

University of Groningen

Hydrogenation of edible oils and fats

Jonker, Geert Hilbertus

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version

Publisher's PDF, also known as Version of record

Publication date:
1999

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Jonker, G. H. (1999). *Hydrogenation of edible oils and fats*. s.n.

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Notation

| | |
|-----------------------|---|
| a_c | external particle surface [m_c^2/m_i^3] |
| Bo | Bodenstein number, $Bo = vd_p/D_{ax}$ |
| Bi | Biot number, $Bi = Sh_{ex} = k_s d_p/D_e$ |
| C | concentration [mol/m_i^3] |
| C_{H_2} | ($=m_{H_2} P_{H_2}/R_{gas}T$) hydrogen bulk-liquid concentration [mol/m_i^3] |
| C_{inj} | injected concentration in pulse experiment [mol%] |
| C_s | concentration in solid [mol/m_c^3] |
| D | diffusion coefficient [m^2/s] |
| D_{ax} | axial dispersion coefficient [m^2/s] |
| $\langle d_c \rangle$ | mean pore size [m] |
| D_e | effective intraparticle diffusion coefficient [$(m_c^2/s)(m_i^3/m_c^3)$] |
| df | degrees of freedom |
| d | diameter [m] |
| $d_{p,s}$ | mean-surface-based spherical particle diameter [m] |
| E_a | activation energy [kJ/mol] |
| $E(q)$ | normalized column response |
| ΔH | enthalpy of adsorption [kJ/mol] |
| $\Delta \tilde{H}$ | adsorption enthalpy, relative to the solvent [kJ/mol] |
| ΔH_{iso} | enthalpy of isomerization reaction [kJ/mol] |
| H | number of models |
| J | mole flux [$mol/(m_c^2 s)$] |
| \dot{k} | (pseudo) first-order rate constant [$mol/(kg_{Ni} s)$] or [$m^3/kg_{Ni} s$] |
| k_a | adsorption rate constant [$m_i^3/(kg_{Ni} s)$] |
| k_b, k_d, k_f, k_h | surface rate constant [$mol/(kg_{Ni} s)$] |
| k_i | lumped parameter in time domain, [$mol/(kg_{Ni} s MPa)$] or [MPa^{-1}] or [-] |
| k_i^c | lumped parameter in conversion domain, see section 2.4.1 |
| \bar{k}^{iso} | overall isomerization rate constant, see Table 2.3 [$mol/(kg_{Ni} s)$] |
| $k_1 a$ | volumetric gas-liquid mass-transfer coefficient [s^{-1}] |

notation

| | |
|--------------------|--|
| k_s | L to S mass transfer coefficient, see page 74 [m/s] |
| K | (Langmuir) equilibrium constant [m^3/mol] or [MPa^{-1}] |
| K_s | adsorption constant from tracer pulse experiments [$\text{m}_1^3/\text{m}_s^3$] |
| K_I | equilibrium constant first hydrogen insertion, see Table 2.3 |
| K_{iso} | isomerization equilibrium constant (eq 2.1) |
| L | column length [m] |
| L_p | characteristic particle or crystallite diffusion length [m] |
| m | amount of catalyst added (chapter 5) [kg] |
| m_c | catalyst load [$\text{kg}_{\text{Ni}}/\text{m}_1^3$] |
| m_{H_2} | partition coefficient of hydrogen in FAME [$\text{m}_g^3/\text{m}_1^3$] |
| M | molecular mass [kg/mol] |
| MO1 | first moment of residence time distribution curve [s] |
| m_{Ni} | nickel load of catalyst [$\text{kg}_{\text{Ni}}/\text{kg}_c$] |
| n | number of molecules [mol] |
| n_{hyd} | amount hydrogenated [mol/kg _c] |
| $n_i^{\sigma(n)}$ | reduced surface excess of component i [mol] |
| n^{max} | specific catalyst capacity [mol/kg _c] |
| N_e | number of experiments |
| $N_{h,\text{fit}}$ | number of fitted parameters (of model h) |
| Pe_{ax} | Peclet number for axial dispersion, $Pe_{\text{ax}} = vL/D_{\text{ax}}$ |
| P_{H_2} | hydrogen pressure [MPa] |
| $\Delta P/L$ | pressure drop per column length [Pa/m] |
| P_r | reactor pressure [mbar] |
| r_p | radius [m] |
| R_i | reaction rate of component i [$\text{mol}/(\text{m}_1^3 \text{ s})$] |
| R_i^c | reaction rate in conversion domain, see eqs 2.17–2.18 |
| R_{iso} | isomerization reaction rate [$\text{mol}/(\text{m}_1^3 \text{ s})$] |
| R_{ES} | reaction rate of elementary reaction step [$\text{mol}/(\text{m}_1^3 \text{ s})$] |
| R_{gas} | gas constant [8.314 J/(mol K)] |
| R_{H_2} | hydrogen reaction rate [$\text{mol}/(\text{m}_1^3 \text{ s})$] |

| | |
|------------------|---|
| R_p | maximum particle radius [m] |
| $R_{V,i}$ | ($=r_c m_{Ni} R_i / m_c$) volumetric catalyst reaction rate [mol/(m _c ³ s)] |
| S_{av}^2 | average variance (eq 2.A4) |
| S_c | specific internal catalyst surface [m ² /g] |
| S_h^2 | variance of a single experimental series (eq 2.A3 or eq 4.10) |
| S_I | diene selectivity, see eq 3.28. |
| Sh | Sherwood number ($Sh = k_s d_p / D_b$) |
| t | time [s] |
| T | absolute temperature [K] |
| u | superficial velocity [m/s] |
| v | interstitial velocity [m/s] |
| V_c | specific catalyst pore volume [mL/g] |
| V | column volume [m ³] |
| V_r | retention volume [m ³] |
| x | mole fraction |
| $x_{l,i}$ | liquid mole fraction of component i |
| $x_{s,i}$ | surface mole fraction of component i |
| x_i^0 | initial fraction of i , corrected for hydrogenation (chapter 5) |
| $\Delta x_{l,i}$ | change in liquid mole fraction of i due to adsorption (chapter 5) |

