LIST OF SYMBOLS

<u>Chapter 1</u>

L	length of the bubble column	m
T	diameter of the bubble column	m

<u>Chapter 2</u>

a	interfacial area per unit volume of dispersion	m^{-1}
A	cross-sectional area of the bubble column	m^2
A_t	total surface area of the gas bubbles in the dispersion	m^2
b	coefficient	1
$\overline{C}_p$	average mass of dry catalyst particles in the slurry per unit volume of liquid	$kg\ m^{-3}$
C_p	mass of dry catalyst particles in the slurry per unit volume of liquid	$kg\ m^{-3}$
C_w	drag coefficient for gas bubble	1
d_b	gas bubble diameter	m
d_i	arithmetic mean diameter of a bubble of class i	m
d_{max}	maximum stable bubble diameter	m
d_o	diameter of the orifice in the gas distributor	m
d_p	catalyst particle diameter	m
d_{p_n}	number-average particle diameter	m
d_{p_w}	weight-average particle diameter	m
d_s	Sauter mean bubble diameter ($d_s = \sum n_i d_i^3 / \sum n_i d_i^2$)	m
d_{si}	Sauter mean bubble diameter in the on-stream zone	m
D	diffusion coefficient	$m^2\ s^{-1}$
$f(d_b)$	probability density function of the bubble diameter	m^{-1}
$f_1(w)$	volume-fraction distribution of the gas bubbles as a function of their velocity of rise ($_0\int^\infty f_1(w)\ dw = 1$)	$s\ m^{-1}$
$f_2(d_b)$	volume-fraction distribution of the gas bubbles as a function of their diameter ($_0\int^\infty f_2(d_b)\ d(d_b) = 1$)	m^{-1}
g	acceleration due to gravitation	$m\ s^{-2}$
g(w)	volume fraction of the gas bubbles with a velocity of rise smaller than H(t')/t' which has left the dispersion at t = t'	1
h	difference between manometer levels corresponding to static and dynamic pressure in the Prandtl-tube	m
h_1	height of the upper measuring point ($h_1 = 1.67$ m)	m
$h_{0,1}$	height of manometer level above upper measuring point	m
$h_{n,n+1}$	difference between manometer levels corresponding to the points n and n + 1	m
H(t')	height of the dispersion during gas disengagement at t = t'	m
H_D	height of the dispersion	m
H_F	height of the dispersion without foam	m
H_w	height of the dispersion at the moment that the bubbles with velocity of rise w have left the dispersion during gas disengagement	m
H_0	clear liquid height	m
H_i	height of the dispersion during gas disengagement at time t_i	m
k_L	liquid-film mass transfer coefficient	$m\ s^{-1}$
K_L	overall mass transfer coefficient based on the concentration in the liquid phase	$m\ s^{-1}$
n	parameter	1
n_i	number of gas bubbles belonging to diameter-class i	1

p	pressure	Pa
r	cylindrical coordinate	m
R	radius of the bubble column	m
R_d	radius of the core of the dispersion in the bubble column	m
t	time	s
t'	sampling time	s
t_w	time at which the bubbles with velocity of rise w have left the dispersion during gas disengagement	s
T	bubble column diameter	m
u_G	superficial gas velocity	m s^{-1}
u_L	superficial liquid velocity	m s^{-1}
$v(t')$	velocity of a rising gas bubble with respect to the surface of the dispersion moving downwards during gas disengagement at $t = t'$	m s^{-1}
$\overline{v}_c$	time-average axial liquid velocity at the centre of the bubble column	m s^{-1}
v_d	velocity of rise of a gas bubble in a swarm of bubbles	m s^{-1}
v_i	velocity of rise of a single gas bubble	m s^{-1}
v_o	terminal velocity of a single bubble	m s^{-1}
v_{or}	gas velocity in the orifice of the gas sparger	m s^{-1}
$\underline{v}_r$	relative gas velocity	m s^{-1}
$\overline{v}_r$	time-average radial liquid velocity	m s^{-1}
$v_s(t')$	velocity of the surface of the dispersion moving downwards during gas disengagement at $t = t'$	m s^{-1}
$\overline{v}_w$	time-average axial liquid velocity near the wall of the bubble column	m s^{-1}
$\overline{v}_z$	time-average axial liquid velocity at distance r from the axis of the bubble column	m s^{-1}
$\underline{v}_\infty$	terminal velocity of a single catalyst particle	m s^{-1}
$\overline{v}_\theta$	time-average angular liquid velocity	m s^{-1}
V_G	volume of gas in the dispersion	m^3
$V_G(t')$	volume of gas in the dispersion during gas disengagement at $t = t'$	m^3
V_L	volume of liquid in the dispersion	m^3
V_D	volume of the dispersion	m^3
w	velocity of rise of the gas bubbles	m s^{-1}
x	rectangular coordinate	m
z	cylindrical coordinate (distance from the bottom of the bubble column)	m
$z_{n,n+1}$	axial distance between measuring points n and n + 1	m

