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Design of multi-phase and catalytic chemical reactors: a simulation tool for pollution prevention

Jack R. Hopper, Jamal M. Saleh, Ralph Pike

Abstract A comprehensive chemical reactor analysis tool was required to complete a project to develop and advanced on-line process optimization analysis system for pollution prevention. The advanced process analysis system integrates programs (reactors, on-line optimization, pinch analysis, and process flow-sheeting) to analyze and modify chemical processes for waste minimization. The reactor analysis program is to be used to evaluate and analyze multi-phase and catalytic reactors to suggest to the plant and process engineers the best reactor type and operating conditions. A multi-phase catalytic reactor design and analysis tool, ReaCat, has been developed. ReaCat incorporates models to design the following reactor types: plug flow, CSTR, batch, catalytic fixed-bed, catalytic fluidized-bed, gas–liquid stirred tank, trickle-bed, three-phase fixed bubble-bed, bubble slurry column, CSTR slurry, and three-phase fluidized-bed. This paper gives a summary of the multi-phase and catalytic reactors: classifications, theory and design models, numerical methods, and solution algorithms. A description of the reactor analysis tool including comparison cases with experimental data is presented.

List Of Symbols

A_i	Heat transfer area (m²)
$C_{G,i}$	Gas bulk concentration of component i (mol/l)
$C^{ib}_{G,i}$	Inlet bulk gas concentration of component i (mol/l)
$C^{ob}_{G,i}$	Outlet bulk gas concentration of component i (mol/l)
$C_{L,i}$	Liquid bulk concentration of component i (mol/l)
$C^{i}_{L,i}$	Inlet bulk liquid concentration of component i (mol/l)
$C^{ob}_{L,i}$	Outlet bulk liquid concentration of component i (mol/l)
$C_{S,i}$	Concentration of component i at catalyst surface (mol/l)
C_{pg}	Specific heat capacity of gas [(BTU/°F lb.) cal/Kg]
C_{pL}	Specific heat capacity of liquid [(BTU/°F lb.) cal/Kg]
D_{Ab}	Bulk diffusivity (cm²/s)
$D_{L,i}$	Liquid-phase axial dispersion coefficient (cm²/s)
E_i	Energy of activation (kJ/mol)
F_{gas}	Flow rate of gas (m³/s)
F^{ib}_{i}	Inlet flow rate for component i
ΔH_{ri}	Heat of reaction of the component i ((kJ/mol)
H_i	Henry's constant for component i
K_i	First-order reaction constant
K_{BC}	Gas-phase (buble-phase) mass transfer coefficient (1/s)
K_{CE}	Intermediate (cloud-wake) phase mab transfer coefficient (1/s)
$K_{cb\,cb}$	Liquid–solid mab transfer coefficient (1/s)
$(K_{Lb\,g})_i$	Gas–liquid mab transfer coefficient for component i ((1/s)
$(K_{cb\,c})_i$	Liquid–solid mab transfer coefficient for component i ((1/s)
$K_{gb\,Lb}$	Gas-phase mab transfer coefficient (1/s)
$K_{Lb\,Lb}$	Liquid-phase mass transfer coefficient (1/s)
N_i	First-order reaction constant
P^{ib}_{i}	Number of species in mixture
P^{ob}_{i}	Inlet bulk gas partial pressure of component i ([(psi) bar]
Q_{Gb}	Outlet bulk gas partial pressure of component i ([(psi) bar]
Q_{Lb}	Gas volumetric flow rate (cm³/s)
Q_{Gmaxb}	Liquid volumetric flow rate (cm³/s)
R_i	Maximum gas flow rate (cm³/s)
$(-r_i)$	Gas constant (lb atm/mol K)
t_i	Net rate of disappearance of component i
T_{ib}	Time (s)
T_{ob}	Inlet temperature [(°F) K]
T_{ab}	Outlet temperature [(°F) K]
U_i	Ambient temperature [(°F) K]
U_{Gb}	Overall heat transfer coefficient [BTU/hr ft² °F (cal/s cm² K)]
U_i	Gas superficial velocity (cm/s)
U_{Lb}	Bulk gas-phase velocity (cm/s)
V_{Rb}	Liquid superficial velocity (cm/s)
V_{Tb}	Reactor volume (m³)
	Volume of the reservoir (m³)

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z(Axialbpositionb (cm)b
ρ_{Lb} Densitybofbliquidb(g/cm^3)b
τ Gas-spacebtimeb(V_R/Q_G)b(s)b

IntroductionE

Tobperformbanbadvancedbprocessbsystembanalysis,bwhichbisb usedbtobevaluatebchemicalbandbrefinerybprocessesbforbwasteb minimizationb(Telangb1996,bPikebetbal.b1998),banbadvancedb chemical reactorbtoolbisbessential. The reactorbdesignbtoolbisb to bebusedbtobevaluatebandbanalyzebthebvariousbtypesbofb industrialbmulti-phasebabdbcatalyticbreactors.bIn anbeffec-b tivebandbtimebsavingbmanner,bplantbandbprocessbengineersb needbabreactorbdesignbtoolbtobanalyzebandbstudybthebeffectb ofboperatingbconditionsbonbthebpollutionbindex.bForbthisb purposeb,bReaCat,babmulti-phasebcatalyticbreactorbanalysisb imulatiob tool,bhas beenbdevelopedbwithbthebfollowingb featuresb:b

1.bUser-friendlybinput/outputbinterfaceb
2.bGraphicalbandbtabularbdataboutputb
3.bReactorbmodelsbincludedb:

- ib Homogeneousbreactorsb(plugbflow,bCSTR, batch)b
- iib Heterogeneousbreactorsb
- I Catalyticbgasbfixed-bedb
- II Catalyticbliquidbfixed-bedb
- III Catalyticbgasbfluidized-bedb
- IVb Catalyticbliquidbfluidized-bedb
- Vb Gas–liquidbcontinuousbstirredbtankb
- VI Three-phasebtrickle-bedb
- VII Three-phase bub lebfixed-bedb
- VIII Three-phaseb catalyticb gas–liquidb slurryb tirredb tankb
- XI Three-phasebcatalyticbgas–liquidbslurryb ub le-bedb
- Xb Three-phasebcatalyticbgas–liquidbfluidized-bedb

4.bPower-lawbreactionbratebforbthebLangmuir–Hinshelwoodb modelbtobaccountbforbthebcatalyticbadsorptionbeffectsb
5.bEquippedbwithbacorrelationbtobestimatebthebexternalbmassb transferbeffectsb(gas–liquid,bandbliquid–solid),bandbdis-b persionbcoefficientsb
6.bEstimationbofbthebcatalyticbeffectivenessbfactorbtobac-b countbforbthebintra-particlebresistanceb
7.bIsothermalbandbnon-isothermal/non-adiabaticbcondi-b tionsb
8.bMulti-reactionbsystemsb withbupbtob30breactionsbandb36b componentsb
9.bPredictionbofbreactorbhydrodynamicsbsuchbasbpressureb drop,bpowerbconsumption,bcatalystbwettingbfactor,bandb flowbregimes.b

