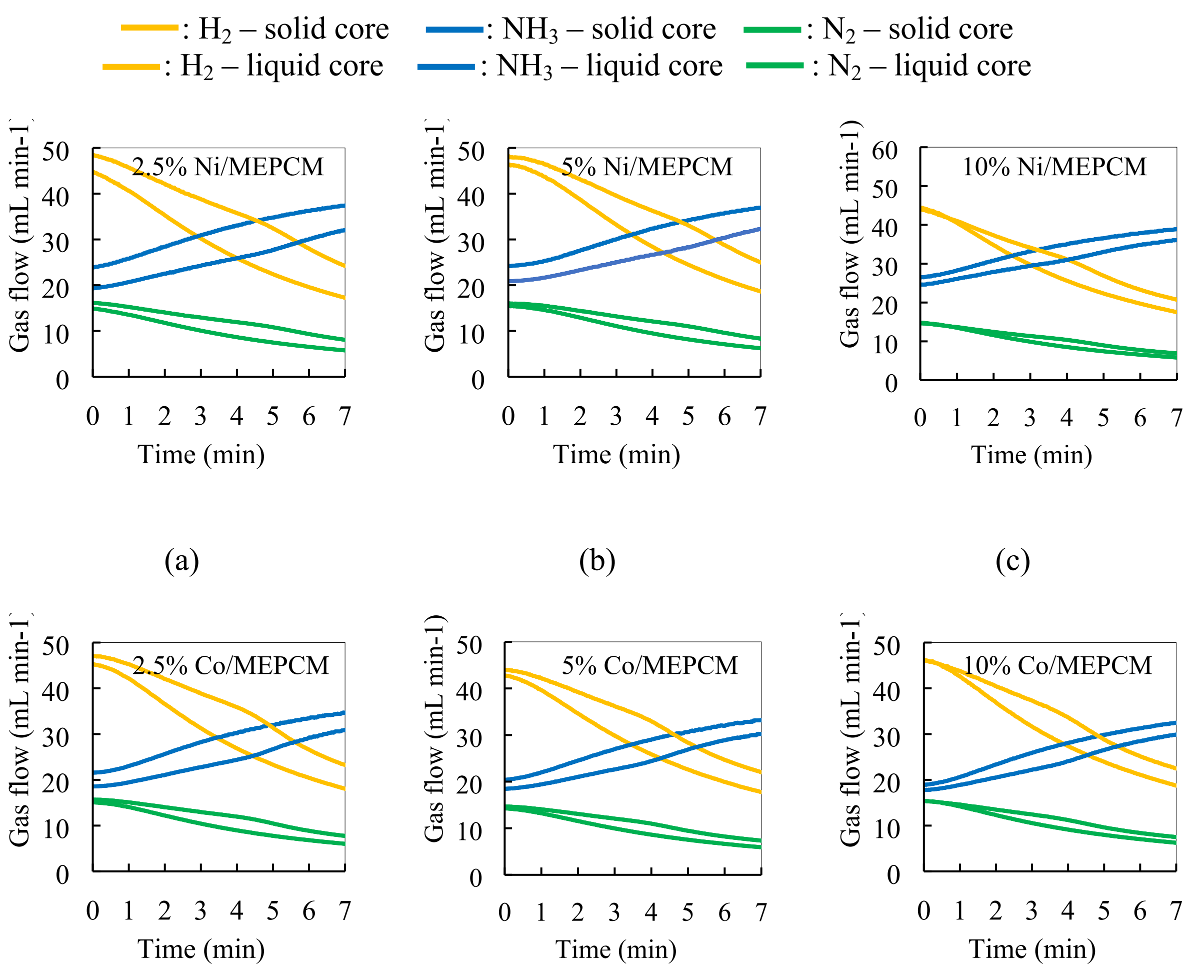
Thermo-regulating Effect of Al–Si Microencapsulated Phase Change Material-based Catalyst Support on Ammonia Decomposition

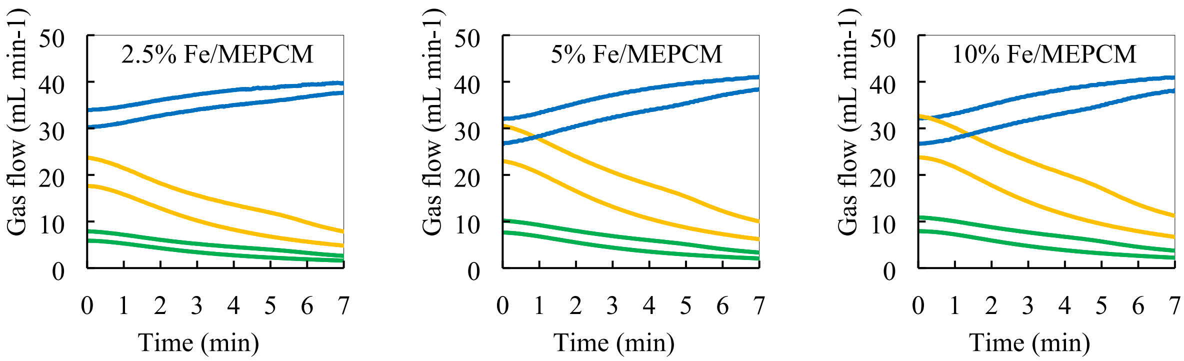
Supplementary Data

1. Reaction performance

The reactor output gas flows were measured during the cooling process for various catalysts. A decrease in the temperature of the endothermic reaction decreases the conversion, resulting in an increase in the output reactant (NH_3) and a decrease in the output products (H_2 and N_2), as shown in Figure S1.