Greek symbols

ε	gas holdup	1
$\langle\varepsilon\rangle$	average gas holdup of the cross-sectional area of the column	1
ε_{av}	average gas holdup	1
$\varepsilon_{n,n+1}$	average gas holdup between measuring points n and n + 1	1
ε_p	porosity of the catalyst particle	1
$\varepsilon_{0,1}$	average gas holdup between the surface of the dispersion and the upper measuring point	1
ε_∞	average gas holdup for $u_G \to \infty$	1
η_G	viscosity of the gas	Pa s
η_L	viscosity of the liquid	Pa s
μ_n	nth moment of the probability density function of bubble diameters ($\mu_n = {}_0\int^\infty d_b{}^n\ f(d_b)\ d(d_b)$)	m^n
ν_t	turbulent kinematic viscosity	m^2 s^{-1}
ν_L	kinematic viscosity of the liquid	m^2 s^{-1}
ρ	density	kg m^{-3}

124

ρ_s	density of the solid part of the catalyst particle	kg m^{-3}
ρ_d	density of the dispersion	kg m^{-3}
ρ_G	density of the gas	kg m^{-3}
ρ_L	density of the liquid	kg m^{-3}
ρ_p	density of the catalyst particle (pores included)	kg m^{-3}
$\Delta\rho$	difference of density between the liquid and the gas ($\Delta\rho = \rho_L - \rho_G$)	kg m^{-3}
σ	surface tension	N m^{-1}
τ_{rz}	shear stress	Pa
τ_w	shear stress at the wall of the bubble column	Pa
Φ	volume flow rate of the gas	m^3 s^{-1}
ϑ	cylindrical coordinate	rad
Ψ	dimensionless solids concentration ($\Psi = C_p(z)/\overline{C}_p$)	1
Ω	volume fraction of gas which has left the dispersion during gas disengagement at t = t' ($\Omega = (H_D - H(t'))/(H_D - H_0)$)	1

Dimensionless numbers

Bo	Bond number (Bo $= gT^2\rho_L/\sigma$)	1
Ca	Capillary number (Ca $= \eta_L u_G/\sigma$)	1
Fr	Froude number (Fr $= u_G/(gT)^{\frac{1}{2}}$)	1
Fr$_{or}$	Froude number (Fr$_{or} = v_{or}/(gd_o)^{\frac{1}{2}}$)	1
Ga	Galilei number (Ga $= gT^3\rho_L^2/\eta_L^2$)	1
Mo	Morton number (Mo $= \sigma^3\rho_L/(\eta_L^4 g)$)	1
Re$_b$	Reynolds number for gas bubbles (Re$_b = \rho_L v_o d_b/\eta_L$)	1
Re$_p$	Reynolds number for catalyst particle (Re$_p = \rho_L d_p v_\infty/\eta_L$)	1
Sc	Schmidt number (Sc $= \eta_L/(\rho_L D)$)	1
Sh	Sherwood number (Sh $= k_L T/D$)	1

Mathematical functions

$$F_1(v(t')) = \int_0^{v(t')} f_1(w) \, dw \qquad\qquad 1$$

Chapter 3

a	interfacial area per unit volume of dispersion	m^{-1}
a_L	interfacial area per unit volume of liquid	m^{-1}
b_e	barometric pressure after gas desorption	Pa
b_o	barometric pressure before gas desorption	Pa
C_A	concentration of gas A in a liquid	mol m^{-3}
C_{Ab}	concentration of gas A in the bulk of the liquid	mol m^{-3}
C_{As}	solubility of gas A in a liquid	mol m^{-3}
d_s	Sauter mean bubble diameter	m
D	diffusion coefficient	m^2 s^{-1}
g	acceleration due to gravitation	m s^{-2}
G	graduation reading	1
G_e	graduation reading after gas desorption	1
G_o	graduation reading before gas desorption	1
h_m	difference between manometer levels indicating overpressure of saturation column	m
h_b	height of liquid sample in gas burette after gas desorption	m
H_D	height of the dispersion	m
H_0	clear liquid height in column A$_1$	m
J_A	molar flux of gas A	mol m^{-2} s^{-1}
k_L	liquid-film mass transfer coefficient	m s^{-1}
$\overline{k}_L$	mean liquid-film mass transfer coefficient	m s^{-1}

L	length of the stream of liquid	m
m	mass of liquid sample saturated with gas	kg
m_1	mass of vessel with saturated liquid	kg
m_2	mass of vessel	kg
N_A	amount of gas A desorbed from a sample of saturated liquid	mol
N_e	amount of gas in the gas burette after desorption	mol
N_o	amount of gas in the gas burette before desorption	mol
N_v	amount of vapour in the gas burette after desorption	mol
p_{Ab}	partial pressure of gas A in the gas burette	Pa
p_{As}	partial pressure of gas A in the saturation column	Pa
p_b	pressure in the gas burette after desorption	Pa
p_s	pressure in the saturation column	Pa
p_{vb}	vapour pressure of a liquid in the gas burette	Pa
p_{vs}	vapour pressure of a liquid in the saturation column	Pa
R	gas constant ($R = 8.314$ J mol^{-1} K^{-1})	J mol^{-1} K^{-1}
R_b	radius of the stream of liquid	m
t	time	s
t_c	contact time ($t_c = L/v_b$)	s
T	temperature	K
T_b	temperature in the gas burette	K
T_s	temperature in the saturation column	K
v_b	velocity of liquid at the gas-liquid interface	m s^{-1}
V_b	volume of gas in the gas burette	m^3
V_D	volume of the dispersion	m^3
V_e	volume of gas in the gas burette after desorption	m^3
V_L	volume of liquid in the dispersion	m^3
V_o	volume of gas in the gas burette before desorption	m^3
V_1	constant ($V_1 = 2.3 \ 10^{-7}$ m^3)	m^3
V_2	constant ($V_2 = 6.3 \ 10^{-9}$ m^3)	m^3
x	rectangular coordinate	m
z	cylindrical coordinate	m