Multi-phaseEandEcatalyticEreactor,EdefinitionsE andEclassificationsE

In industrialbchemicalbprocesses,bmulti-phasebreactorsb havebabwidebrangebofbapplicationsbsuchbasboxidation,b hydrogenation,bhydro-desulfurization,bandbthebFischer–b Tropschbynthesis.bTablebS1.1blistsbthebdefinitionb forbthebdifferentbreactorbtypesbincludedbinbthisbstudy.bMulti-phaseb reactorsbarebdefinedbasbreactorsbwithbatbleastbtwobdistinctb phasesbinbcontact.bReactors,bingeneral,bmay bebclassified basedbonbthebnumberbofbphasebcoexistencebintobthebfol-b lowingbcategory:b

i)b Homogeneous:bonebphasebsuchbasbgasborbliquid existsbinb thebreactor.bThebhydrodynamicbflowbcharacteristicbofb thebmixturebdeterminesbthebreactorbtypebsuchbasbplug,b CSTR,bor batch.b
ii)bHeterogeneous:btwobdistinctbphasesbofbreactantsb(orb catalyst)bcoexist.bThisbcategorybmay bebclassifiedbintobb thebfollowingbsubcategories:b

ab Catalytic reactors:bgasborbliquidbphaseb(or both)bisbinb contactbwithbabcatalystb(mainlybolid, butbcould beb anotherbliquidbphase).bExamplesbofbthisbcategoryb includebthebcatalyticbpacked-bedb(catalyticbgasbre-b actionb)bandbthebthree-phasebtrickle-bedb(catalyticb gas–liquidbreactionb).

b Non-catalyticbreactors:bgas–liquidborbliquid–liquidb reactionsbarebcarriedbinbabvarietybofbcontactbvesselsb suchbasbthebgas–liquidbcontinuousbstirredbtankb reactor.b

Eachbreactorbtypebexhibitsbcertainbcharacteristicsbabdbad-b vantagesbthatbmay make itbthe bestbcandidatebfor absspecificb reaction;bthebpowerbof abimulationb tool becomesbverybclearb forbsuchban analysis.bForbabcompletebdisbussionbonbexam-b ples,bclassificationsbdefinitions,bandbadvantagesborbdisad-b vantagesbofbmulti-phasebandbcatalyticbindustrialbreactors,b thebreaderbisbreferredbtobOstergaardb(1974),bShahb(1979),b Tarhanb(1979),bRamachandranbandbChaudharib(1983),b Tsutsumibetbal.b(1987),bandbSalehb(1994).b

TableS1.S Definitionsbofbreactorsb

Catalyticbpacked-bedb	Gab orbliquidbreactantsbflowboverbabfixed-bedbofbcatalystsb
Catalyticbfluidized-bedb	Thebup-flowbgasborbliquidbphasebuspendsb thebfinebcatalystbparticlesb
CSTRbgas–liquidb	Liquidbandbgasbphaseb arebmechanicallybagitatedb
Bub lebgas–liquid bedb	Liquidbphasebisbagitated bybthe bub lebrisebofbthebgasbphaseb.bLiquidbphasebisbcontinuousb
Trickle-bedb	Concurrentbdown-flowbofbgasbandbliquidboverbabfixed-bedbofbcatalyst.bLiquidbtricklesbdown,b whilebgasbphasebisbcontinuousb
Bub lebfixed-bedb	Concurrentbup-flowbofbgasbandbliquid.bCatalyst bedbisbcompletelybimmersedbinbabcontinuousb liquidbflowbwhilebgab risesbas bub lesb
CSTRbslurryb	Mechanicallybagitatedbgas–liquidbcatalystbreactor.bThebFinebcatalystbparticlesbarebuspendedbinbtheb liquidbphase bybmeab ofbagitation.b(Batchbliquidbphasebmaybalsob ebused)b
Bub lebslurrybcolumb	Liquidbisbagitated bybmeansbofbthebdispersedbgas bub les.bGas bub lebprovidesbthebmomentumb tobuspendbdbthebcatalystbparticlesb
Three-phasebfluidized-bedb	Catalystbparticlesbarebfluidized bybab upwardbliquidbflowbwhilebgab phasebrisesbinbabdispersed bub lebregimeb

