APPENDIX A1

aspentech	LEGENDS Burlington, MA USA	Case Name:	Hydrodeoxygenation of oleic acid and stearic acid.hsc
		Unit Set:	SI
		Date/Time:	Fri Mar 06 14:57:35 2015

Pure Component: OleicAcid

Identification

Family / Class	Chemical Formula	ID Number	Group Name	CAS Number
Carboxilic_Acid	C18H34O2	3097		---

UNIFAC Structure

CH3 (CH2)14 CH=CH COOH

User ID Tags

Tag Number	Tag Text

Critical/Base Properties

Base Properties			Critical Properties		
Molecular Weight		282.5	Temperature	(C)	496.9
Normal Boiling Pt	(C)	358.9	Pressure	(kPa)	1390
Std Liq Density	(kg/m3)	893.4	Volume	(m3/kgmole)	1.000
			Acentricity		1.178

Temperature Dependent Properties

		Vapour Enthalpy	Vapour Pressure	Gibbs Free Energy
Minimum Temperature	(C)	-270.0	13.38	25.00
Maximum Temperature	(C)	5000	496.9	426.9
Coefficient Name		IdealH Coefficient	Antoine Coefficient	Gibbs Free Coefficient
a		3.520e-007	175.2	-6.716e+005
b		-0.2042	-2.002e+004	1577
c		3.543e-003	0.0000	0.1282
d		-1.856e-006	-21.91	0.0000
e		6.040e-010	5.918e-006	0.0000
f		-8.948e-014	2.000	---
g		1.000	0.0000	---
h		0.0000	0.0000	---
i		0.0000	0.0000	---
j		0.0000	0.0000	---

	LEGENDS Burlington, MA USA	Case Name:	Hydrodeoxygenation of oleic acid and stearic acid.hsc
		Unit Set:	SI
		Date/Time:	Fri Mar 06 14:58:42 2015

Pure Component: StearicAcid

Identification

Family / Class	Chemical Formula	ID Number	Group Name	CAS Number
Carboxilic_Acid	C18H36O2	3046		---

UNIFAC Structure

COOH (CH2)16 CH3

User ID Tags

Tag Number	Tag Text

Critical/Base Properties

Base Properties			Critical Properties		
Molecular Weight		284.5	Temperature	(C)	525.9
Normal Boiling Pt	(C)	375.2	Pressure	(kPa)	1350
Std Liq Density	(kg/m3)	881.7	Volume	(m3/kgmole)	1.020
			Acentricity		1.084

Temperature Dependent Properties

		Vapour Enthalpy	Vapour Pressure	Gibbs Free Energy
Minimum Temperature	(C)	-270.0	69.60	25.00
Maximum Temperature	(C)	5000	525.9	426.9
Coefficient Name		IdealH Coefficient	Antoine Coefficient	Gibbs Free Coefficient
a		2.389e-007	171.6	-7.806e+005
b		3.128e-002	-1.898e+004	1711
c		2.974e-003	0.0000	0.1343
d		-1.070e-006	-21.74	0.0000
e		1.434e-010	7.231e-006	0.0000
f		5.141e-015	2.000	---
g		1.000	0.0000	---
h		0.0000	0.0000	---
i		0.0000	0.0000	---
j		0.0000	0.0000	---

APPENDIX A3

LEGENDS Burlington, MA USA	Case Name:	Hydrodeoxygenation of oleic acid and stearic acid.hsc
	Unit Set:	SI
	Date/Time:	Sat Mar 07 09:34:14 2015

Conversion Reactor: Hydrodeoxygenation reactor

CONNECTIONS

Inlet Stream Connections

Stream Name	From Unit Operation
Oleic acid	
Stearic acid	
H2	

Outlet Stream Connections

Stream Name	To Unit Operation
Steam	
Biofuel	

Energy Stream Connections

Stream Name	From Unit Operation
Q Reactor	

PARAMETERS

Physical Parameters		Optional Heat Transfer	
Delta P	**Vessel Volume**	**Duty**	**Energy Stream**
0.0000 kPa	---	2.414e+006 kJ/h	Q Reactor

User Variables

REACTION DETAILS

Reaction: Oleic +H2

Component	Mole Weight	Stoichiometric Coeff.
OleicAcid	282.5	-1.000 *
Hydrogen	2.016	-3.989 *
n-C18	254.5	1.000 *
H2O	18.02	2.000 *

Reaction: Stearic + H2

Component	Mole Weight	Stoichiometric Coeff.
StearicAcid	284.5	-1.000 *
Hydrogen	2.016	-2.989 *
n-C18	254.5	1.000 *
H2O	18.02	2.000 *

REACTION RESULTS FOR : HDO

Extents

Name	Rank	Specified % Conversion	Use Default	Actual % Conversion	Base Component	Reaction Extent
Oleic +H2	0 *	90.00	Yes	81.56	OleicAcid	2.492e-003
Stearic + H2	0 *	90.00 *	No	90.00	StearicAcid	2.250e-003

Balance

Components	Total Inflow	Total Reaction	Total Outflow
OleicAcid	3.056e-003	-2.492e-003	5.636e-004
StearicAcid	2.500e-003	-2.250e-003	2.500e-004
LinoleicAcid	0.0000	0.0000	0.0000

* Specified by user.