Greek symbols

δ	penetration depth	m
ε_{av}	average gas holdup	1
η_L	viscosity of the liquid	Pa s
ρ_b	density of the degassed liquid in the gas burette	kg m^{-3}
ρ_G	density of the gas in the saturation column	kg m^{-3}
ρ_s	density of the liquid in the saturation column	kg m^{-3}
$\Delta\rho$	difference between the density of the liquid and the gas in the saturation column ($\Delta\rho = \rho_s - \rho_G$)	kg m^{-3}
σ_{He}	standard deviation of the Henry number	1

Dimensionless numbers

Fo	Fourier number (Fo $= Dt_c/R_b^2$)	1
He	Henry number (He $= c_{As}RT_s/p_{As}$)	1
Sc	Schmidt number (Sc $= \eta_L/(\rho_s D)$)	1

Chapter 4

a	thermal diffusivity of the liquid	m^2 s^{-1}
A_c	area of blocked segment of the sphere	m^2
c_a	concentration of additives	mol m^{-3}
c_A	concentration of gas A in the solution	mol m^{-3}
c_p	polymer concentration in the solution	kg kg^{-1}

c_R	molar concentration of gas in the solution at the gas-liquid interface	mol m^{-3}
c_∞	molar concentration of gas in the solution at t = 0 and at r $\to \infty$ for t > 0	mol m^{-3}
d	diameter of the gas bubble	m
d^o	diameter of the gas-bubble projection on the screen	m
d_c	diameter of the top of the truncated cone	m
d_c^o	diameter of the top of the truncated-cone projection on the screen	m
d_{max}	maximum diameter of a gas bubble that stays fixed at the tip of the needle	m
d_N	diameter of the needle	m
d_N^o	diameter of the needle projection on the screen	m
D	diffusion coefficient	m^2 s^{-1}
D_{AB}	diffusion coefficient of solute A in solvent B	m^2 s^{-1}
D_G	diffusion coefficient of the solvent vapour	m^2 s^{-1}
D_w	diffusion coefficient of gas in the pure solvent	m^2 s^{-1}
g	acceleration due to gravitation	m s^{-2}
$\Delta H_{vap,B}$	enthalpy of vaporization of solvent B	J mol^{-1}
$\Delta H_{vap,w}$	enthalpy of vaporization of water	J mol^{-1}
J_A	molar flux of gas A	mol m^{-2} s^{-1}
k	Boltzmann constant (k = 1.38 10^{-23} J K^{-1} molecule^{-1})	J K^{-1} molecule^{-1}
ℓ	length of slab of gas in the needle	m
L	radius of the inner cell	m
m	slope of straight line in eqn (4-20)	s^{-1}
M_B	molar mass of solvent B	kg mol^{-1}
n	exponent in eqn (4-45)	1
N_A^*	amount of gas absorbed in the solvent	mol
p_R	partial pressure of gas at the gas-liquid interface	Pa
r	polar coordinate	m
R	radius of the gas bubble	m
$\tilde{R}$	gas constant ($\tilde{R}$ = 8.314 J mol^{-1} K^{-1})	J mol^{-1} K^{-1}
R_A	radius of a molecule of solute A	m
R_B	radius of curvature of the bottom of the gas bubble	m
R_T	radius of curvature of the top of the gas bubble	m
ΔR	difference of radii ($\Delta R = R_T - R_B$)	m
t	time	s
t'	sampling time	s
T	temperature	K
ΔT	temperature difference	K
V_A	molar volume of the solute A	m^3 mol^{-1}
V_A^*	volume of gas A absorbed in the solvent	m^3
V_b	volume of the gas bubble	m^3
V_B	molar volume of the solvent B	m^3 mol^{-1}
z	argument ($z = (r - R)/(2(D_{AB}t)^{\frac{1}{2}})$)	1

Greek symbols

α	heat transfer coefficient	W m^{-2} K^{-1}
α	cone angle (see Fig. 4.2.)	rad
β	thermal expansion coefficient of the solvent	K^{-1}
γ	fraction of the bubble surface available for mass transfer	1
η	viscosity	Pa s
η_B	viscosity of solvent B at 20 ^{o}C	Pa s
η_0	zero-shear viscosity	Pa s
η_∞	infinite-shear viscosity	Pa s
η_w	viscosity of water	Pa s
θ	polar coordinate	rad
λ	heat conductivity of the liquid	W m^{-1} K^{-1}

ν	kinematic viscosity of the liquid	$m^2\ s^{-1}$
ρ_G	density of the gas	$kg\ m^{-3}$
ρ_L	density of the liquid	$kg\ m^{-3}$
σ	surface tension	$N\ m^{-1}$
σ_D	standard deviation of the mean diffusion coefficient	$m^2\ s^{-1}$
σ_n	standard deviation of n	1
ϕ_A	molar rate of gas absorption from a sphere	$mol\ s^{-1}$
ϕ_A^*	molar rate of gas absorption from the bubble on the needle	$mol\ s^{-1}$
χ	association parameter	1

