Electronic Supplementary Material (ESI) for RSC Advances.

Impact of heterogeneous nanoparticulate Ruthenium catalysts on the greenness of hydrogenation reactions

Dörthe Gericke[a], Dana Kralisch[a]*, Denise Ott[a], Valentina G. Matveeva[b], Esther Sulman[b], Atte Aho[c], Dmitry Yu. Murzin[c], Stefan Roggan[d], Lyudmila Danilova[e], Volker Hessel[f], Patrick Loeb[g]

[a] Friedrich Schiller University of Jena, Institute of Pharmacy, Department of Pharmaceutical Technology, Otto-Schott-Str. 41, D-07745 Jena, Germany. Fax: +49 3641 949942; Phone: +49 3641 949951; E-mail: dana.kralisch@uni-jena.de

[b]Tver Technical University, A.Nikitina str. 22, 170026, Tver, Russia. Tel./Fax: +7(4822)449317; E-mail: sulman@online.tver.ru

[c]Process Chemistry Centre, Åbo Akademi University, Biskopsgatan 8, 20500, Turku/Åbo, Finland. Fax: +359 2215 4479; Phone:+358 2215 4985; E-mail:dmurzin@abo.fi

[d]Bayer Technology Services GmbH, D-51368 Leverkusen, Germany. Fax: +49-214-30-81118; Phone: +49-214-30-48420; E-mail: stefan.roggan@bayer.com

[d]Clariant (RUS), LLC, Andropov ave. 18/6, 115432, Moscow, Russia. Fax: +7(495)7972598; Phone: +7(495)7972599; E-mail: Lyudmila.Danilova@clariant.com

[e]Laboratory of Chemical Reactor Engineering/Micro Flow Chemistry and Process Technology, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherland; Phone: +40-247 2973; E-mail: v.hessel@tue.nl

s[f]Fraunhofer ICT-IMM Continuous Chemical Engineering Department, Carl-Zeiss-Str. 18-20, 55129 Mainz, Germany. Fax: +49 6131 990-205; Phone: +49 6131 990-377; E-Mail: Patrick.Loeb@imm.fraunhofer.de

Evaluation of data quality according to Kralisch et al. 2014[1]

ESI Table 1. Data quality indicators for general modules used in the study.

Process	Source	Completeness	Representativeness	Reliability
Process Auxiliaries				
Water , deionized	Ecoinvent database v3.0[2]	3	4	5
Electricity	Ecoinvent database v3.0	-	-	-
Transport	Ecoinvent database v3.0	-	-	-
Infrastructure	Ecoinvent database v3.0	2	4	3
Heat from natural gas at industrial furnace	Ecoinvent database v3.0	-	-	-
Heat, chemical industry	Ecoinvent database v3.0	-	-	-
Heat from waste treatment in municipal incineration	Ecoinvent database v3.0	-	3	2
Heat from light fuel oil	Ecoinvent database v3.0	-	-	-
Waste Treatment				
Treatment of organic waste	Ecoinvent database v3.0	2	3	2
Wastewater treatment	Ecoinvent database v3.0	3	3	3
Treatment of hazardous waste	Ecoinvent database v3.0	2	3	2
Treatment of non-hazardous waste	Ecoinvent database v3.0	-	3	2

ESI Table 2. Data quality indication of the inventory of the HPS based system.

Process	Source	Completeness	Representativeness	Reliability
Glucose Hydrogenation				
Energy demand	Measured data; thermodynamic calculation	2	2	2
Mass balance	Measured data	1	1	1
Waste treatment	Qualified assumptions	2	4	5
H_2	Ecoinvent database v3.0	1	3	2
*Glucose				
*HPS/Ru				
Glucose				
Energy demand	Process specific demands according to Rosenberger-Süß et al.[3]	3	4	2
Mass balance	Miyawaki and Kaneko[4]	2	1	1
Waste treatment	Qualified assumptions	2	4	5
HCl	Ecoinvent database v3.0	3	3	3
Maize starch	Ecoinvent database v3.0	4	3	3
Kieselguhr	Ecoinvent database v3.0; substituted by silica sand	2	5	5
HPS/Ru				
Energy demand	Measured data			
Mass balance	Measured data	1	1	1
Waste treatment	Qualified assumptions	2	4	5
H_2O_2	Ecoinvent database v3.0	-	-	-
NaOH	Ecoinvent database v3.0	-	-	-
MeOH	Ecoinvent database v3.0	2	3	2
THF	Ecoinvent database v3.0	3	4	4
*HPS				
*$Ru(OH)Cl_3$				
HPS				
Energy demand	Process specific demands	3	4	2
Mass balance	Tsyurupa and Davankov[5]	1	4	3
Waste treatment	Process specific demands	3	4	2
Polystyrene	Ecoinvent database v3.0	1	2	1
Dichloroethane	Ecoinvent database v3.0	1	2	2
Chlorodimethylether	Ecoinvent database v3.0	4	4	2
*$SnCl_4$				

