

# CONTENTS

CONTRIBUTORS . . . . .	ix
PREFACE . . . . .	xi

## Dynamic Behavior and Characterization of Automobile Catalysts

SHINICHI MATSUMOTO AND HIROFUMI SHINJOH

I. Introduction . . . . .	2
II. Automotive Exhaust Catalyst and its Specific Features . . . . .	3
A. Introduction of Exhaust Catalyst . . . . .	3
B. Catalytic Performance in Fluctuating Condition . . . . .	5
III. Oxygen Storage and Release in TWC . . . . .	8
A. Introduction . . . . .	8
B. OSC of Mixed Oxide: $(\text{Ce},\text{La})\text{O}_{2-x}$ , $(\text{Ce},\text{Zr})\text{O}_2$ . . . . .	9
C. Heat Resistant Oxygen Storage Material: ACZ . . . . .	10
D. Atomic Arrangement of Oxygen Storage Materials and their OSC . . . . .	12
E. Dynamic Oxygen Mobility in $\text{Pt}/\text{CeO}_2\text{-ZrO}_2$ . . . . .	15
IV. Sintering of PGM . . . . .	18
A. Introduction . . . . .	18
B. Sintering Inhibition Mechanism of Platinum Supported on Ceria-based Oxide . . . . .	19
C. Re-dispersion of Platinum Supported on Ceria-based Oxide . . . . .	22
V. NO <sub>x</sub> Storage and Reduction Catalyst and Reaction Mechanism . . . . .	23
A. NO <sub>x</sub> Reduction Method Under Lean Conditions . . . . .	23
B. Outlook of NSR Catalyst . . . . .	25
C. Mechanism of NSR Catalyst . . . . .	26
D. SO <sub>x</sub> Poisoning . . . . .	30
VI. Improvement of NSR Catalyst and Engine System . . . . .	32
A. NSR Catalyst Formulation . . . . .	32
B. Improvement of Durability against Sulfur Poisoning . . . . .	33
C. Combination of Catalysts . . . . .	39
VII. Conclusions . . . . .	42
References . . . . .	44

## Simulation of Automotive Emission Control Systems

MEHRDAD AHMADINEJAD, MAYA R. DESAI, TIMOTHY C. WATLING  
AND ANDREW P.E. YORK

I. Introduction . . . . .	48
II. Applications of Modelling/Rational Design of Emissions Control System . . . . .	49
A. Catalyst System Design . . . . .	50
B. Modification of Engine Calibration . . . . .	53
III. Monolith Reactor Model . . . . .	56
IV. Model Development, Illustrated by 3-Way Catalysis . . . . .	59
A. Approach/Methodology . . . . .	59
B. Reactions Involved . . . . .	62
C. Developing Kinetics from Microreactor Data . . . . .	63
D. Model Validation . . . . .	71
V. Other (Diesel) Aftertreatment Systems . . . . .	76
A. Diesel Oxidation Catalysts . . . . .	78
B. Ammonia SCR . . . . .	83
C. NO <sub>x</sub> Traps . . . . .	88
D. Filters . . . . .	91
VI. Future Directions . . . . .	97
Acknowledgement . . . . .	98
List of Symbols . . . . .	98
Abbreviations . . . . .	99
References . . . . .	100

## Current Status of Modeling Lean Exhaust Gas Aftertreatment Catalysts

ANKE GÜTHENKE, DANIEL CHATTERJEE, MICHEL WEIBEL, BERND KRUTZSCH,  
PETR KOČÍ, MILOŠ MAREK, ISABELLA NOVA AND ENRICO TRONCONI

I. Introduction . . . . .	104
II. Simulation of Combined Exhaust Gas Aftertreatment Systems . . . . .	109
III. Monolith Reactor Modeling . . . . .	111
A. Monolith Channel . . . . .	112
B. Spatially 1D Model . . . . .	114
C. Heat and Mass Transfer between Bulk Gas and Catalytic Washcoat . . . . .	115
D. Internal Diffusion in the Washcoat . . . . .	117
E. Spatially 2D (1D+1D) Model with Internal Diffusion . . . . .	119
F. Detailed 3D Model of Porous Catalytic Washcoat . . . . .	121
G. Numerical Solution . . . . .	122
IV. Development of Global Reaction Kinetics . . . . .	124
A. Microreactor Scale . . . . .	124
B. Monolith Reactor Scale . . . . .	129
C. Engine Test Bench Scale . . . . .	129
V. Diesel Oxidation Catalyst . . . . .	130
A. Functions of DOC . . . . .	130
B. Development of a DOC Global Kinetic Model . . . . .	131
C. Validation and Applications of the DOC Global Kinetic Model . . . . .	139

VI. NO <sub>x</sub> Storage and Reduction Catalyst . . . . .	142
A. NO <sub>x</sub> Storage and Reduction Principles . . . . .	142
B. Discussion on Surface Reaction Mechanisms . . . . .	144
C. Development of Effective NSRC Kinetic Model . . . . .	150
D. NSRC Model Validation and Simulation Results . . . . .	158
VII. Selective Catalytic Reduction of NO <sub>x</sub> by NH <sub>3</sub> (Urea-SCR) . . . . .	164
A. Microreactor Scale . . . . .	166
B. Monolith Reactor Scale . . . . .	188
C. Engine Test Bench Scale . . . . .	192
VIII. Combined Aftertreatment Systems . . . . .	198
IX. Summary and Conclusions . . . . .	201
List of Symbols . . . . .	202
Abbreviations . . . . .	205
Acknowledgments . . . . .	206
References . . . . .	206

## Advances in the Science and Technology of Diesel Particulate Filter Simulation

ATHANASIOS G. KONSTANDOPOULOS, MARGARITIS KOSTOGLOU,  
NICKOLAS VLACHOS AND EVDOKIA KLADOPOULOU

I. Introduction . . . . .	214
II. The Many Scales of DPF Systems . . . . .	216
III. Filter Wall Scale . . . . .	216
A. Classic Flow in Porous Media Descriptors . . . . .	217
B. Microflow Simulation Technology . . . . .	219
C. Soot Deposit Microstructure . . . . .	223
D. Soot Deposit Compaction . . . . .	226
E. Deep-bed Filtration . . . . .	228
F. Microflow Deposition in Filter Wall . . . . .	231
G. Effect of Microstructure on Oxidation Kinetics . . . . .	234
H. The Role of NO <sub>2</sub> Turnover/Recycling . . . . .	238
IV. Filter Channel Scale . . . . .	242
A. Inertial Losses at Channel Inlet/Outlet . . . . .	242
B. Asymmetric Channel Geometries . . . . .	245
C. Ash and Soot Entrainment Phenomena . . . . .	246
D. Channel to Porous Wall Heat Transfer . . . . .	250
V. Entire Filter Scale . . . . .	254
A. The Effective Conductivity of DPFs . . . . .	254
B. Multichannel Phenomena . . . . .	257
VI. Conclusion . . . . .	261
Nomenclature . . . . .	265
Greek Letters . . . . .	266
Abbreviations . . . . .	267
Acknowledgments . . . . .	267
References . . . . .	268
Appendix. Microstructural Model of Soot Oxidation: The Effect of Catalyst . . . . .	270
INDEX . . . . .	277
CONTENTS OF VOLUMES IN THIS SERIAL . . . . .	279

**SEE COLOR PLATE SECTION AT THE END OF THIS BOOK**