

ADVANCES IN DIGITALIZATION OF CATALYSIS; HOW IR4.0 IS REVOLUTIONIZING THE WAY WE GO ABOUT CATALYSIS

A technical investigation
commissioned by the members of the
Catalytic Advances Program

Client Private
July 2020





The Catalytic Advances Program (CAP)

The Catalytic Advances Program (CAP) is an information resource for research and development organizations in the petroleum, chemical, and polymer industries. By the direction of the member companies (through balloting and other interactive means), the program delivers a range of timely and insightful information and analyses which are accessible exclusively to members and protected by confidentiality agreements. The objective is to provide a technical update on commercially viable advances in catalysis as well as benchmark commercial advances in catalysis and process technology.

Members receive three in-depth **CAP Technical Reports** which are written and peer reviewed by leading scientists and experienced industry professionals in areas selected by the membership (via ballot); weekly *CAP Communications* (delivered via e-mail) which provide the latest updates on technical breakthroughs, commercial events and exclusive development opportunities; and attendance at the **CAP Annual Meeting**.

The **Catalytic Advances Program (CAP)** is available on a membership basis from The Catalyst Group Resources (TCGR). For further details, please contact John J. Murphy at John.J.Murphy@catalystgrp.com or +1.215.628.4447 (x1121).



P.O. Box 680
Spring House, PA 19477 U.S.A
ph: +1.215.628.4447
fax: +1.215.628.2267
website: www.catalystgrp.com

CONTENTS

EXECUTIVE SUMMARY	ix
1. INTRODUCTION	1
1.1 THE ROLE OF DIGITALIZATION IN CATALYSISIS	3
1.1.1 Initiatives by Enterprises Active in the Field of Catalysis and Process Engineering Involving Catalysis as Documented by Publications and Press Releases	7
1.1.2 Initiatives by Enterprises Active in the Field of Chemical and Petrochemical Engineering	8
1.1.3 Initiatives by Enterprises Active as Catalyst Producers	9
1.1.4 Initiatives in the Oil and Gas Industry.....	9
1.1.5 National and International Initiatives in the Field of Catalysis and Materials Science.....	10
1.2 CHALLENGES AND HURDLES	14
1.3 CONCLUSION AND PERSPECTIVES.....	17
1.4 AUTHORS AND CONTRIBUTORS	18
1.5 REFERENCES	19
2. DIGITALIZATION IN CATALYST RESEARCH, DEVELOPMENT, DISCOVERY	27
2.1 INTRODUCTION, THE CATALYSIS GAP	27
2.2 SYNTHESIS	30
2.2.1 Catalyst Conditioning.....	32
2.2.2 Catalyst Scale-up.....	34
2.2.3 3D Printing	35
2.3 CHARACTERIZATION AND SPECTROSCOPIC DATA.....	37
2.3.1 Catalyst Characterization	37
2.3.2 Operando Characterization.....	38
2.4 EXPERIMENTATION, DATA MANAGEMENT AND EXPECTATIONS	39
2.4.1 Data Quality and Data Handling in Laboratory Environments	39
2.4.2 Data Quality and Data Handling in Environments on Pilot and Plant Scale	40
2.4.3 Data Collection and Data Management in High Throughput Experimentation	40
2.4.4 Analysis of Data, Statistical Analysis and Visualization	50
2.4.5 Chemometrics.....	52
2.4.6 Case Studies	53
2.4.7 Automation and Robotics	56
2.5 INDUSTRIAL PERFORMANCE DATA / HISTORICAL DATA	63

