U_G	=	superficial gas velocity	[cm/s]
U_L	=	superficial liquid or slurry velocity	[cm/s]
U_T	=	U_G+U_L, total fluid velocity	[cm/s]
U_T^*	=	$(U_G\rho_G+U_L\rho_L)/\rho^*$, modified total fluid velocity	[cm/s]
u_L	=	$U_L/(1-\varepsilon_G)$, apparent linear velocity of slurry	[cm/s]
ε_G	=	gas holdup	[—]
λ	=	thermal conductivity	[$W \cdot m^{-1} \cdot K^{-1}$]
λ^*	=	$\{\varepsilon_G\rho_G\lambda_G+(1-\varepsilon_G)\rho_L\lambda_L\}/\rho^*$, modified thermal conductivity	[—]
μ	=	viscosity	[Pa·s]
μ_b	=	viscosity of fluid at average fluid temperature	[Pa·s]
μ_w	=	viscosity of fluid at the average wall temperature	[Pa·s]
μ^*	=	$\{\varepsilon_G\mu_G+(1-\varepsilon_G)\mu_L\}/\rho^*$, modified viscosity	[Pa·s]
ρ	=	density	[$kg \cdot m^{-3}$]
ρ^*	=	$\varepsilon_G\rho_G+(1-\varepsilon_G)\rho_L$, modified density	[$kg \cdot m^{-3}$]

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THE REACTION CHARACTERISTICS OF PARALLEL CONSECUTIVE REACTIONS IN A FLUIDIZED BED

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Key Words: Fluidized Bed Modeling, Scale Up, Fluidized Catalytic Reactor, Reactor Design, Process Simulation

The reaction characteristics (the reactant conversion and the yield of the intermediate product) of a parallel consecutive reaction in a fluidized bed were analyzed on the basis of the "Bubble Assemblage Model." The effects of rate constants, particle size and bed diameter upon the reaction characteristics were investigated theoretically. When the rate constants and the size of particles were small, the reaction characteristics for a fluidized-bed reactor closely approached those for a plug-flow reactor and scale-up of the fluidized bed reactor became easy.

Introduction

To develop an industrial fluidized-bed reactor, it is very important to estimate correctly the reactant conversion and the yield of intermediate product from operating conditions. To analyze the reaction performance of the fluidized-bed catalytic reactor, many models[4-8] have been published. The reaction performance of small-scale fluidized bed reactors were analyzed by these models. However, the effects of fluidized particle size, gas velocity, reactor size and reaction rate constants upon the reaction characteristics have not yet been systematically investigated.

In this paper the reaction characteristics of a parallel consecutive reaction in a gas-solid catalytic fluidized bed reactor are analyzed on the basis of the "Bubble Assemblage Model" (B.A. model).[2] The effects of individual reaction rate constants, size of fluidized particles, superficial gas velocity and bed diameter upon reactant conversion and yield of the intermediate product were investigated theoretically.

1. Computational Method

The B.A. model has no adjustable parameter. Therefore, the effects of the above-mentioned factors

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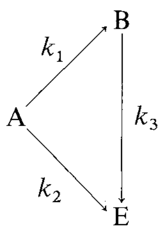
upon the reaction characteristics are reasonably easily evaluated. The B.A. model is briefly described in Appendix. In addition to the usual assumptions of the B.A. model, the following assumption is made: The maximum bubble holdup in the bed is 0.5; that is, the maximum bed expansion ratio L/L_{mf} is 2.

Let us consider the following parallel consective reaction:



Each path is assumed to be a first-order reaction with no change in total number of moles during the reaction. The reaction rates are given by

$$-r_A=(k_1+k_2)C_A \tag{1}$$

$$r_B=k_1C_A-k_3C_B \tag{2}$$

$$r_E=k_2C_A+k_3C_B \tag{3}$$

The following equations are obtained from the material balances of the reactant A, the intermediate product B and the final product E around the n-th compartment. For component A:

$$(SUC_{bA})_{n-1}=\{F'oV_b(C_{bA}-C_{eA})\}_n+(SUC_{bA})_n + \{(k_1C_{bA}+k_2C_{bA})V_c\}_n \tag{4}$$