Conversion Reactor: Hydrodeoxygenation reactor (continued)

REACTION RESULTS FOR : HDO

Balance

Components	Total Inflow	Total Reaction	Total Outflow
1C16oicAcid	0.0000	0.0000	0.0000
Hydrogen	1.667e-002	-1.667e-002	0.0000
n-C18	0.0000	4.742e-003	4.742e-003
n-C16	0.0000	0.0000	0.0000
H2O	0.0000	9.484e-003	9.484e-003

CONDITIONS

Name		Oleic acid	Stearic acid	H2	Biofuel
Vapour		0.0000	0.0000	1.0000	0.0000
Temperature	(C)	30.0000 *	30.0000 *	30.0000 *	300.0000 *
Pressure	(kPa)	220.0000 *	220.0000 *	220.0000 *	220.0000
Molar Flow	(kgmole/h)	10.0000 *	10.0000 *	60.0000 *	6.6710
Mass Flow	(kg/h)	2833.7421	2833.7421	120.9600	1741.1244
Std Ideal Liq Vol Flow	(m3/h)	3.1909	3.1909	1.7315	2.1518
Molar Enthalpy	(kJ/kgmole)	-8.402e+005	-8.402e+005	142.1	-3.959e+005
Molar Entropy	(kJ/kgmole-C)	247.2	247.2	155.4	886.3
Heat Flow	(kJ/h)	-8.4017e+06	-8.4017e+06	8.5286e+03	-2.6412e+06
Name		Steam	Q Reactor		
Vapour		1.0000	---		
Temperature	(C)	300.0000	---		
Pressure	(kPa)	220.0000	---		
Molar Flow	(kgmole/h)	47.4713	---		
Mass Flow	(kg/h)	4047.3197	---		
Std Ideal Liq Vol Flow	(m3/h)	4.9368	---		
Molar Enthalpy	(kJ/kgmole)	-2.473e+005	---		
Molar Entropy	(kJ/kgmole-C)	387.5	---		
Heat Flow	(kJ/h)	-1.1740e+07	2.4141e+06		

PROPERTIES

Name		Oleic acid	Stearic acid	H2	Biofuel	Steam
Molecular Weight		283.4	283.4	2.016	261.0	85.26
Molar Density	(kgmole/m3)	3.053	3.053	8.728e-002	2.274	4.617e-002
Mass Density	(kg/m3)	865.2	865.2	0.1760	593.6	3.936
Act. Volume Flow	(m3/h)	3.275	3.275	687.4	2.933	1028
Mass Enthalpy	(kJ/kg)	-2965	-2965	70.51	-1517	-2901
Mass Entropy	(kJ/kg-C)	0.8725	0.8725	77.10	3.396	4.545
Heat Capacity	(kJ/kgmole-C)	542.2	542.2	28.43	794.8	221.0
Mass Heat Capacity	(kJ/kg-C)	1.913	1.913	14.10	3.045	2.592
LHV Vol Basis (Std)	(kJ/kgmole)	1.050e+007	1.050e+007	2.419e+005	1.106e+007	3.145e+006
LHV Mass Basis (Std)	(kJ/kg)	3.704e+004	3.704e+004	1.200e+005	4.239e+004	3.689e+004
Phase Fraction [Vol. Basis]		0.0000	0.0000	1.000	---	1.000
Phase Fraction [Mass Basis]		0.0000	0.0000	1.000	0.0000	1.000
Partial Pressure of CO2	(kPa)	0.0000	0.0000	0.0000	0.0000	0.0000
Cost Based on Flow	(Cost/s)	0.0000	0.0000	0.0000	0.0000	0.0000
Act. Gas Flow	(ACT_m3/h)	---	---	687.4	---	1028
Avg. Liq. Density	(kgmole/m3)	3.134	3.134	34.65	3.100	9.616
Specific Heat	(kJ/kgmole-C)	542.2	542.2	28.43	794.8	221.0
Std. Gas Flow	(STD_m3/h)	236.4	236.4	1419	157.7	1122
Std. Ideal Liq. Mass Density	(kg/m3)	888.1	888.1	69.86	809.1	819.8

Conversion Reactor: Hydrodeoxygenation reactor (continued)