2.6	DATA EXCHANGE WITH THEORY / SUMMARY	64
2.7	ARTIFICIAL INTELLIGENCE(AI) IN THE CONTEXT OF CATALYSIS	65
2.7.1	Definition Artificial Intelligence.....	65
2.7.2	Data Requirements.....	66
2.7.3	AI Trends in Industry.....	66
2.7.4	Critical Comments on the Potential Role of AI in Catalysis	66
2.7.5	Specific Use Cases for AI in Catalysis	69
2.7.6	Challenges and Outlook.....	71
2.7.7	Impact of the FAIR Principles on AI.....	72
2.8	CONCLUSIONS AND RECOMMENDATIONS	72
2.9	GLOSSARY	75
2.10	REFERENCES	74
3.	IR4.0 IN THE CATALYST INDUSTRY	87
3.1	PROVIDERS OF DIGITAL SERVICES	89
3.1.1	Software Vendors.....	92
3.1.2	Equipment Providers with Software	97
3.1.3	Catalyst Manufacturers	104
3.2	IMPLEMENTATION OF DIGITAL SERVICES.....	105
3.2.1	Scale-up to Commercial.....	106
3.2.2	Data Collection and Integration	107
3.3.	DIGITAL TOOLS IN CATALYST OPERATION.....	108
3.3.1	Planning and Implementation for Catalyst Operation	109
3.3.2	Reliability for Catalyst Operation	112
3.3.3	Control for Catalyst Operation.....	113
3.3.4	Quality for Catalyst Operation.....	115
3.4	DIGITAL TOOLS IN CATALYST MANUFACTURE.....	116
3.4.1	Planning and Implementation for Catalyst Manufacture	118
3.4.2	Reliability for Catalyst Manufacture	120
3.4.3	Control for Catalyst Manufacture	121
3.4.4	Quality for Catalyst Manufacture	122
3.5	APPLICATION CASE STUDIES.....	124
3.5.1	Case Study: Scale-up to Commercial	124
3.5.2	Case Study: Data Collection and Integration.....	125
3.5.3	Case Study: Planning and Implementation	126
3.5.4	Case Study: Reliability	126

3.5.5	Case Study: Control.....	127
3.5.6	Case Study: Quality	128
3.6	APPLICATION OF EMERGING TECHNOLOGIES	129
3.7	CONCLUSIONS AND RECOMMENDATIONS.....	131
3.8	GLOSSARY	132
3.9	REFERENCES.....	134
4.	INDEX	141

FIGURES

Figure 1.1	Economic gains of AI adoption.....	3
Figure 1.2	Digital maturity for production in heavy industries	4
Figure 1.3	Opportunities from digitalization as viewed by BASF	5
Figure 1.4	Challenges and hurdles depending on company size	15
Figure 2.1	Hydrodesulfurization activity of catalysts (Procatalyse HR 306) activated according to different procedures at different temperatures	33
Figure 2.2	Properties that determine the catalyst performance	35
Figure 2.3	Different geometries for catalyst supports	36
Figure 2.4	Comparison between pellet and 3D printed structures.....	36
Figure 2.5	The one database principle for catalyst development	43
Figure 2.6	Key features of hte's proprietary software solution myhte	46
Figure 2.7	Screenshot of hte's latest development – a new module to collect all relevant data during catalyst synthesis	49
Figure 2.8	Fully integrated feedback loop	54
Figure 2.9	Correlation of IR spectra with the yields of the most important products for the DTO reaction	55
Figure 2.10	Cellular workflow approach – migration strategy.....	57
Figure 2.11	Multi-floor system and key elements	59
Figure 2.12	Mobile robot transportation – the shortest path planning.....	60
Figure 2.13	Schematic multi-floor navigation with an UR cobot.....	60
Figure 2.14	Artificial intelligence in the field of catalysis	69
Figure 2.15	Natural language processing and explainable artificial intelligence used for catalysis.....	71
Figure 3.1	Enabling digital technologies	88
Figure 3.2	ISA-95 hierarchy of control and optimization	90
Figure 3.3	Performance Engineering for Engineering, Procurement, & Construction.....	106
Figure 3.4	Progress toward autonomous operations	130

TABLES

Table 1.1	Enabling Technologies for Industry 4.0.....	1
Table 1.2	The Five Pillars of the Digitalization Strategy at Evonik	6
Table 1.3	Overview of Different Initiatives for Industry Players. Activities Have Been Monitored Based on Publicly Accessible Information Like Press Releases and Publications.....	10
Table 1.4	National and International Initiatives in the Field of Catalysis and Materials Science	14
Table 2.1	Different Synthesis Methods for Solid Catalysts.....	31
Table 2.2	Summary and Comparison Of Different Systems and Functionalities Applied in Digitalization	47
Table 3.1	Digital Dexterity Capabilities as Defined by Gartner.....	89
Table 3.2	Leading Providers of Digital Technologies to Chemical and Refining Industries, with Major Products Shown.....	92
Table 3.3	New Technology Applications Chemicals and Refining.....	129