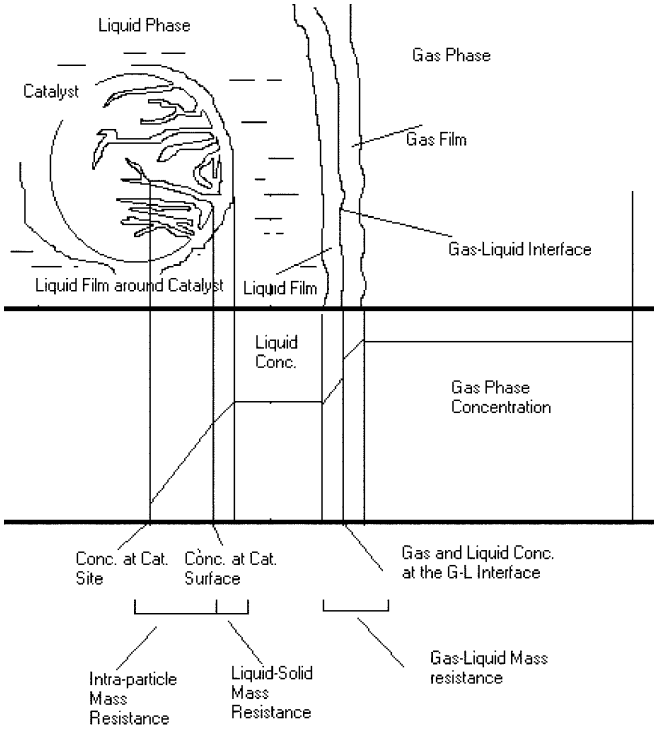

Fig. S1.S Gas–liquid–solid contact in three-phase reactors

Design Models

Design of multi-phase and catalytic reactors is more complex than that of homogeneous reactors due to the following: the coexistence of more than one phase introduce the mass transfer resistance (Fig 1), the intra-particle diffusion, adsorption effects, and the flow regimes, which may be different for each phase. The details of the mathematical model, assumptions, and solution algorithm for each of the reactor types are listed in Sale (1994), Hedge (1999), and Wagh choure (1999). Tables 2, 3, 4, 5, 6, and 7 show the design model, assumption s, and solution algorithms for the three-phase trickle-bed, three-phase catalytic slurry CSTR, and gas–liquid (non-catalytic) agitated tank, catalytic liquid fluidized-bed, catalytic gas fluidized-bed, and catalytic fixed-bed, respectively. The trickle-bed model (Table 2) is applicable to the three-phase fixed-bed, three-phase fluidized-bed, and three-phase bub les slurry-bed as well. A complete list of the correlations implemented in the ReaCat program to predict the mass transfer and hydrodynamic parameters are listed in Sale (1994), Hedge (1999), and Wagh choure (1999). The selection of these correlation is based on the recommendation, found in literature review, of the other authorities in this area. For examples, the correlation implemented for the three-phase reactors are those recommended by Ramachandran and Chaudhari (1983). Since most of the correlations were developed for laboratory and pilot reactors, program users are allowed to skip correlation when experimental data are available. Tables 8 and 9 give a summary of the correlations used in the program. For catalytic reactors, intra-particle diffusion is accounted for by multiplying the intrinsic reaction rate by the catalytic effectiveness factor. The procedure to estimate the catalytic effectiveness factor is listed in Table 10. Procedures to warn the user of conditions that violate the model assumption are also included. For example, when the catalyst-wetting factor is not unity or when the flow regime

Table S2.S Three-phase gas–liquid catalytic reactors design models (trickle-bed, fixed-up-flow bub le-bed, bub le slurry bed, three-phase fluidized-bed)

Non-volatile liquid-phase mass balance	$D_{L,i}\frac{d^2C_{L,i}}{dz^2} - U_L\frac{dC_{L,i}}{dz} - (K_{c\ c})_i(C_{L,i} - C_{S,i}) = 0.0$	(1)
Volatile liquid-phase mass balance	$D_{L,i}\frac{d^2C_{L,i}}{dz^2} - U_L\frac{dC_{L,i}}{dz} + (K_{L\ g})_i(\frac{C_{G,i}}{H_i} - C_{L,i}) - (K_{c\ c})_i(C_{L,i} - C_{S,i}) = 0.0$	(2)
Boundary conditions	At $z = 0$ $\quad -D_{L,i}\frac{dC_{L,i}}{dz} = U_L\left(C_{L,i} - C^i_{L,i}\right)$	
	At $z = L$ $\quad \frac{dC_{L,i}}{dz} = 0$	
Gas-phase mass balance	$-U_g\frac{dC_{g,i}}{dz} - (K_{L\ g})_i(\frac{C_{G,i}}{H_i} - C_{L,i}) = 0.0$	(3)
Component mass balance around the catalyst	$(K_{c\ c})_i(C_{L,i} - C_{S,i}) = (-r_i)$	(4)

Model assumption
1. Complete radial mixing
2. Axial back mixing is accounted for by the dispersion parameter
3. Gas and liquid concentration and temperature profiles are function of reactor length only
4. Complete catalyst-wetting factor and uniform catalyst concentration and activity
5. The catalytic effectiveness factor accounts for the intra-particle diffusion resistance

Solution algorithm
1. Equation 1–4 are developed for each component in mixture
2. At the inlet of reactor, $z = 0$, the nonlinear algebraic system of Eq. (4) is solved for concentration at the catalyst surface by the Newton-Raphson numerical method
3. When plug flow model is assumed, Eqs. (2), (3), and (4) are integrated using the previously calculated surface concentration. For the dispersion model, the shooting method is applied
4. Steps 1–3 are repeated for the entire reactor length

developed is other than the assumed, a warning message will be displayed at the end of the calculation. Each of the mathematical models has been tested versus other published experimental or simulation work. Table 1 lists some comparison examples; for more examples the reader may refer to Saleh (1994).

Program Description

A user-friendly input/output program has been developed to solve and analyze the different reactor types. Figures 2, 3, and 4 show a few of the input screens. A complete user manual may be requested from the authors. Results may be viewed in graphical or tabular format. The user can view conversion, concentration, temperature, and pressure, which may be displayed as a function of reactor length, volume, catalyst weight, or reaction time (Fig. 5). Another version of ReaCat was built to allow simple flow-sheeting capability, such as connecting reactors in series or parallel, generic mixing and splitting of streams, and generic heat transfer equipment (Fig. 6).

Example 1, Sulfuric Acid Production By Contact Process

The production of sulfuric acid by the contact process is a three-step process that produces sulfuric acid and steam from air, molten sulfur, and water. The process consists of three sections: (1) the feed preparation section, (2) the reactor section; (3) the absorber section. The feed preparation section, molten sulfur feed is combusted with dry air in the sulfur burner to produce SO_2. The converter section is the reactor or converter section. Gases from the feed section, sulfur dioxide and air, enter at 787 °F (419.4 °C) and (19.4 psia) 133,759.12 Pa. Sulfur dioxide and

Table 3. S Three-phase gas–liquid catalytic reactors design model (CSTR/slurry)

Non-volatile component mass balance around liquid-phase	$Q_{Li}\left(C^{ib}_{L,i} - C^{ob}_{L,i}\right) - V_{Ri}(K_c)_i\left(C^{ob}_{L,i} - C_{S,i}\right) = 0.0$	(1)
Non-volatile component mass balance around liquid-phase	$Q_{Li}\left(C^{ib}_{L,i} - C^{ob}_{L,i}\right) + V_{Ri}(K_{La})_i\left(\frac{C^{o}_{G,i}}{Hi} - C^{ob}_{L,i}\right) - V_R(K_c)_i\left(C^{ob}_{L,i} - C_{S,i}\right) = 0.0$	(2)
Gas-phase mass balance around	$Q_{Gi}\left(C^{ib}_{G,i} - C^{ob}_{G,i}\right) - V_{Ri}(K_{La})_i\left(\frac{C^{o}_{G,i}}{Hi} - C^{ob}_{L,i}\right) = 0.0$	(3)
Component mass balance around the catalyst	$V_R(K_c)_i\left(C^{ob}_{L,i} - C_{S,i}\right) = V_R(-r_i)$	(4)

Model assumption
1. Gas and liquid phases are well agitated
2. Uniform concentration and temperature within each phase in the entire reactor volume
3. Complete and homogeneous catalyst suspension
4. Continuous flow

Solution algorithm
1. Equation 1–4 are developed for each component in mixture
2. An initial guess for the surface concentration is assumed
3. For a given reactor volume, the system of non-linear algebraic equation is solved iteratively by the Newton–Raphson method to find the exit conditions