PROPERTIES

Name		Oleic acid	Stearic acid	H2	Biofuel	Steam
Act. Liq. Flow	(m3/s)	9.098e-004	9.098e-004	---	8.148e-004	---
Z Factor		2.859e-002	2.859e-002	1.000	---	---
Watson K		11.78	11.78	47.60	12.66	12.85
User Property		---	---	---	---	---
Partial Pressure of H2S	(kPa)	0.0000	0.0000	0.0000	0.0000	0.0000
Cp/(Cp - R)		1.016	1.016	1.413	1.011	1.039
Cp/Cv		1.124	1.124	1.413	1.191	1.039
Heat of Vap.	(kJ/kgmole)	1.034e+005	1.034e+005	1246	1.156e+005	8.589e+004
Kinematic Viscosity	(cSt)	36.26	36.26	50.39	0.4610	3.624
Liq. Mass Density (Std. Cond)	(kg/m3)	875.3	875.3	---	807.6	859.9
Liq. Vol. Flow (Std. Cond)	(m3/h)	3.237	3.237	---	2.156	4.707
Liquid Fraction		1.000	1.000	0.0000	1.000	0.0000
Molar Volume	(m3/kgmole)	0.3275	0.3275	11.46	0.4397	21.66
Mass Heat of Vap.	(kJ/kg)	364.9	364.9	618.0	443.0	1007
Phase Fraction [Molar Basis]		0.0000	0.0000	1.0000	0.0000	1.0000
Surface Tension	(dyne/cm)	22.04	22.04	---	7.873	---
Thermal Conductivity	(W/m-K)	0.1210	0.1210	0.1771	8.503e-002	3.373e-002
Viscosity	(cP)	31.37	31.37	8.867e-003	0.2737	1.427e-002
Cv (Semi-Ideal)	(kJ/kgmole-C)	533.8	533.8	20.12	786.5	212.6
Mass Cv (Semi-Ideal)	(kJ/kg-C)	1.884	1.884	9.980	3.014	2.494
Cv	(kJ/kgmole-C)	482.5	482.5	20.12	667.3	212.6
Mass Cv	(kJ/kg-C)	1.703	1.703	9.980	2.557	2.494
Cv (Ent. Method)	(kJ/kgmole-C)	---	---	---	8124	---
Mass Cv (Ent. Method)	(kJ/kg-C)	---	---	---	31.13	---
Cp/Cv (Ent. Method)		---	---	---	9.784e-002	---
Reid VP at 37.8 C	(kPa)	1.013e-006	1.013e-006	---	2.299e-004	2.839e-004
True VP at 37.8 C	(kPa)	1.013e-006	1.013e-006	---	0.2935	5.797
Liq. Vol. Flow - Sum(Std. Cond)	(m3/h)	3.237	3.237	0.0000	2.156	4.707
Viscosity Index		29.64	29.64	30.89	-10.27	16.74

LIST OF PUBLICATIONS

1. **O. B. Ayodele**, Hamisu U. Farouk, Jibril Mohammed, Y. Uemura, W.M.A.W. Daud, (2015). Effect of precursor acidity on Zeolite supported Pd catalyst properties and hydrodeoxygenation activity for the production of biofuel, *Journal of Molecular Catalysis A: Chemical*, http://dx.doi.org/10.1016/j.molcata.2015.01.033 (**Tier 1 ISI/Scopus indexed article, Elsevier Publisher, Impact Factor = 3.679).**

2. **O. B. Ayodele**, Hamisu U. Farouk, Jibril Mohammed, Y. Uemura, W.M.A.W. Daud, (2015). Hydrodeoxygenation of oleic acid into n- and iso-paraffin biofuel using zeolite supported fluoro-oxalate modified molybdenum catalyst: Kinetics study, *Journal of the Taiwan Institute of Chemical Engineers*, *http://dx.doi.org/10.1016/j.jtice.2014.12.014* (**Tier 1 ISI/Scopus indexed article, Elsevier Publisher, Impact Factor = 2.637**).

3. **O. B. Ayodele**, W. M. A. W Daud (2014). Optimization of catalytic hydrodeoxygenation of oleic acid into biofuel using fluoroplatinum oxalate zeolite supported catalyst, *Journal of the Taiwan Institute of Chemical Engineers*, *http://dx.doi.org/10.1016/j.jtice.2014.09.031* (**Tier 1 ISI/Scopus indexed article, Elsevier Publisher, Impact Factor = 2.637**).

4. **O. B. Ayodele**, H. F. Abbas, W. M. A. W Daud (2014). Hydrodeoxygenation of stearic acid into normal and iso-octadecane biofuel with zeolite supported palladium-oxalate catalyst, *Energy and Fuels*, 2014, 28 (9), 5872–5881 (**Tier 1 ISI/Scopus indexed article, America Chemical Society Publisher, Impact Factor = 2.733**).