Process	Source	Completeness	Representativeness	Reliability
$Ru(OH)Cl_3$				
Energy demand	Process specific demands	3	4	2
Mass balance	Gutbier and Trenkner, Remy and Lührs[6]	2	5	3
Waste treatment	Process specific demands	3	4	2
Ru	Ecoinvent database v3.0; modelled by platinum group metal	2	5	4
KOH	Ecoinvent database v3.0	-	-	-
KNO_3	Ecoinvent database v3.0	3	4	2
$SnCl_4$				
Energy demand	Process specific demands	3	4	2
Mass balance	Graf [7]	4	5	2
Waste treatment	Process specific demands	3	4	2
Sn	Ecoinvent database v3.0	-	-	-
Cl_2	Ecoinvent database v3.0	-	-	-

ESI Table 3. Data quality indication for the NCNT-based system.

Process	Source	Completeness	Representativeness	Reliability
Glucose Hydrogenation (GH)				
Energy demand	Measured data; thermodynamic calculations	2	2	2
Mass balance	Measured data	2	1	1
Waste treatment	Qualified assumptions	2	4	5
H_2	Ecoinvent database v3.0	1	3	2
*Glucose				
*NCNT/Ru				
NCNT/Ru				
Energy demand	Measured data; thermodynamic calculations	2	2	2
Mass balance	Measured data	2	1	1
Waste treatment	Qualified assumptions	3	4	5
H_2O_2	Ecoinvent database v3.0	-	-	-
*NCNT				
*$Ru(OH)Cl_3$				
NCNT				
Energy demand	Process specific demands	3	4	2
Mass balance	Aurel and colleagues[8]	3	1	2
Waste treatment	Process specific demands	3	4	2
Acetonitrile	Ecoinvent database v3.0	3	3	3
N_2	Ecoinvent database v3.0	-	-	-
H_2	Ecoinvent database v3.0	1	3	2
NCNT-Cat*				
NCNT Catalyst				
Energy demand	Process specific demands	3	4	2
Mass balance	Aurel and colleagues	2	1	1
Waste treatment	Process specific demands	3	4	2
$Co(NO_3)_2 \cdot 6H_2O$				
$Mn(NO_3)_2 \cdot 4H_2O$				
$Al(NO_3)_3 \cdot 9H_2O$				
$Mg(NO_3)_2 \cdot 6H_2O$				
NaOH	Ecoinvent database v3.0	-	-	-

Process	Source	Completeness	Representativeness	Reliability
HNO_3	Ecoinvent database v3.0	1	2	3
$Co(NO_3)_2 \cdot 6H_2O$				
Energy demand	Process specific demands	3	4	2
Mass balance	Donaldson and Beyersmann[9]	4	3	3
Waste treatment	Process specific demands	3	4	2
Co	Ecoinvent database v3.0	2	3	4
HNO_3	Ecoinvent database v3.0	1	2	3
$Mn(NO_3)_2 \cdot 4H_2O$				
Energy demand	Process specific demands	3	4	2
Mass balance	Reidies[10]	4	3	3
Waste treatment	Process specific demands	3	4	2
MnO_2	Ecoinvent database v3.0	2	3	3
HNO_3	Ecoinvent database v3.0	1	2	3
$Al(NO_3)_3 \cdot 9H2O$				
Energy demand	Process specific demands	3	4	2
Mass balance	Sitzmann[11]	4	3	3
Waste treatment	Process specific demands	3	4	2
$Al(OH)_3$	Ecoinvent database v3.0	2	3	1
HNO_3	Ecoinvent database v3.0	1	2	3
$Mn(NO_3)_2 \cdot 4H_2O$				
Energy demand	Process specific demands	3	4	2
Mass balance	-	5	5	4
Waste treatment	Process specific demands	3	4	2
$Mg(OH)_2$	Ecoinvent database v3.0; substituted by MgO	-	5	-
HNO_3	Ecoinvent database v3.0	1	2	3

ESI Table 4. Data quality indication for the RaNi-based system.

Process	Source	Completeness	Representativeness	Reliability
Glucose Hydrogenation (GH)				
Energy demand	Thermodynamic calculations	2	2	2
Mass balance	Schiweck et al.[12]	2	2	2
Waste treatment	Qualified assumptions	2	4	5
H_2	Ecoinvent database v3.0	1	3	2
*Glucose				
*Raney Nickel				
RaNi				
Energy demand	Thermodynamic calculations	3	4	5
Mass balance	Ertl and Knözinger[13]	3	1	2
Waste treatment	Qualified assumptions	2	4	5
Nickel	Ecoinvent database v3.0	-	-	-
Aluminium	Ecoinvent database v3.0	-	-	-

\- Data quality information was not given in the Ecoinvent database v3.0.
* Item is evaluated in more detail below.

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