Table 4. S Gas–liquid agitated tank, design model

Gas-phase component mass balance	$(Q_G/RT)\left(P^i_i - P^o_i\right) + V_R E K_{GLi}\left(P^o_i/Hi - C^{ob}_{Li}\right) = 0$	(1)
or	$F_{gas}/P_T\left(P^i_i - P^o_i\right) - V_R E K_{GLi}\left(P^o_i/Hi - C^{ob}_{Li}\right) = 0$	
Liquid-phase volatile-component mass balance	$Q_{Li}\left(C^{ib}_{Li} - C^{ob}_{Li}\right) + V_R E K_{Li}\left(P^o_i/Hi - C^{ob}_{Li}\right) + r_i V_R = 0$	(2)
Liquid-phase non-volatile-component mass balance	$Q_{Li}\left(C^{ib}_{Li} - C^{ob}_{Li}\right) + r_i V_R = 0$	(3)
Energy balance	$\Sigma F^i_i\left[\alpha_i(T_i - T_o) + \beta_i/2\left(T_i^2 - T_o^2\right) + \gamma_i/3\left(T_i^3 - T_o^3\right)\right] - \left[V_R\Sigma(\Delta H_{ri} r_i)\right] + UA(T_a - T_o) = 0$	(4)

Model assumption
1. Steady state
2. Both phases are assumed to be perfectly macro-mixed
3. Uniform gas and liquid temperature

Solution algorithm
1. Provide an initial guess for the design variables: gas and liquid concentration and temperature
2. Estimate the hydrodynamic parameters: mass transfer coefficients, power consumption, and minimum gas flow rate
3. Equation 1–4 are developed for each component in mixture
4. The system of non-linear algebraic equation is solved simultaneously by the Newton–Raphson method

oxygen from air reacts with each other to produce SO_3 and reacts with water to form sulfuric acid. In the actual process plant, four converters are used to obtain maximum possible conversion with intermediate removal of the heat and the reactor section is passed to the absorber section where it

Table S5.S Catalytic liquid fluidized-bed reactors, design model

Liquid-phase component balance

Plug flow

$$-U_{\mathrm{L}}\frac{dC_{i\mathrm{L}}}{dZ} = K_{\mathrm{L}}(C_{i\mathrm{L}} - C_{i\mathrm{S}}) \quad (1)$$

Dispersion

$$D_{\mathrm{L}}\frac{d^2C_{i\mathrm{L}}}{dZ^2} - U_{\mathrm{L}}\frac{dC_{i\mathrm{L}}}{dZ} = K_{\mathrm{L}}(C_{i\mathrm{L}} - C_{i\mathrm{S}}) \quad (2)$$

Catalyst (emulsion) phase

$$K_{\mathrm{L}}(C_{i\mathrm{L}} - C_{i\mathrm{S}}) = (R)_{i\mathrm{CatalystPhase}} \quad (3)$$

Energy balance

$$\rho_{\mathrm{L}} U_{\mathrm{L}} C_{p\mathrm{L}}\frac{dT}{dZ} = \sum_{j=1}^{NR} Rj\Delta Hr_j + Ua(T_{\mathrm{ambient}} - T_{\mathrm{Reactor}}) \quad (4)$$

Assumptions

1. The reaction in the liquid phase is assumed negligible
2. By neglecting internal convection effects, the catalyst and the liquid are assumed to be at the same temperature as and on the extremely small particle sizes. (in μm)
3. Steady state

Solution algorithm

1. Estimate the required parameters. (U_{L}, K_{L}, expanded length of bed)
2. Catalyst surface concentration (Eq. 3) are converged using the Newton–Raphson method with the Gauss–Jordan elimination method. A bad starting guess, catalyst phase concentration are assumed to be equal to concentrations in liquid phase
3. Liquid concentration (Eq. 1 or 2) for the next interval are calculated depending on type of the flow selected. (4th order Runge–Kutta for plug flow, finite difference for the dispersion model)

Table S6.S Catalytic gas-fluidized-bed reactor, design model

Design equations

Bulk (gas phase (bubble phase)

Plug flow

$$-U\frac{dC_i}{dZ} = K_{\mathrm{BC}}(C_i - C_{ic}) \quad (1)$$

With axial dispersion

$$D_{\mathrm{ga}}\frac{d^2C_i}{dZ^2} - U\frac{dC_i}{dZ} = K_{\mathrm{BC}}(C_i - C_{ic}) \quad (2)$$

Intermediate (cloud-wake) (phase)

$$K_{\mathrm{BC}}(C_i - C_{ic}) = \gamma_c(R)_{i\mathrm{CloudPhase}} + K_{\mathrm{CE}}(C_{ic} - C_{ie}) \quad (3)$$

Catalyst (emulsion) (phase)

$$K_{\mathrm{CE}}(C_{ic} - C_{ie}) = \gamma_e(R)_{i\mathrm{EmulsionPhase}} \quad (4)$$

Energy (balance)

$$\rho_{\mathrm{g}} U(C_{pg}\frac{dT}{dZ} = \sum_{j=1}^{NR} Rj\Delta Hr_j + Ua(T_{\mathrm{ambient}} - T_{\mathrm{Reactor}}) \quad (5)$$

Assumptions

1. Three phases present in a gas fluidized-bed reactor. Bulk gas phase is known as bubble phase. Intermediate phase contains both gas and the solids. Catalyst (emulsion) phase has solids in higher concentration
2. The gas bubbles formed are assumed to be spherical in nature
3. Mass transfer is believed to be happening in all the three phases
4. The reaction occurring in bulk gas (bubble) phase is both significant and hence is neglected
5. Steady state

Solution algorithm

1. Estimate the required parameter using correlations (D, U, γ_c, γ_e, K_{BC}, K_{CE})
2. Intermediate and bolid surface concentrations (Eqs. 3 and 4) are converged using the Newton–Raphson method with the Gauss–Jordan elimination method
3. Bulk gas concentrations (Eqs. 1 or 2) for the next interval are calculated depending on type of the flow selected. (4th order Runge–Kutta for plug flow, finite difference for the dispersion model)
4. For non-isothermal cases, the temperature for the next interval is calculated by Eq. 5 and used to find reaction rates for the next length interval
5. Steps 3 and 4 are repeated over the total reactor length

the product, SO_3. The removal increases the equilibrium conversion. The reaction takes place on a vanadium pentoxide catalyst. Two types of this catalyst LP-110 and LP-120 are used in these reactors. The reaction is:

$$SO_2 + (1/2)O_2 \rightarrow SO_3$$

The kinetic model for this reaction was given by Harris and Norman (1972). The reaction rate is predicted by the following expression:

$$r_{SO2} = \frac{P_{SO2} P_{O2}^{1/2}}{\left(A + BP_{O2}^{1/2} + CP_{SO2} + DP_{SO3}\right)^2} \left[1 - \frac{P_{SO3}}{K_P P_{SO2} P_{O2}^{1/2}}\right]$$

where

Table 7. Catalytic fixed-bed, design model

Mass balance around the catalyst	$(\quad c \quad c)_i (C_{Gb} - C_S) i (= \eta (-R (et\ )_{i(}$	(1)
Gas-phase component mass balance (plug flow model)	$-U_G \frac{dCGi(}{dz} - (\quad c \quad c)_{i(} (C_{Gb} - C_S) i (= 0.0$	(2)
Gas-phase component mass balance (dispersio model)	$D_G i \frac{d^2 CGi(}{d^2 z(} - U_G \frac{dCGi(}{dz} - (\quad c \quad c)_{i(} (C_{Gb} - C_S) i (= 0.0$	(3)
Energy model	$U_G \rho_G C p_G \frac{dT}{dz(} = \sum (Rj \Delta HRj) + UA(T(- Ta)$	(4)