5. **O. B. Ayodele**, H. F. Abbas, W. M. A. W Daud. Preparation and characterization of alumina supported nickel-oxalate catalyst for the hydrodeoxygenation of oleic acid into normal and iso-octadecane biofuel, *Energy Conversion and Management*, 88

(2014) 1111–1119. http://dx.doi.org/10.1016/j.enconman.2014.05.099 (**Tier 1 ISI/Scopus indexed article, Elsevier Publisher, Impact Factor = 3.590**).

6. **O. B. Ayodele**, H. F. Abbas, W. M. A. W Daud (2014). Catalytic upgrading of oleic acid into biofuel using Mo modified zeolite supported Ni oxalate catalyst functionalized with fluoride ion, *Energy Conversion and Management*, DOI:10.1016/j.enconman.2014.02.014 (**Tier 1 ISI/Scopus indexed article, Elsevier Publisher, Impact Factor = 3.590**).
7. **O. B. Ayodele**, H. F. Abbas, W. M. A. W Daud, (2014). Preparation and Characterization of Zeolite Supported Fluoro-palladium Oxalate Catalyst for Hydrodeoxygenation of Oleic Acid into Paraffinic Fuel, *Industrial Engineering and Chemistry Research*, 53 (2), 650–657. (**Tier 1 ISI/Scopus indexed article, America Chemical Society Publisher, Impact Factor = 2.235**).
8. **O. B. Ayodele,** H.F. Abbas, Wan Mohd Ashri Wan Daud (2014). Hydrodeoxygenation of Shea butter to produce diesel-like fuel using acidified and basic Al_2O_3 supported molybdenum oxalate catalyst based on Aspen Hysys simulation study- with Aspen Hysys simulation study, *Energy Education Science and Technology Part A: Energy Science and Research*, 32 (1) 447-460. **(Tier 1 Scopus cited).**
9. **O. B. Ayodele**, H. F. Abbas, W. M. A. W Daud. Effect of oxalic acid functionalization on alumina supported Ni catalyst on the isomerization, kinetics and Arrhenius parameters of oleic acid hydrodeoxygenation into biofuel, Applied Energy, (Manuscript under review), June 2014. **(Tier 1 ISI/Scopus cited).**

Conference Proceedings

1. **O. B. Ayodele,** Wan Mohd Ashri Wan Daud, "Hydrodeoxygenation of Shea butter to produce diesel-like fuel using acidified and basic Al_2O_3 supported molybdenum oxalate catalyst based on Aspen Hysys simulation study" digital proceedings of the 8th SDEWES Conference on Sustainable Development of Energy, Water and Environment Systems, 22 - 27 September 2013, Dubrovnik, Croatia.

Other Publications during Candidature Year

1. N.H.M. Azmi, **O.B. Ayodele**, V.M. Vadivelu, B. H. Hameed (2014). Fe-modified local clay as effective and reusable heterogeneous photo-Fenton catalyst for the decolorization of Acid Green 25, *Journal of the Taiwan Institute of Chemical Engineers*, http://dx.doi.org/10.1016/j.jtice.2014.03.002 **(Tier 1 ISI/Scopus cited)**
2. **O. B. Ayodele,** O.S. Togunwa (2014). Catalytic activity of synthesized bentonite supported cuprospinel oxalate catalyst on the degradation and mineralization kinetics of Direct Blue 71, Acid Green 25 and Reactive Blue 4 pollutants in photo-Fenton process, *Applied Catalysis A*, 470, 285– 293. **(Tier 1 ISI/Scopus cited)**
3. **O. B. Ayodele**, B. H. Hameed (2013). Development of kaolin supported ferric oxalate heterogeneous catalyst for degradation of 4-nitrophenol in photo Fenton process, *Applied Clay Science*, 83–84, 171-181. (**Elsevier**)
4. **O. B. Ayodele**, (2013). Effect of phosphoric acid treatment on kaolin clay supported ferrioxalate catalyst for the degradation of amoxicillin in batch photo-Fenton process, *Applied Clay Science*, 72, 74–83. **(Tier 1 ISI/Scopus cited)**

5. **O. B. Ayodele**, B. H. Hameed (2013). Synthesis of copper pillared bentonite ferrioxalate catalyst for degradation of 4-nitrophenol in visible light assisted Fenton process, *Journal of Industrial and Engineering Chemistry*, 19, (3), 966–974. **(Tier 1 ISI/Scopus cited)**
6. **O. B. Ayodele**, H. S. Auta, N. Md Nor, (2012). Artificial Neural Networks, optimization and kinetic modeling of amoxicillin degradation in photo-Fenton process using aluminum pillared montmorillonite supported ferrioxalate catalyst, *Industrial and Engineering Chemistry Research Journal*, 51, 16311−16319. **(Tier 1 ISI/Scopus cited)**