Dimensionless numbers

Bo	Bond number (Bo = $\rho_L g R^2/\sigma$)	1
Fo	Fourier number (Fo = $D_G t/l^2$)	1
He	Henry number (He = $c_R \hat{R} T/p_R$)	1
Nu	Nusselt number (Nu = $\alpha L/\lambda$)	1
Ra	Rayleigh number (Ra = $L^3 g \beta \Delta T/(a\nu)$)	1

Mathematical function

erfc (z) complementary error function

$$erfc(z) = (2/\sqrt{\pi}) \int_z^\infty e^{-x^2}\ dx \qquad\qquad 1$$

Chapter 5

a_L	interfacial area of the gas per unit volume of liquid	m^{-1}
A_L	interfacial area of the gas	m^2
a_s	interfacial area of the catalyst particles per unit volume of liquid	m^{-1}
C_A	molar concentration of gas A	$mol\ m^{-3}$
C_{Ab}	molar concentration of gas A in the bulk of the liquid	$mol\ m^{-3}$
C_{Ai}	molar concentration of gas A at the gas-liquid interface	$mol\ m^{-3}$
C_{As}	molar concentration of gas A at the liquid-solid interface	$mol\ m^{-3}$
C_B	molar concentration of component B in the liquid	$mol\ m^{-3}$
C_p	mass of dry catalyst particles per unit volume of liquid	$kg\ m^{-3}$
d_p	catalyst particle diameter	m
d_s	Sauter mean bubble diameter	m
D	diffusion coefficient	$m^2\ s^{-1}$
D^*	effective diffusion coefficient ($D^* = D\epsilon_p/\tau$)	$m^2\ s^{-1}$
E	enhancement factor ($E = \Phi_A/(k_L a_L C_{Ai})$)	1
k_o	reaction-rate constant for reaction of zero order in gas component A and m^{th} order in component B	$(mol\ m^{-3})^{1-m}\ s^{-1}$
k_1	reaction-rate constant for reaction of first order in gas component A and m^{th} order in component B	$(mol\ m^{-3})^{-m}\ s^{-1}$
k_L	liquid-film mass transfer coefficient at gas-liquid interface	$m\ s^{-1}$
k_n	reaction-rate constant for reaction of nth order in gas component A and m^{th} order in component B	$(mol\ m^{-3})^{1-m-n}\ s^{-1}$
k_s	liquid-film mass transfer coefficient at liquid-solid interface	$m\ s^{-1}$
m	order of reaction for component B	1
n	order of reaction for component A	1
n_p	number of catalyst particles per unit volume of bulk	m^{-3}

	liquid	
r	polar coordinate	m
R^*	radial distance in the catalyst particle at which $C_A = 0$	m
R_p	radius of the catalyst particle	m
x	rectangular coordinate	m
v_p	volume of the catalyst particles (pores included) per unit volume of liquid	l
v_L	volume of liquid	m^3

Greek symbols

Γ, Γ'	dimensionless ratio ($\Gamma = k_s a_s/(k_L a_L)$; $\Gamma' = k_s a_s/(k_L a_L(1 - a_L \delta))$)	1
δ	thickness of the liquid film ($\delta = D/k_L$)	m
δ^*	linear distance in the liquid film at which $C_A = 0$	m
ε_p	porosity of the catalyst particle	1
η_0	effectiveness of the catalyst particle for zero-order reaction in gas component A	1
η_1	effectiveness of the catalyst particle for first-order reaction in gas component A	1
Θ_0	modified Hatta number for heterogeneously catalyzed reaction of zero order in gas component A ($\Theta_0 = Ha_0 \phi^{\frac{1}{2}}$)	1
Θ_1	modified Hatta number for heterogeneously catalyzed reaction of first order in gas component A ($\Theta_1 = Ha_1 \phi^{\frac{1}{2}}$)	1
Θ_n	modified Hatta number for heterogeneously catalyzed reaction of nth order in gas component A ($\Theta_n = Ha_n \phi^{\frac{1}{2}}$)	1
λ	coefficient for heterogeneously catalyzed reaction of first order in gas component A ($\lambda = (k_1 C_B^m \phi/D)^{\frac{1}{2}}$)	m^{-1}
λ'	coefficient for heterogeneously catalyzed reaction of first order in gas component A ($\lambda' = (k_1 C_B^m/D^*)^{\frac{1}{2}}$)	m^{-1}
λ''	coefficient for heterogeneously catalyzed reaction of first order in gas component A ($\lambda'' = (k_1 C_B^m \phi''/D)^{\frac{1}{2}}$)	m^{-1}
Λ_0	coefficient for heterogeneously catalyzed reaction of zero order in gas component A ($\Lambda_0 = k_0 C_B^m d_p^2/(24D^* C_{Ai})$)	1
Λ_1	coefficient for heterogeneously catalyzed reaction of first order in gas component A ($\Lambda_1 = k_1 C_B^m d_p^2/(12D^*)$)	1
Λ_n	coefficient for heterogeneously catalyzed reaction of nth order in gas component A ($\Lambda_n = k_n C_B^m d_p^2 C_{Ai}^{n-1}(n + 1)/(24D^*)$)	1
ρ_p	density of the catalyst particles (pores included)	kg m^{-3}
τ	tortuosity	1
ϕ	volume of the catalyst particles per unit volume of liquid film ($\phi = \bar{C}_p/(\rho_p a_L \delta)$)	1
ϕ'	volume of the catalyst particles per unit volume of bulk liquid ($\phi' = \bar{C}_p/(\rho_p(1 - a_L \delta))$)	1
ϕ''	volume of the catalyst particles per unit volume of liquid ($\phi'' = \bar{C}_p/\rho_p$)	1
Φ_A	gas absorption rate per unit volume of liquid	mol m^{-3} s^{-1}