Model assumption
1. Complete radial mixing
2. Dispersion coefficient is used to account for the axial back mixing
3. Effectiveness factor accounts for the intra-particle resistance
4. Steady state

Solution algorithm
1. At the reactor inlet, develop Eq. 1 for each component in the mixture
2. Solve the system of non-linear algebraic equations for the concentration at the catalyst surface, $C($. This is an iterative procedure as follow: Guess $C($, solve for the effectiveness factor, evaluate the net intrinsic reaction rate for each component, then using the Newton–Raphson method to solve the system of Eqs. 1, new values for $C($ are estimated. The process is repeated till no further change in $C($ is occurring
3. Develop Eqs. 2 or 3 (depending on the model choice, plug or dispersion) for each component in mixture; solve for the next increment in reactor length using the 4th order Runge–Kutta method for finite difference
4. Repeat the above steps for the next reactor length increment

Table 8. Correlation used for the three-phase catalytic reactors

Correlation	Trickle-bed	Fixed up-flow	CSTR slurry	Bub le slurry	Three-phase fluidized
Pressure drop	Larkins et al. (1961) Ellman et al. (1988)	Turpin and Hintington (1967)	–	–	–
L and G hold up < 1	Sato et al. (1973) Ellman et al. (1990)	Fukushima and Kusaka (1979) Achwal and Stepanek (1976)	Calderbank (1958) Yung et al. (1979)	Yamashita and Aeon (1975) Maselker (1970)	Kim et al. (1975)
G–L mass transfer coefficient	Ellman et al. (1988) Sato et al. (1973)	Reiss (1967)	Bern et al. (1976)	Akita and Yoshida (1974)	Dhanuka and Stepanek (1980) Dakshinamurthy et al. (1974)
L–S mass transfer coefficient	Van Krevelen and Krekels (1948) Dharwadker and Sylvester (1977)	Specchia et al. (1978)	Sano et al. (1974)	Kobayashi and Saito (1965)	Lee et al. (1974)
L dispersion coefficient	Michell and Furzer (1972)	Stiegel and Shah (1977)	–	Deckwer et al. (1974)	El-Temtamy et al. (1979)
G dispersion coefficient	Hochman and Effron (1969)	–	–	Mangartz and Pilhofer (1981)	–
Wall heat transfer coefficient	Specchia and Baldi (1979)	–	–	Fair (1967)	–
Power consumption	–	–	Luong and Volesky (1979) Michel and Miller (1962)	–	–

P_{SO2}, P_{O2}, P_{SO3} are interfacial partial pressures of SO_2, O_2, and SO_3 (atm)

K_P is the thermodynamic equilibrium constant ($atm^{-1/2}$)

Constants A, B, C, and D are the function of the temperature T (P denotes interfacial partial pressures of SO_2 and O_2 zero conversion under total pressure at the point or reactor (atm)

For catalyst type LP-110

$$A = e^{-6.8+4960/T}, B = 0, C = e^{10.32-7350/T}, D = e^{-7.38+6370/T(}$$

For catalyst type LP-120

$$A = e^{-5.89+4060/T}, B = 0, C = e^{6.45-4610/T}, D = e^{-8.59+7020/T(}$$

For the heat of reaction, an empirical formula is used, which was also derived by Harris and Norman (1972):

$$\Delta H_{\text{reaction}} = 1.827(-24097 - 0.26T + 1.69 \times 10^{-3}T^2 + 1.5 \times 10^{+5}/T) \rightarrow \text{BTU/lbmol (cal/gmol)}$$

The complete list of input parameters and operating conditions is provided for the ReaCatPro gram is given in Kunii and Levenspiel (1969).

Results

An SO_2 conversion of 59.74% is obtained (catalyst type: LP-120) at the exit point of the reactor and the outlet temperature is (1014 °F) 545.55 °C. If LP-110 catalyst is used, a 45.99% conversion is obtained with an exit temperature of (950 °F) 510 °C. It can be seen that conversion is higher for LP-120, hence SO_2 emission will be less. Keeping the catalyst type constant and varying the inlet flow rate shows that decreasing the flow rate increases the conversion thus reducing SO_2 emission. Since this is an exothermic reaction, conversion decreases at higher temperatures. The process uses intermediate coolers to lower the temperature, which gives a better conversion and reduces SO_2 emission.

Example 2, Catalytic Oxidation of Ethanol in Waste Water

Organic pollutant dissolved in liquid water are usually removed by the biological oxidation process. However, some pollutant with aromatic structure decomposes slowly under this process. Liquid-phase oxidation of organic pollutant in water with a solid catalyst provides a method that may remove dissolved organic compounds. This is a typical case where three-phase reactors are applied since the process contains liquid (aqueous

Table 9. Correlation used for the two-phase reactors

Gas–liquid continuous stirred tank reactor	
1. Maximum gas flow rate (Q_{Gmax})	Charpentier (1981)
2. Bubble diameter (d)	Van Dierendonck (1970)
3. Gas holdup (ϵ_G)	Van Dierendonck (1970)
4. Liquid side mass transfer coefficient (k_L)	Van Dierendonck (1970)
Catalytic liquid fluidized-bed	
Mass transfer coefficient (K_L)	Chu et al. (1953)
Catalytic gas fluidized-bed	
1. Voidage at minimum fluidization (ϵ_{mf})	Broadhurst and Becker (1975)
2. Velocity at minimum fluidization (U_{mf})	Kunii and Levenspiel (1969)
3. Bubble diameter (D_B)	Horio and Nonaka (1987)
4. Mass transfer coefficients (K_{BC} and K_{CE})	Kunii and Levenspiel (1969)
5. Coefficient for axial dispersion (D_{GA})	Kunii and Levenspiel (1969)
Catalytic gas fixed-bed	
1. Coefficient for axial-dispersion	Kunii and Levenspiel (1969)