$$\{F'oV_b(C_{bA}-C_{eA})\}_n=\{(k_1C_{eA}+k_2C_{eA})V_e\}_n \tag{5}$$

For component B:

$$(SUC_{bB})_{n-1}=\{F'oV_b(C_{bB}-C_{eB})\}_n - \{(k_1C_{bA}-k_3C_{bB})V_c\}_n+(SUC_{bB})_n \tag{6}$$

$$\{F'oV_b(C_{bB}-C_{eB})\}_n=-\{(k_1C_{eA}-k_3C_{eB})V_e\}_n \tag{7}$$

For component E:

$$(SUC_{bE})_{n-1}=\{F'oV_b(C_{bE}-C_{eE})\}_n - \{(k_2C_{bA}+k_3C_{bB})V_c\}_n+(SUC_{bE})_n \tag{8}$$

$$\{F'oV_b(C_{bE}-C_{eE})\}_n=-\{(k_2C_{eA}+k_3C_{eB})V_e\}_n \tag{9}$$

Boundary conditions are

$$n=0 \qquad \begin{aligned} &C_{bA}=C_{eA}=C_{Ao} \\ &C_{bB}=C_{eB}=C_{bE}=C_{eE}=0 \end{aligned} \tag{10}$$

Using the boundary conditions given by Eq. (10), the concentrations of each component in the bed are numerically calculated from Eqs. (4)–(9). The conversion of component A is defined as

$$X=\frac{C_{Ao}-C_{A\,out}}{C_{Ao}} \tag{11}$$

The yield ϕ of component B is calculated by

$$\phi=\frac{C_{B\,out}}{C_{Ao}-C_{A\,out}} \tag{12}$$

2. Results of Calculations and Discussion

When a parallel consecutive reaction takes place in a fluidized bed, the factors affecting the conversion of reactant gas A and the yield of intermediate B are the minimum fluidizing gas velocity of fluidized particles, the superficial gas velocity, bed diameter, the reaction rate constants k_1, k_2, k_3 and the ratios of the reaction rate constants $\alpha=k_2/k_1$, $\beta=k_3/k_1$. In this calculation, the effects of these factors upon the conversion of A and yield of B are quantitatively investigated. The calculation was performed for a 100 cm-diameter reactor. In many industrial chemical reactions with first-order kinetics, the reaction rate constants fall within the range of 0.02–2.0 1/s.

As a general rule, the characteristics of complex reactions such as a parallel consecutive reaction can be satisfactorily analyzed on the basis of the conversion of reactant gas A and the yield of B from A. Provided that the fluid flow within the reactor is ideal flow, that is, plug flow or perfect mixing flow, the conversion of A can be expressed as a function of the dimensionless rate constant, $(k_1+k_2)L_{mf}/U$, and the yield of B can be expressed as a function of X. For the investigation of the effects of the parallel reaction and the consecutive reaction upon the reaction characteristics, the parameters $\alpha=k_2/k_1$ and $\beta=k_3/k_1$ are used. The minimum fluidization gas velocity U_{mf} is used as a general factor that expresses properties of fluidized particles such as particle size, particle density and shape factor.

Figures 1a and **1b** show, respectively, the relationship between the conversion of reactant gas A and the value of $(k_1+k_2)L_{mf}/U$ in the case of $k_1=0.2$ with superficial gas velocity U as parameter in the case of $U_{mf}=0.26$ cm/s and $U_{mf}=4.6$ cm/s. **Figures 2a** and **2b** show the relationship between yield of intermediate B and conversion of A with U as a parameter in the case of $U_{mf}=0.26$ cm/s and $U_{mf}=4.6$ cm/s. It can be seen from Figs. 1 and 2 that when U_{mf} is small (fluidized particles are small), the conversion of A and the yield of B in a fluidized-bed reactor are approximately equal to those in the plug-flow reactor. When $U_{mf}=4.6$, however, these two values are appreciably smaller than those for the plug-flow reactor. This fact means that when small particles are fluidized, the fluidized-bed reactor is the reactor in which catalyst's capability can be used to the maximum value. The axial concentration distribution of each component in the bubble phase and the emulsion phase was calculated, and no appreciable difference in concentration was found between the