Dimensionless numbers

Ha_0	Hatta number for zero-order reaction in gas component A ($Ha_0 = (1/k_L)\{2k_0 C_B^m D/C_{Ai}\}^{\frac{1}{2}}$)	1
Ha_1	Hatta number for first-order reaction in gas component A ($Ha_1 = (1/k_L)\{k_1 C_B^m D\}^{\frac{1}{2}}$)	1
Ha_n	Hatta number for n^{th} order reaction in gas component A ($Ha_n = (1/k_L)\{2k_n C_B^m C_{Ai}^{n-1} D/(n + 1)\}^{\frac{1}{2}}$)	1

a_L	interfacial area of the gas per unit volume of liquid	m^{-1}
a_s	interfacial area of the catalyst particles per unit volume of liquid	m^{-1}
b	slope of straight line in eqn (6-7)	s^{-1}
c_A	molar concentration of gas A in the bulk of the liquid	$mol\ m^{-3}$
$c_A{}^0$	molar concentration of gas A in the bulk of the liquid at $t = 0$	$mol\ m^{-3}$
c_{Ai}	molar concentration of gas A at the gas-liquid interface	$mol\ m^{-3}$
c_B	molar concentration of component B in the liquid	$mol\ m^{-3}$
$\overline{c}_p$	mass of dry catalyst particles per unit volume of liquid	$kg\ m^{-3}$
d_i	inside diameter of the syringe	m
d_p	catalyst particle diameter	m
D	diffusion coefficient	$m^2\ s^{-1}$
D^*	effective diffusion coefficient ($D^* = D\varepsilon_p/\tau$)	$m^2\ s^{-1}$
D_w	inside diameter of the Whitman cell	m
E	enhancement factor ($E = \Phi_A/(k_L a_L c_{Ai})$)	1
k_o	reaction-rate constant for reaction of zero order in hydrogen and half order in hydroxylamine	$(mol\ m^{-3})^{\frac{1}{2}}\ s^{-1}$
$k_o{}^*$	modified reaction-rate constant for reaction of zero order in hydrogen and half order in hydroxylamine ($k_o{}^* = k_o/\rho_p$)	$(mol\ m^{3})^{\frac{1}{2}}\ kg^{-1}\ s^{-1}$
k_1	reaction-rate constant for reaction of first order in hydrogen and zero order in styrene	s^{-1}
$k_{\frac{1}{2}}$	reaction-rate constant for reaction of half order in hydrogen and zero order in 3-pentanone	$(mol\ m^{-3})^{\frac{1}{2}}\ s^{-1}$
k_L	liquid-film mass transfer coefficient at gas-liquid interface	$m\ s^{-1}$
k_s	liquid-film mass transfer coefficient at gas-solid interface	$m\ s^{-1}$
$\Delta\ell$	displacement of the plunger of the syringe	m
m	order of reaction for component B	1
M_L	mass of the liquid in the Whitman cell	kg
n	order of reaction for component A	1
p_{H_2}	partial pressure of hydrogen in the gas phase	Pa
p_t	total pressure in the Whitman cell	Pa
p_v	vapour pressure of the liquid in the Whitman cell	Pa
$\tilde{R}$	gas constant ($\tilde{R} = 8.314\ J\ mol^{-1}\ K^{-1}$)	$J\ mol^{-1}\ K^{-1}$
S_p	internal specific surface area of the catalyst particles	$m^2\ kg^{-1}$
t	time	s
Δt	sampling time	s
T	temperature	K
V_L	volume of the liquid in the Whitman cell	m^3
V_p	volume of the pores in the catalyst particles	$m^3\ kg^{-1}$

Greek symbols

Γ, Γ'	dimensionless ratio ($\Gamma = k_s a_s/(k_L a_L)$, $\Gamma' = k_s a_s/(k_L a_L(1 - a_L\delta))$)	1
δ	thickness of the liquid film ($\delta = D/k_L$)	m
δ_p	pore diameter	m
ε_p	porosity of the catalyst particle	1
η_o	effectiveness of the catalyst particle for zero-order reaction in gas component A	1
η_1	effectiveness of the catalyst particle for first-order	1