Table 10. Calculation of catalytic effectiveness factor

Catalytic effectiveness factor	$\eta = \frac{1}{\phi}\left(\coth 3\phi - \frac{1}{3\phi}\right)$ where ϕ is the Thiele modulus
First order reaction rate	
Spherical pellet	$\phi = \frac{R}{3}\sqrt{kSa\rho_P/De}$
Cylindrical pellet	$\phi = \frac{R}{2}\sqrt{kSa\rho_P/De}$
Slap pellet	$\phi = L\sqrt{kSa\rho_P/De}$
General non-linear reaction rate	$\phi = \frac{R}{3}\rho_P(-r(CS))\{\int_0^{C_S} 2De(-r(CS))dCS\}^{-0.5}$
where	
	Limiting reactant index
D_{ek}	Effective diffusivity for the limiting reactant
C_{Sk}	Limiting reactant concentration at catalyst surface
$(-r(C))$	Intrinsic reaction rate as non-linear function of surface concentration
$R($	Catalyst pellet radius
ρ_P	Catalyst density
Limiting reactant is found by the following criterion	$D_{eB}C_{SB} > 10 D_{eA}C_{SA}$
	Stoichiometry of B when stoichiometry of A = 1
D_e	Effective diffusivity
$C($	Surface concentration

organic),bgasb(oxygen),bandbsolidb(catalystb).bThebobjec-b tivebofbthib analysisbisbtobcomparebthebethanolbconver-b ionb profilesbforbthebdifferentbtypesbofbthebthree-phaseb reactors.b

AbtypicalbcatalystbusedbinbthisbreactionbisbPd–Al_2O_{3b}atb 30b°C.bThebreactionbhas beenbhownbto bebfirstborderbwithb respectbtoboxygeb andbzeroborderbwithbrespectbtobethanol.b Thebreactionbstoichiometrybisbrepresentedbas:b

$A_{gb}+ B_{lb}\rightarrow$ productsb

whereb

AbOxygenb
BbEthanolb
gbGab phaseb
lbLiquidbphaseb

Thebratebconstantb,b ,bib 0.0177bcm^3/gbs.bTablebl2blistsb otherbparametersbandboperatingbconditionsbneededbtobrunb thebReaCatbpackage.bSincebfixed-bedsbandbuspended- bedsb havebdifferentbcharacteristicsbregardingbthebcatalystbloadb andbcatalystbparticlesbdiameter,bdifferentbsizesbofbcatalytb particlesbandbcatalystbloadsbwerebusedbinbfixed-bedsbandb suspended-beds.bHowever,ballbotherbparametersbandb operatingbconditionsbarebessentiallybthebsamebib thib comparison.bTablebl2bhowsbthebdifferentbcatalystbandb reactorbcharacteristicsbasbusedbinbthebtudy.b

DesignEmodelsEandEsolutionEalgorithmsE

Abdispersiob modelbisbusedbtobdescribebthebliquid-phaseb componentbmaterial balancesbinbthebfollowingbreactors:b trickle-bed, bub lebfixed-bed, bub lebslurry,bandbthree-b phasebfluidized.bThebgasbphasebwasbassumedbtobmovebinb plugbflow.bTablebl2bhowsbthebcomponent balanbebforbtheb catalyst,bgas,bandbliquidbphasebforbthebabovebreactors.b Tablebl3blistsbthebcomponentbmaterial balancesbinbthebwell-b agitatedbslurrybreactorb(CSTRbslurry).b

Thebcatalyticbeffectivenessbfactorbwasbcalculatedbac-b cordingbtobequationsbpresentedbinbTablebl0.bThebgas–liquidb andbliquid–solidbmab transferbcoefficientsbwerebfoundb usingbthebcorrelationsbpresentedbib Tablebl9.bValuesbcal-b culatedbforbthebmassbtransferbcoefficientsbandbcatalyticbef-b fectivenessbfactorsbarebgivenbinbTablebl3.b

ResultsEandEdiscussionsE

Thebconversiob profilesbforbthebfixed-bedb(tricklebandb bub lebfixed-bed)bandbthebsuspended-bedb(slurrybandb fluidized)breactorbgroupsbwerebcomparedbseparately be-b causebofbthebdifferencesbib catalystbloadbandbparticlebize.b Howeverbthebcatalystbloadbandbparticlebsizebarebthebameb withinbeachbgroup.b

Figurebl7bhowsbthebethanolbconversionbprofilesbinbtheb trickle-bedbandbthe bub lebfixed-bedboverbthebtrickle-bedb (aboutb4%bathlength=500bcm)bisbprobablybduebtobhigherb valueb of bub lebfixed-bedbmassbtransferbcoefficientsb.Theb catalyticbeffectivenessbfactorbfor bothbofbthebfixed-bedbre-b actorsbwasbfoundbto beb0.13,bwhilebdispersionbcoefficientsb werebnegligiblebfor bothbofbtheseb reactorsbinbcomparisonb withbthosebforbsuspended-bedsb(Tablebl3).b

Figureb8bhowsbabcomparisob ofbthebethanolbconversionb profilesbinbsuspended-bedbreactors.bSimilarbcatalystbload-b ingbandbparticlebdiameterbwerebusedbinbthebthreebtypesbofb

TableSl1.S ReaCat,btestbcasesb

Catalyticbgasbfluidized-bedb
Multiplebreactionbsystembforbthebproductiob ofbphthalicbanhydridebfrombnaphthaleneb(KuniibandbLevenspiel)b

Literatureb	ReaCatb(1)b	ReaCatb(2)b	ReaCatb	
	Plugbflowb	Plugbflowb	Plugbflowb	Dispersionb
Conversionb	97%b	94.93%b	85.49%b	81.26%b

(1)bExperimental bub lebdiameterbvaluesbhas beenbused bybthebprogramb
(2)bThebcorrelationbofbHoriobandbNonakab(1984)bhas beenbusedbtobfindbthe bub lebdiameterb

Continuousbgas–liquidbstirredbtankbreactorb
Liquidbphaseboxidationbofbo-xylenebintobo-methylbenzoicbacid bybmeansbofbairb(FromentbandbBischoffb1979)b

	Literatureb	ReaCatb
Conversionb	83.39%b	83.95%b

Trickle-bedb
Liquid-phaseboxidatiob ofbformicbacidbinbthebpresencebofbCuO.ZnObcatalystb(Baldibetbal.b1974;bGotobandbSmithb1975)b

	Experimentalb	ReaCatb(plugbflow)b	ReaCatb(dispersiob)b
Conversionb	88.5%b	91.0%b	89.8%b

Continuousbcatalyticbgas–liquidblurrybstirredbtankbreactorb
Hydrogenationbofbanilinebtobcyclohexylaminebb(supportedbnickelbcatalyst)b(GovindaraobandbMurthyb1975;bRamachandranbandb Chaudharib1983)b

