

Tables used in manuscripts

Table S1. Reaction pathways in 2-way DPF/SCR.....	2
Table S2. Rate expressions for SCR reactions.....	3
Table S3. Catalyst Core dimension of blended DPF/SCR sample and aging conditions	4
Table S4. Test Conditions for NO oxidation and NO ₂ dissociation	4
Table S5. Test conditions for soot oxidation studies	5
Table S6. Activation energy determined from soot oxidation measurements	5
Table S7. Comparison of mass transfer inside filter wall between clean and soot loaded conditions.....	6
Table S8. Test condition for the results in Figure 11 to Figure 14	6
Table S9. Test condition for the results in Figure 15 to Figure 18	7

Table S1. Reaction pathways in 2-way DPF/SCR

Domain	Reaction Type	Reaction Pathway
Soot cake layer	Soot oxidation by O ₂	$C + (1 - f_{CO}/2)O_2 \rightarrow f_{CO}CO + (1 - f_{CO}/2)CO_2$
	Soot oxidation by NO ₂	$C + (2 - g_{CO})NO_2 \rightarrow g_{CO}CO + (1 - g_{CO})CO_2 + (2 - g_{CO})NO$
Catalytic filter wall	Catalytic soot oxidation by O ₂	$C + (1 - f_{CO,cat}/2)O_2 \rightarrow f_{CO,cat}CO + (1 - f_{CO,cat}/2)CO_2$
	Soot oxidation by NO ₂	$C + (2 - g_{CO})NO_2 \rightarrow g_{CO}CO + (1 - g_{CO})CO_2 + (2 - g_{CO})NO$
	Ammonia adsorption	$NH_3 + S \rightarrow NH_3-S$
	Ammonia desorption	$NH_3-S \rightarrow NH_3 + S$
	Ammonia oxidation	$2NH_3-S + 3/2O_2 \rightarrow N_2 + 3H_2O + 2S$
	NO oxidation	$NO + 1/2O_2 \leftrightarrow NO_2$
	Standard SCR reaction	$4NH_3-S + 4NO + O_2 \rightarrow 4N_2 + 6H_2O + 4S$
	Fast SCR reaction	$2NH_3-S + NO + NO_2 \rightarrow 2N_2 + 3H_2O + 2S$
	NO ₂ SCR reaction	$3NO_2 + 4NH_3-S \rightarrow 3.5N_2 + 6H_2O + 4S$
	N ₂ O formation	$2NO_2 + 2NH_3-S \rightarrow N_2O + N_2 + 3H_2O + 2S$

Table S2. Rate expressions for SCR reactions

Reaction type	Rate Expression
Ammonia adsorption	$RR_{ads} = A_1 C_{NH_3} (1 - \theta)$ $A_1 = 3.737$
Ammonia desorption	$RR_{des} = A_2 \exp\left(\frac{-E_{A,2}}{R_u T}\right) \theta$, where $E_{A,2} = E_{A,des1} e^{-\delta \theta} + E_{A,des2}$ $A_2 = 1E+11$, $E_{A,des1} = 50000$ [J/mol], $\delta = 4.5$, $E_{A,des2} = 102000$ [J/mol]
Ammonia oxidation	$RR_{NH_3,oxi} = A_3 \exp\left(\frac{-E_{A,3}}{R_u T}\right) C_{O_2} \cdot \theta$ $A_3 = 1.44E+11$, $E_{A,3} = 162400$ [J/mol]
NO oxidation	$RR_{NO,oxi} = A_4 \exp\left(\frac{-E_{A,4}}{R_u T}\right) C_{NO} \sqrt{C_{O_2}} \cdot \theta - k_{4,b} C_{NO_2}$ $k_{4,b} = A_4 \exp\left(\frac{-E_{A,4}}{R_u T}\right) / K_{eq}$ $K_{eq} = \exp\left(\frac{-\Delta S}{R_u}\right) \exp\left(\frac{-\Delta H}{R_u T}\right)$ $A_4 = 3.0E+1$, $E_{A,4} = 48000$, $\Delta S = -76.1$ [J/K-mol], $\Delta H = 58279$ [J/mol]
Standard SCR reaction	$RR_{std,SCR} = A_5 \exp\left(\frac{-E_{A,5}}{R_u T}\right) C_{NO} \cdot \theta$ $A_5 = 5.04E+8$, $E_{A,5} = 84300$ [J/mol]
Fast SCR reaction	$RR_{fast,SCR} = A_6 \exp\left(\frac{-E_{A,6}}{R_u T}\right) C_{NO} C_{NO_2} \cdot \theta$ $A_6 = 9E+11$, $E_{A,6} = 66100$ [J/mol]
NO ₂ SCR reaction	$RR_{NO_2,SCR} = A_7 \exp\left(\frac{-E_{A,7}}{R_u T}\right) C_{NO_2} \cdot \theta$ $A_7 = 1.1E+7$, $E_{A,7} = 71800$ [J/mol]
N ₂ O formation	$RR_{N_2O} = A_8 \exp\left(\frac{-E_{A,8}}{R_u T}\right) C_{NO_2} \cdot \theta$ $A_8 = 3.6E+4$, $E_{A,8} = 43300$ [J/mol]