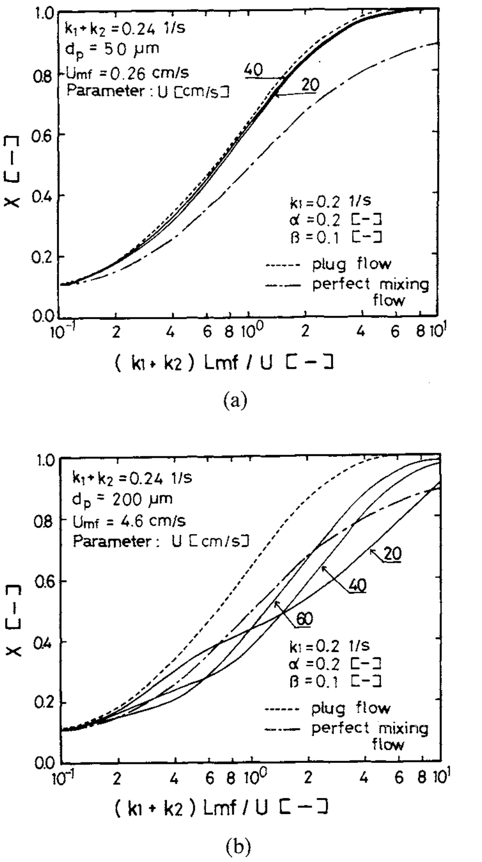


Fig. 1. Effect of U on reactant conversion.

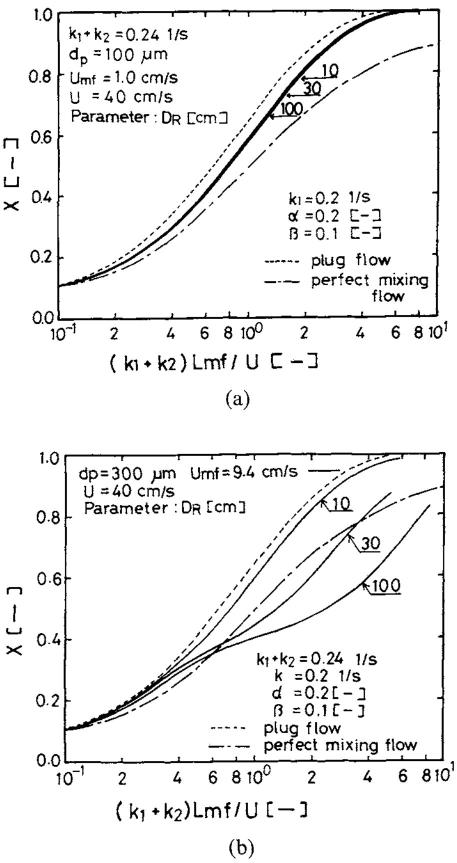


Fig. 3. Effect of reactor diameter on reactant conversion.

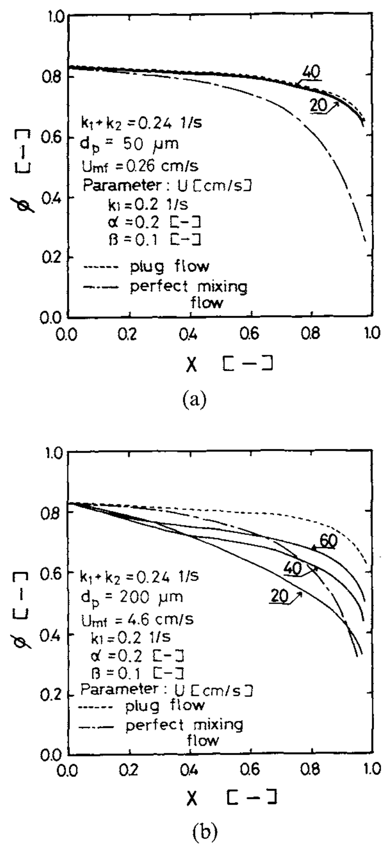


Fig. 2. Effect of U on yield of an intermediate product.

two phases in the case of small particles. When small particles with small U_{mf} are fluidized, the bubble size and the maximum stable bubble size in the bed become small, and the gas interchange coefficient between the two phases and the fraction of particles in the bubble phase become large. Therefore, the mass transfer resistance between the two phases becomes small. This is the reason why the conversion of A and the yield of B in the fluidized bed with small U_{mf} value are approximately equal to the values in the plug-flow reactor as shown in Figs. 1 and 2. From Figs. 1 and 2, when U_{mf} is small, the effects of the superfical gas velocity upon X and ϕ are small and these values are determined by the residence time of gas in the bed. This fact is quite convenient for scale-up of the fluidized-bed reactor.