	reaction in gas component A	
Θ_0	modified Hatta number for heterogeneously catalyzed reaction of zero order in gas component A ($\Theta_0 = Ha_0\phi^{\frac{1}{2}}$)	1
$\Theta_{\frac{1}{2}}$	modified Hatta number for heterogeneously catalyzed reaction of half order in gas component A ($\Theta_{\frac{1}{2}} = Ha_{\frac{1}{2}}\phi^{\frac{1}{2}}$)	1
Θ_1	modified Hatta number for heterogeneously catalyzed reaction of first order in gas component A ($\Theta_1 = Ha_1\phi^{\frac{1}{2}}$)	1
λ''	coefficient for heterogeneously catalyzed reaction of first order in gas component A ($\lambda'' = (k_1C_B^m\phi''/D)^{\frac{1}{2}}$)	m^{-1}
Λ_0	coefficient for heterogeneously catalyzed reaction of zero order in gas component A ($\Lambda_0 = k_0C_B^md_p^2/(24D*C_{Ai})$)	1
ρ_s	density of the catalyst solid	$kg\ m^{-3}$
ρ_L	density of the liquid in the Whitman cell	$kg\ m^{-3}$
ρ_p	density of the catalyst particles (pores included)	$kg\ m^{-3}$
τ	tortuosity ($\tau = 3$ for carbon particles [119])	1
ϕ	volume of the catalyst particles per unit volume of liquid film ($\phi = \overline{C}_p/(\rho_pa_L\delta)$)	1
ϕ'	volume of the catalyst particles per unit volume of bulk liquid ($\phi' = \overline{C}_p/(\rho_p(1 - a_L\delta))$)	1
ϕ''	volume of the catalyst particles per unit volume of liquid ($\phi'' = \overline{C}_p/\rho_p$)	1
Φ_A	gas absorption rate per unit volume of liquid	$mol\ m^{-3}\ s^{-1}$

Dimensionless numbers

Ha_0	Hatta number for zero-order reaction in gas component A ($Ha_0 = (1/k_L)\{2k_0C_B^mD/C_{Ai}\}^{\frac{1}{2}}$)	1
$Ha_{\frac{1}{2}}$	Hatta number for half-order reaction in gas component A ($Ha_{\frac{1}{2}} = (1/k_L)\{4k_{\frac{1}{2}}D/(3C_{Ai}^{\frac{1}{2}})\}^{\frac{1}{2}}$)	1
Ha_1	Hatta number for first-order reaction in gas component A ($Ha_1 = (1/k_L)\{k_1C_B^mD\}^{\frac{1}{2}}$)	1
Sh_p	Sherwood number for the catalyst particles ($Sh_p = k_sd_p/D$)	1

Chapter 7
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a_L	interfacial area of the gas per unit volume of liquid	m^{-1}
a_s	interfacial area of the catalyst particles per unit volume of liquid	m^{-1}
b	coefficient	1
C_{Ai}	molar concentration of gas A at the gas-liquid interface	$mol\ m^{-3}$
C_B	molar concentration of component B in the liquid	$mol\ m^{-3}$
$\overline{C}_p$	mass of dry catalyst particles per unit volume of liquid	$kg\ m^{-3}$
$C_p^{\ o}$	mass of dry catalyst particles per unit volume of liquid film	$kg\ m^{-3}$
d_L	outside diameter of spherical layer (film and bulk) of liquid around the gas bubble	m
d_p	catalyst particle diameter	m
d_s	Sauter mean bubble diameter	m
D	diffusion coefficient	$m^2\ s^{-1}$
D*	effective diffusion coefficient ($D* = D\epsilon_p/\tau$)	$m^2\ s^{-1}$
D_w	inside diameter of Whitman cell	m
E	enhancement factor ($E = \Phi_A/(k_La_LC_{Ai})$)	1
f_0	fraction of gas-bubble surface area occupied by the projection of the catalyst particles in a monolayer	1
H_0	clear liquid height	m
k_G	gas-film mass transfer coefficient	$m\ s^{-1}$

k_L	liquid-film mass transfer coefficient at gas-liquid interface	m s^{-1}
k_n	reaction-rate constant for reaction of nth order in gas component A and mth order in component B	(mol m^{-3})$^{1-m-n}$ s^{-1}
k_s	liquid-film mass transfer coefficient at gas-solid interface	m s^{-1}
m	order of reaction for component B	1
n	order of reaction for component A	1
n_b	number of gas bubbles in the dispersion	1
n_c	number of catalyst particles per gas bubble in cross-sectional view with depth d_p	1
n_p	number of catalyst particles in the dispersion	1
n_p*	number of catalyst particles per gas bubble	1
n_p^o	number of catalyst particles per gas bubble in the liquid film	1
p_A	partial pressure of gas component A	Pa
S_p	internal specific surface area of the catalyst particles	m^2 kg^{-1}
T	bubble column diameter	m
T'	temperature	K
u_G	superficial gas velocity	m s^{-1}
u_L	superficial liquid velocity	m s^{-1}
v_o	terminal velocity of a single gas bubble	m s^{-1}
V_F	volume of the liquid film	m^3
V_G	gas volume in the dispersion	m^3
V_L	liquid volume in the dispersion	m^3
V_p	volume of the pores in the catalyst particles	m^3 kg^{-1}