	Literatureb	ReaCatb
Reactorbvolumeb (46%bconversionbofbAnilineb)b	98blb	99blb

Semi-batchbcatalyticbgas–liquidblurrybstirredbtankbreactorb
Butynediolbynthesis bybthebreactionbofbgaseousbacetylenebwithbaqueousbformaldehydebib thebpresencebofbcopperbacetylideb catalystbs(Kalebetbal.b1981)b

	Experimentalb	ReaCatb(1)b	ReaCatb(2)b
Conversionb	62%b	61.0%b	68.5%b

(1)bAdsorptionbatbcatalystbsurfacebisbtakingbintobaccoubt bybthebprogramb
(2)bNobadsorptionbeffectsb

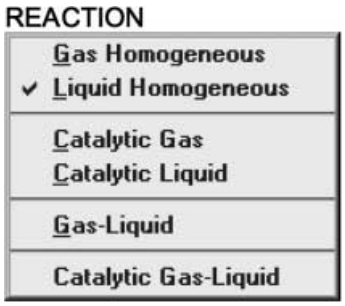

Fig. S2.S Reactionbphasebmenub

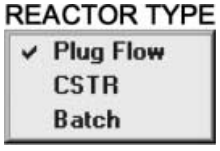

Fig. S3.S Reactorbtypebmenub

suspended-beds.bTheb catalyticb effectivenessbfactorbinbus-b pended-bedsbwab foundbto bebmuchbhigherbthanbthatbforb fixed-bedsb(0.799bcomparedbwithb0.13binfixed-beds)bduebtob finebcatalystbparticles.bThebconversionbprofilesbforbtheb three-phasebfluidized-bedband bub lebslurrybreactorbhadb valueb thatbwerebverybsimilar.bThebconversionbinbthebthree-b phasebfluidized-bedbwasbhigher bybt9%bthanbthatbinbthe bub lebslurrybreactorbatblengthb500bcm.bHowever,btheb conversionbprofilebforbthebCSTRbslurrybreactorbwasbmuchb higherbthanbinbotherbsuspended-beds.bThebconversionbofb ethanolbinbCSTRbslurrybwasb52%bhigherbthanbinbthe bub leb lurry- bedbandb37%bhigherbthanbinbthebthree-phasebflui-b dized-bedbatblengthb500bcm.bThebhighbconversionbinbtheb CSTRbslurrybreactorbcan bebexplained bybthebmuchbhigherb massbtransferbcoefficientsbduebtobthebmechanicalbagitationb asbseenbinbTablebl3.bThebCSTRbslurrybreactorbgavebthe bestb ethanolbconversionbamongbthebsuspended-beds,bwhilebthe bub lebfixed-bedbgavebthe bestbconversionbforbthebfixed-beds.b

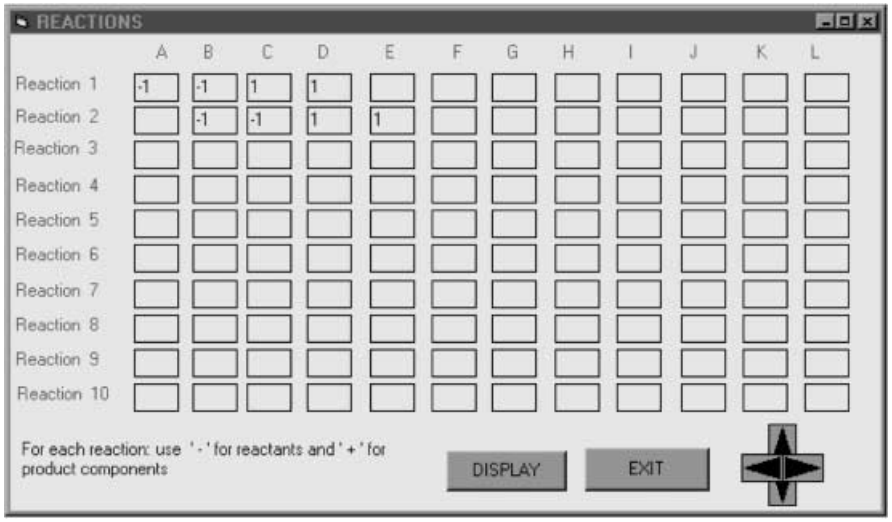

Fig. S4.S Reactionbtoichiometryb inputb creenb

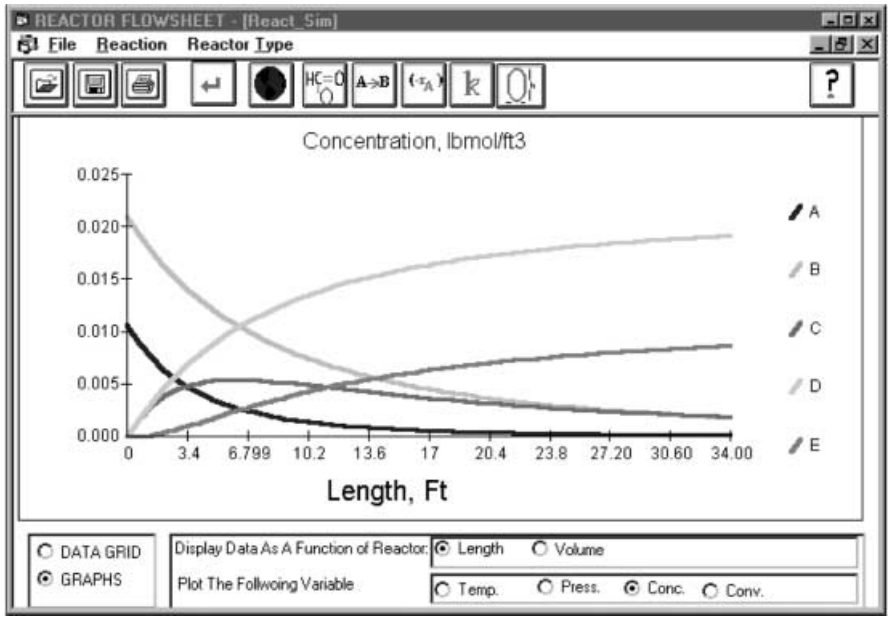

Fig. S5.S Anbillustrationbofbthebgraphicalb outputbofbReaCatbprogramb

TableS12.S Parametersbandboperationbconditionsbforbtheboxidationbofbethanolb

Parameterborboperatingbconditionb	
Catalystbbparticlebdiameterb(cm)b	Fixed-bedsb(trickle-bedband bub lebfixed-bed)=0.5b Suspendded-bedsb(slurrybandbfluidized-beds)=0.05b
Catalystbloadb(g/cm^3)b	Fixed-beds=1.04b Suspendded-beds=0.1b
Reactorbdiameterb(cm)b	20b
Gasbflowbrateb(cm^3/s)b	3140.0b
Liquidbflowbrateb(cm^3/s)b	62.8b
Ethanolbconcentrationbinbliquid-phasebatbinletb(mol/cm^3)b	4×10^{-4}
Oxygeb concentratiob atbsaturationb(mol/cm^3)b	4.2×10^{-6}
Molecularbdiffusivityb(cm^2b/s)b	4.7×10^{-5}
Effectivebdiffusivityb(cm^2b/s)b	4.16×10^{-5}
Catalystbdensityb(g/cm^3)b	1.2b