Table S3. Catalyst Core dimension of blended DPF/SCR sample and aging conditions

Catalyst Core Dimensions	Length	0.0605 [m] , 0.95 [in]
	Diameter	0.0241 [m] , 2.38 [in]
	Cell Density	300 CPSI
	Substrate Porosity	59 %
	Mean Pore Diameter	18 [μm]
Aging Conditions		100h / 700 °C + 20h / 750 °C (Air / 10% H ₂ O) , SV=60000 [1/h]

Table S4. Test Conditions for NO oxidation and NO₂ dissociation

Test		NO oxidation to NO ₂	NO ₂ dissociation to NO
Space velocity		23500 1/hr	23500 1/hr
Sample catalyst condition		Clean (free from soot loading)	Clean (free from soot loading)
Feed gas composition	O ₂	5 % / 10 %	5 %
	NO	500 ppm	0 ppm
	NO ₂	0 ppm	100 ppm
	H ₂ O	5 %	5 %
	N ₂	Balance	Balance

Table S5. Test conditions for soot oxidation studies

Test		'test 1'	'test 2'
Space velocity		23500 1/hr	23500 1/hr
Initial soot loading		Soot loaded (3g/L)	Soot loaded (1.9g/L)
Feed gas composition	O ₂	5 %	5 %
	NO	500 ppm	0 ppm
	NO ₂	0 ppm	100 ppm
	H ₂ O	5 %	5 %
	N ₂	Balance	Balance

Table S6. Activation energy determined from soot oxidation measurements

Oxidation Mechanism	Activation Energy (current calibration)	Activation Energy (literature)
Thermal Soot Oxidation by O ₂	158 kJ/mol	125 ~ 177 kJ/mol
Catalytic Soot Oxidation by O ₂	110 kJ/mol	100 ~ 120 kJ/mol
Soot oxidation by NO ₂	70 kJ/mol	40 ~ 70 kJ/mol

Table S7. Comparison of mass transfer inside filter wall between clean and soot loaded conditions

		Clean case	Soot loaded case
Mass transfer	Mechanism	Diffusion	Knudsen diffusion
	Rate	Fast	Slow

Table S8. Test condition for the results in Figure 11 to Figure 14

Space Velocity		23500 1/hr
Initial soot loading		Clean(0g/L) or 1.0g/L
Initial ammonia storage		0 g
Feed gas composition	NO	200 ppm
	NH ₃	180 ppm
	O ₂	5%
	H ₂ O	5%
	N ₂	Balance
Temperature		200 ~ 600 °C (programmed temperature)

Table S9. Test condition for the results in Figure 15 to Figure 18

Space Velocity		23500 1/hr
Initial soot loading		3.0g/L
Feed gas composition	NO _x	200 ppm
	NO ₂ /NO _x	0.25, 0.375, 0.5, 0.625, 0.75 respectively
	NH ₃	180 ppm
	O ₂	5%
	H ₂ O	5%
	N ₂	Balance
Temperature		400 °C