Greek symbols

Γ, Γ'	dimensionless ratio ($\Gamma = k_s a_s/(k_L a_L)$; $\Gamma' = k_s a_s/(k_L a_L(1 - a_L\delta))$)	1
δ	thickness of the liquid film ($\delta = D/k_L$)	m
ε	gas holdup	1
ε_{av}	average gas holdup	1
ε_p	porosity of the catalyst particle	1
η	viscosity	Pa s
Θ_n	modified Hatta number for heterogeneously catalyzed reaction of nth order in gas component A ($\Theta_n = Ha_n\phi^{\frac{1}{2}}$)	1
Λ_n	coefficient for heterogeneously catalyzed reaction of nth order in gas component A ($\Lambda_n = k_n C_B^m d_p^2 C_{A1}^{n-1}(n + 1)/(24D*)$)	1
μ	mass fraction of catalyst on catalyst particles	1
ρ	density	kg m^{-3}
ρ_p	density of the catalyst particles (pores included)	kg m^{-3}
σ	surface tension	N m^{-1}
τ	tortuosity	1
ϕ	volume of the catalyst particles per unit volume of liquid film ($\phi = \bar{C}_p/(\rho_p a_L\delta)$)	1
ϕ'	volume of the catalyst particles per unit volume of bulk liquid ($\phi' = \bar{C}_p/(\rho_p(1 - a_L\delta))$)	1
ϕ''	volume of the catalyst particles per unit volume of liquid ($\phi'' = \bar{C}_p/\rho_p$)	1
Φ_A	gas absorption rate per unit volume of liquid	mol m^{-3} s^{-1}

Dimensionless numbers

| Ha_n | Hatta number for nth order reaction in gas component A ($Ha_n = (1/k_L)\{2k_n C_{A1}^{n-1}C_B^m D/(n + 1)\}^{\frac{1}{2}}$) | 1 |
| He | Henry number (He $= C_{A1}\tilde{R}T'/p_A$) | 1 |

Sh_p Sherwood number for the catalyst particles   1
           $(Sh_p = k_s d_p/D)$

$C_1,..,C_{20}$ locally defined constants

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SAMENVATTING

In dit proefschrift worden de resultaten weergegeven van een onderzoek van het stoftransport in een driefasige slurry reactor dat is uitgevoerd in de periode april 1977 tot juni 1981 in het Laboratorium voor Chemische Technologie van de Universiteit van Amsterdam.
Het onderzoek heeft betrekking gehad op de gas-geroerde slurry reactor waarin de vloeistof de continue fase en het gas de disperse fase is. Het gas stroomt in opwaartse richting. De vaste stof bestaat uit katalysator die is aangebracht op actieve kooldeeltjes welke homogeen in de vloeistof worden gedispergeerd door de gasstroom.
Voor het ontwerp van slurry reactoren is het noodzakelijk te beschikken over informatie betreffende:
- het hydrodynamisch gedrag van het slurrysysteem;
- de kinetiek van de reactie;
- de transporteigenschappen van het reactiesysteem;
- het gas transport naar de actieve plaatsen van de katalysatordeeltjes.
In dit proefschrift wordt aangetoond dat het mogelijk is ontwerpregels voor commerciële slurryreactoren op te stellen m.b.v. informatie verkregen uit afzonderlijke experimenten op kleine schaal voor elk van de vier hierboven genoemde onderwerpen. Juiste combinatie van de vereiste informatie over deze onderwerpen leidt tot betrouwbare ontwerpregels.

In hoofdstuk 1 wordt een overzicht gegeven van gas-vloeistof-vast reactie-systemen en van reactoren die deze systemen bevatten.
In hoofdstuk 2 worden de resultaten van het onderzoek van het <u>hydrodynamisch</u> <u>gedrag</u> van gasbellenkolommen en slurrykolommen besproken.
Deze resultaten hebben betrekking op:
- de gemiddelde volumefractie gas;
- de verdeling van het gasvolume over de reactor;
- de concentratieverdeling van de vaste deeltjes;
- de axiale vloeistofsnelheidverdeling;
- de gemiddelde gasbeldiameter;
- het specifieke gas-vloeistof oppervlak.
De experimenten zijn uitgevoerd in een kolom (T = 0,29 m, 1 = 4 m) waarvan de afmetingen zo zijn gekozen dat de verkregen informatie representatief wordt geacht voor het hydrodynamisch gedrag van het systeem in een commerciële kolom.
In de hoofdstukken 3 en 4 worden methoden besproken voor de bepaling van twee van de transporteigenschappen van het reactiesysteem t.w. de oplosbaarheid en de diffusiecoëfficiënt van matig oplosbare gassen in de betreffende vloeistof.
Een methode voor de bepaling van de <u>oplosbaarheid</u> van matig oplosbare gassen in vloeistoffen alsmede resultaten van het onderzoek van de oplosbaarheid van waterstof in een aantal reactiesystemen worden in hoofdstuk 3 toegelicht.
M.b.t. de <u>diffusiecoëfficiënt</u> van matig oplosbare gassen in vloeistoffen worden theorie, gebruikte apparatuur en resultaten van onderzoek in hoofdstuk 4 beschreven.
De methode (Constant Bubble Size method) is door ons ontwikkeld daar er behoefte bestond aan betrouwbare informatie over de diffusiecoëfficiënt van gassen in vloeistoffen. De CBS-methode leidt tot nauwkeurige en betrouwbare gegevens van de diffusiecoëfficiënt van matig oplosbare gassen in vloeistoffen.
In hoofdstuk 5 worden drie <u>modellen</u> ontwikkeld voor het transport van een gas-vormige component uit de gedispergeerde gasfase naar de actieve plaatsen van de katalysatordeeltjes die in de vloeistof zijn gesuspendeerd.
Er worden modellen besproken waarin de katalysatordeeltjes homogeen verdeeld zijn:
- alleen in de bulk van de vloeistof;
- alleen in de vloeistof film;
- in bulk en vloeistof film.
Voor de berekening van de gasabsorptiesnelheid in een heterogeen gekatalyseerd