Greek Symbols

| | |
|------------------------------|--|
| \mathbf{a} | contribution of macropore mass transfer; eq 4.16 |
| \mathbf{c}^2 | target function in optimisation procedure (eq 2.A1) |
| \mathbf{c}_c^2 | critical χ^2 of Bartlett's test (eq 2.A2) |
| $\mathbf{c}_t^2(\mathbf{H})$ | tabulated χ^2 for H degrees of freedom |
| \mathbf{e}_b | bed porosity |
| \mathbf{e}_G | volume fraction of gas phase in reactor |
| \mathbf{e}_p | particle porosity [m ³ _{pore} /m ³ _c] |
| \mathbf{f}_{H_2} | hydrogen reaction rate, defined by eq 3.24 [mol/s] |
| Φ | Weisz–Prater modulus, see eq 2.12 |

notation

| | |
|------------|--|
| Φ_v | column flow rate [m ³ /s] |
| h | viscosity [Pa s] |
| l | molecule to pore diameter ($d_m/\langle d_c \rangle$) |
| m | effectiveness factor |
| q | surface coverage fraction; dimensionless time, $q = t(v/L)$ |
| q_m | relative mean residence time, eq. 4.14 |
| r | density [kg/m ³] |
| σ^2 | experimental variance |
| t | particle tortuosity; holding time, $t = L/v = e_b V_{cl}/\Phi_v$ [s] |
| Ω | partition coefficient, defined by eq 5.6 |
| x_{DB} | double bonds per fatty acid, defined by eq 3.18 |
| z | conversion |

Abbreviations

A1, A2, B1, B2, C1, C2: see Table 2.1

| | |
|-------------------|---|
| ass | associative hydrogen adsorption function |
| B | (methyl) behenate (C22:0) |
| C | FAME with 1 double bond in the <i>cis</i> configuration |
| CT | FAME with 2 double bonds, <i>cis</i> and <i>trans</i> configuration |
| C1, C2 | column 1 or 2 |
| CH | cholesterol |
| CP | constant-pressure experiment |
| D | diene; all FAME dienes |
| diss | dissociative hydrogen adsorption function |
| E | elaidate (<i>trans</i> -monoene) |
| Er | (methyl) erucate (C22:1) |
| FAME | fatty acid methyl ester |
| GC | gas chromatograph |
| H, H ₂ | hydrogen |
| HD | <i>n</i> -hexadecane |

| | |
|------------------|---|
| HP | Horiuti–Polanyi mechanism |
| HPE; HPO | high percentage of elaidate or oleate mixture |
| HPLC | high-performance liquid chromatography |
| IPM | isopropyl myristate |
| LHHW | Langmuir–Hinshelwood–Hougen–Watson kinetics |
| MCT | medium-chain triacylglyceride |
| MPO | medium percentage of oleate mixture |
| L | (methyl) linoleate (<i>cis,cis</i> -C18:2) |
| M | monoenes; all FAME monoenes |
| O | (methyl) oleate (<i>cis</i> -monoene, C18:1) |
| P | (methyl) palmitate (C16:0) |
| RTD | residence time distribution (curve) |
| S | (methyl) stearate (C18:0); all saturated species |
| SB | soy bean oil |
| SFME | sunflower methyl ester |
| σ ;SH | half-hydrogenated intermediate |
| T | FAME with 1 double bond in the <i>trans</i> configuration |
| TAG | triacylglyceride |
| TO | trioleate |
| V;V _H | vacancy for FAME or hydrogen |
| VP | variable-pressure experiment |

Sub- and Superscripts

| | |
|----|---|
| a | adsorption |
| ax | axial dispersion |
| b | bulk; first hydrogen insertion backward |
| c | catalyst; conversion domain |
| cl | column |
| CR | crystalline |
| d | data point; desorption |

notation

| | |
|------------------|---|
| DB | double bond |
| e | experimental; effective |
| eq | equilibrium |
| E,h | hydrogenation path of E |
| ES | elementary reaction step |
| f | first hydrogen insertion forward |
| <i>h</i> | model number |
| h;hyd | hydrogenation (path) |
| H,H ₂ | hydrogen |
| <i>i</i> | component |
| IH | intercrystalline holes |
| iso | isomerization (path) |
| l | liquid |
| m | model; molecule |
| Ni | nickel |
| O,h | hydrogenation path of O |
| p | particle |
| r | reactor |
| ref | reference |
| s | solid; second hydrogen insertion |
| solv | solvent |
| tot | total |
| 0 | initial |
| \bar{O} | adsorbed (O) |
| $\Delta\bar{H}$ | relative (dimensionless), see e.g., Table 3.3 |