(d) (e) (f)



(g) (h) (i)

Figure S1. Output flow rate of gases during reactor cooling from 570 to 500 °C with different MEPCM catalysts.

2. Heat balance

The calculation of heat balance on the MEPCM catalyst system during transient cooling process described as follows:

a. Latent heat release

$$\lambda_{(t)} = \sum_{i=t0}^{i=t} \lambda_{(i)}$$

Time (min)	Latent heat release (J/min)
1	0.134398923
2	0.965228629
3	3.970877272
4	9.233816917
5	12.23335652
6	9.233816917
7	3.970877272
8	0.965228629
9	0.134398923
Total	40.842 (for 0.2 g catalyst, released over 9 minutes).

b. Reaction enthalpy

$$r\Delta H_{r,NH_3} = \frac{P(V_{in} - V_{out})}{RT}\Delta H_{r,NH_3}$$

Time (min)	NH_3 flow in (mL/min)	NH_3 flow out (mL/min)	Sample temperature (K)	NH_3 reacted (mol/min)	Reaction enthalpy absorption (J/min)
1	50	26	840.1	0.000348391	-32.20522528
2	50	27.9	833	0.000323544	-29.90841215
3	50	29.4	826.9	0.000303809	-28.0840872
4	50	31	820.9	0.00028226	-26.09212375
5	50	33.1	816.3	0.000252478	-23.33904023
6	50	34.8	810.4	0.000228734	-21.14415043
7	50	36.1	800	0.00021189	-19.58713415
8	50	37.5	792.5	0.000192352	-17.78102639
9	50	38.5	786.6	0.000178291	-16.48124376

c. Flow enthalpy in

$$H_{gas,in} = \sum mC_p(T - T_{ref})$$

Cp NH_3	42.3 J/mol.K
Cp Ar	20.8 J/mol.K

Time (min)	Inlet temperature (K)	NH_3 flow in (mol/min)	Ar flow in (mol/min)	Enthalpy gas in (J/min)
1	569.3	0.000725814	0.000725814	24.91487933
2	559.9	0.000732	0.000732	24.69329444
3	551.0	0.0007374	0.0007374	24.46156229
4	543.3	0.00074279	0.00074279	24.2796483
5	536.7	0.000746975	0.000746975	24.10555077
6	529.8	0.000752414	0.000752414	23.95363085
7	523.2	0.000762195	0.000762195	23.9477753
8	517.2	0.000769408	0.000769408	23.88326937
9	511.2	0.000775179	0.000775179	23.7690843

d. Flow enthalpy out

$$H_{gas,out} = \sum mC_p(T - T_{ref})$$

Cp NH_3	42.3 J/mol.K
Cp Ar	20.8 J/mol.K

Cp H_2	28.8 J/mol.K
Cp N_2	29.11 J/mol.K

Time (min)	Bottom temperature (K)	NH_3 flow out (mol/min)	H_2 flow out (mol/min)	N_2 flow out (mol/min)	Ar flow out (mol/min)	Enthalpy gas out (J/min)
1	565.3	0.000377423	0.000522586	0.000174195	0.000725814	-27.65489066
2	555.9	0.000408456	0.000485316	0.000161772	0.000732	-27.1760463
3	547.1	0.000433591	0.000455713	0.000151904	0.0007374	-26.73825901
4	539.3	0.00046053	0.00042339	0.00014113	0.00074279	-26.34655775
5	532.6	0.000494498	0.000378717	0.000126239	0.000746975	-25.90766858
6	525.8	0.00052368	0.000343101	0.000114367	0.000752414	-25.54266897
7	519.2	0.000550305	0.000317835	0.000105945	0.000762195	-25.38163814
8	513.3	0.000577056	0.000288528	9.6176E-05	0.000769408	-25.14744606
9	507.2	0.000596888	0.000267437	8.91456E-05	0.000775179	-24.90859432

e. Sensible heat

$$mC_p\frac{dT}{dt} = \left(H_{gas,in} + \lambda_{(t)}\right) - \left(H_{gas,out} + r\Delta H_{r,NH_3}\right)$$

Time (min)	Sensible heat (J/min)
1	-34.81083769
2	-31.42593538
3	-26.38990666
4	-18.92521629
5	-12.90780151
6	-13.49937164
7	-17.05011971
8	-18.07997446
9	-17.48635486