TableS13.S Massbtransferbcoefficientsbandbcatalyticbeffectivenessbfactorb

Reactorb	Catalyticbeffectivelessb factorb	G–Lbmassbtransferb coefficientb(1/s)b	Liquidbphasebdispersionb coefficientb(cm^2b/s)b	L–Sbmassbtransferb coefficientb(1/s)b
Trickle-bedb	0.13b	0.02b	0.3266b	0.0276b
Bub lebfixed-bedb	0.13b	0.144b	0.9977b	0.0408b
CSTRbslurryb	0.799b	1.05–1.45b	–b	1.14b
Bub lebslurryb	0.799b	0.02677b	43.4b	0.0952b
Three-phasebfluidized-bedb	0.799b	0.252b	47.9b	0.1b

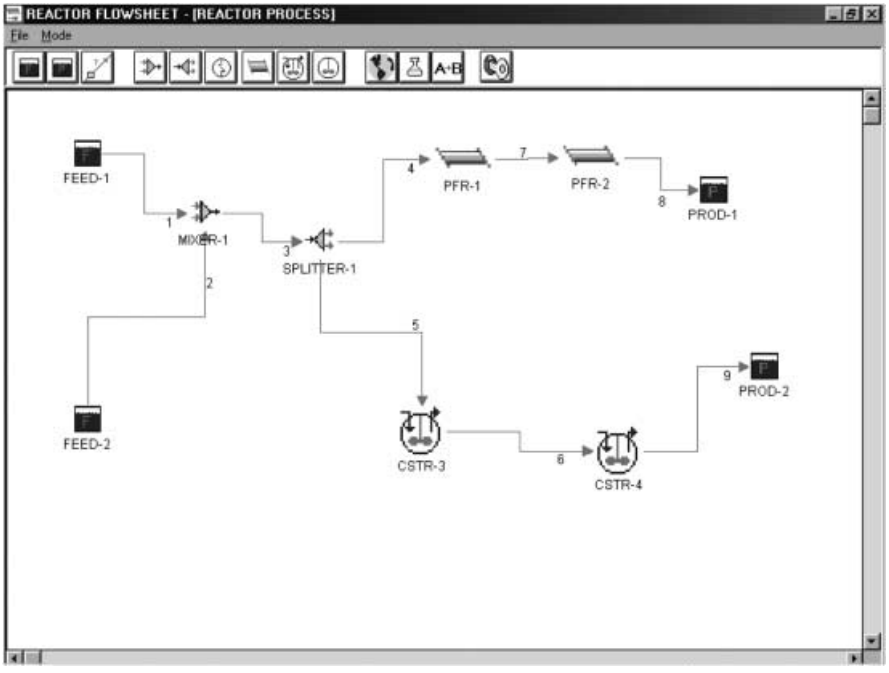

Fig.S6.S Reactorbflow-sheetingb

Thisbillustratiob ofbthebusebofbthebimulationb packageb forbtheseb calculationsbdemonstratesbthebignificanbtbcapa-bilitybtobhandlebabverybcomplexbsetbofbequatiob inbabveryb effectivebandbtimebsavingbmanner.bOtherbexamplesbwhereb imulatiob resultb werebcomparedbagainstbbexperimentalb databhavebalso beenbillustratedb(Salehb1994).b

ConclusionE

Abmulti-phasebcatalyticbreactorbsimulatorbhas beenbdevel-b oped.bThebimulationb packagebhasbmodelsbtobdesignbtheb followingbreactorbtypes:bplugbflow,bCSTR, batch,bcatalyticb fixed-bed,bcatalyticbfluidized-bed,bgas–liquidbstirredbtank,b trickle-bed,bthree-phasebfixed bub le-bed, bub lebslurryb column,bCSTRbslurry,bthree-phasebfluidized-bed.bPower-b lawbreactionbratesborbthebLangmuir–Hinshelwoodbmodelsb arebincluded.bItbisbequippedbwithbcorrelationbtobestimateb thebexternalbmassbtransferbeffectsb(gas–liquidbandbliquid–b solid)bandbdispersionbcoefficients.bEstimationbofbthebcata-b lyticbeffectivenessbfactorbtobaccountbforbthebintra-particleb resistancebisbalsobincluded.bIsothermalbandbnon-isother-b mal/nbn-adiabaticbconditionsbwithbmulti-reactionbsystemsb withbuptob30breactionb andb36bcomponentsbarebpermitted.b

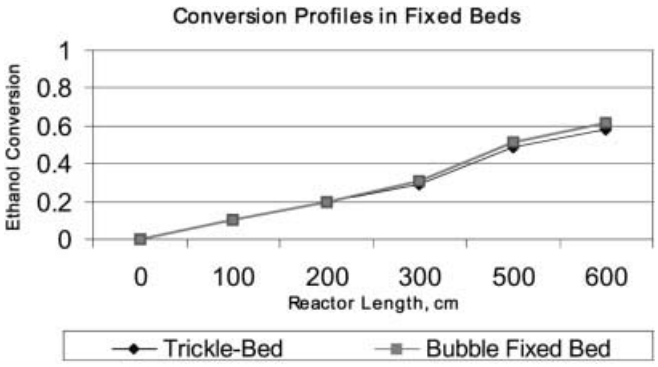

Fig.S7.S Conversionbofbethanolbinbthree-phasebfixed-bedsb

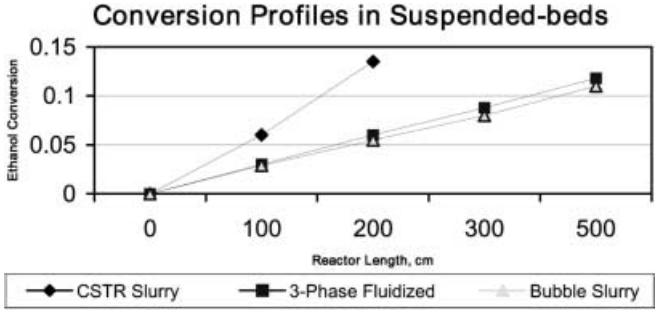

Fig.S8.S Conversionbofbethanolbinbthree-phasebuspended-bedsb

Reactorbhydrodynamicsbsuchbasbpressurebdrop,bpowerb consumptionbbcatalystb-wettingbfactor,bandbflowbregimesb maybalso bebpredicted.b

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