reactiesysteem is een gemodificeerd Hatta getal geïntroduceerd. Dit gemodifi-
ceerde Hatta getal gaat over in het klassieke Hatta getal als de heterogeen
gekatalyseerde reactie overgaat in een homogeen gekatalyseerde reactie.
De theorie van hoofdstuk 5 is in hoofdstuk 6 experimenteel geverifieerd; de
resultaten van de experimenten met enkele driefasige reactiesystemen worden
besproken. Deze experimenten zijn uitgevoerd in een Whitman cel (1.5 dm^3). In
deze cel worden vloeistof en gas afzonderlijk geroerd. Het gas-vloeistof grens-
oppervlak is horizontaal en vlak; het specifiek oppervlak is ongeveer 9 m^{-1}.
In hoofdstuk 7 wordt samengevat welke gegevens van driefasige reactiesystemen
nodig zijn en hoe deze informatie moet worden verwerkt om slurryreactoren te
kunnen ontwerpen.
Tevens wordt nagegaan welke invloed de volumefractie gas, de beldiameter, de
concentratie en de grootte van de katalysatordeeltjes hebben op de gas absorp-
tiesnelheid.

SUMMARY

In this thesis, the results are presented of an investigation into mass transfer in a three-phase slurry reactor. The experimental part of the investigation was carried out from April 1977 to June 1981 in the Laboratory for Chemical Technology of the University of Amsterdam.
This work is related to gas-agitated slurry reactors in which the liquid is the continuous phase and the gas the dispersed phase. The gas flows upwards. The solid consists of catalyst on activated carbon particles, which are homogeneously dispersed in the liquid by the gas flow.
For the design of slurry reactors, information is needed about:
- the hydrodynamic behaviour of the slurry system;
- the kinetics of the reaction;
- the transport properties of the reaction system;
- the gas transport to the active sites of the catalyst particles.
In this thesis it is demonstrated that it is possible to draw up rules for the design of commercial slurry reactors using information obtained from small-scale experiments relating to individual aspects from the list of four items given above. Appropriate combination of the pieces of information obtained lead to reliable design rules.

In Chapter 1, a summary is given of gas-liquid-solid reaction systems and of reactors containing such systems.
In Chapter 2, the results of the investigation of the <u>hydrodynamic behaviour</u> of bubble columns and slurry columns are discussed.
These results relate to:
- the average gas holdup;
- the gas-holdup distribution;
- the solids concentration distribution;
- the axial liquid-phase velocity distribution;
- the Sauter mean gas bubble diameter;
- the specific interfacial area.
The experiments were carried out using a column (T = 0.29 m, 1 = 4 m) whose dimensions were so chosen that the information obtained could be considered representative of the hydrodynamic behaviour of the system in a commercial column. In Chapters 3 and 4, methods are discussed for the determination of two of the transport properties of the reaction system, viz. solubility and diffusion coefficient of slightly soluble gases in the liquid. A method for the determination of the <u>solubility</u> of slightly soluble gases in liquids and the results of the investigation into the solubility of hydrogen in a number of reaction systems are explained in detail in Chapter 3.
Theory, apparatus and experimental results with regard to the <u>diffusion coefficient</u> of slightly soluble gases in liquids are described in Chapter 4.
The experimental method (Constant Bubble Size method) was developed by ourselves in view of the need for reliable information about the diffusion coefficient of gases in liquids. The CBS method provides accurate and reliable data on the diffusion coefficient of slightly soluble gases in liquids.
In Chapter 5, three <u>models</u> have been discussed which relate to the transport of a gas component from the dispersed gas phase to the active sites of the catalyst particles suspended in the liquid.
In the models discussed, the catalyst particles are assumed to be homogeneously dispersed:
- in the bulk of the liquid only;
- in the liquid film only;
- in both the bulk and the liquid film.
For the calculation of the gas absorption rate in a heterogeneously catalyzed reaction system, a modified Hatta number is introduced. This modified Hatta number changes into the classical Hatta number if the heterogeneously catalyzed reaction changes into a homogeneously catalyzed reaction.

139

Experimental verification of the theory of Chapter 5 is provided in Chapter 6, where the results of experiments with a number of three-phase slurry systems are discussed. These experiments were carried out in a Whitman cell (1.5 dm^3). In this cell, liquid and gas are agitated separately. The gas-liquid interface is horizontal and flat; the specific interfacial area is about 9 m^{-1}.

Chapter 7 contains a summary of the data on three-phase reaction systems that are needed and the ways in which they are to be processed to enable the design of slurry reactors.

In addition, it is investigated how the gas holdup, the bubble diameter and the concentration and size of the catalyst particles influence the gas absorption rate.

DANKWOORD

Curriculum vitae

Wilhelmus Jozef de Blok is geboren op 13 maart 1953 te Amsterdam. Na zijn
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In september 1971 ving hij aan met de scheikundestudie aan de Universiteit van
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Op 19 januari 1977 werd door hem het doctoraal examen scheikunde behaald met
als hoofdrichting fysische technologie (cum laude).
Van april 1977 tot juni 1981 was hij werkzaam als wetenschappelijk medewerker
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