Figures 3a and **3b** show the relationship between X and $(k_1+k_2)U_{mf}/U$ with reactor diameter as a parameter in the case of $U_{mf}=1.0\,\text{cm/s}$ and $U_{mf}=9.4\,\text{cm/s}$. **Figures 4a** and **4b** show, respectively, the relationship between ϕ and X with reactor diameter as parameter in the case of $U_{mf}=1.0\,\text{cm/s}$ and $U_{mf}=9.4\,\text{cm/s}$. When the fluidized particles are small, the bubble size is not affected by reactor diameter. Therefore, the reactant conversion and the yield of the intermediate product are not affected by reactor diameter. On the other hand, when the fluidized particles become large the

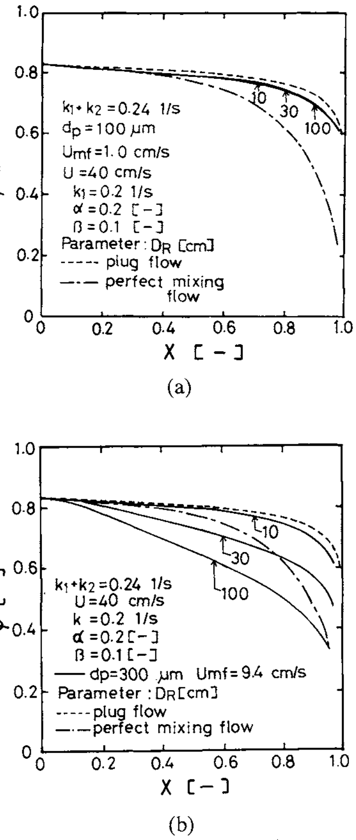


Fig. 4. Effect of reactor diameter on yield of an intermediate.

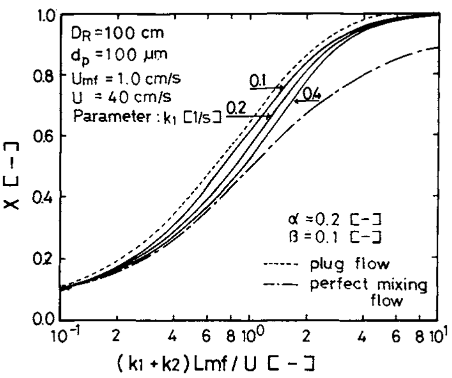


Fig. 5. Effect of reaction rate constant on reactant conversion.

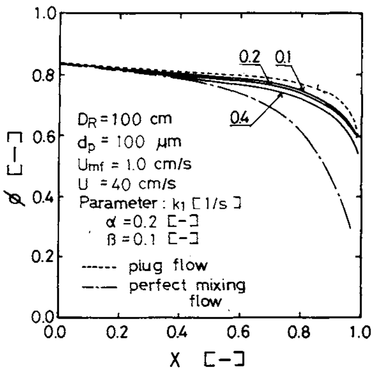


Fig. 6. Effect of reaction rate constant on yield of intermediate product.

reactant conversion and the yield of the intermediate decrease with increasing reactor diameter at constant L_{mf}/U. This fact means that when the fluidized particles are small, scale-up of the fluidized-bed reactor becomes easy. When the fluidized particles are large, however, the reaction characteristics are strongly affected by the reactor diameter. Therefore, scale-up becomes difficult. In this case, suitable internals such as packings or baffles are quite effective in improving the reaction characteristics.

Figure 5 shows the relationship between the conversion of A and $(k_1+k_2)L_{mf}/U$ with k_1 as parameter in the case of $U_{mf}=1.0\,\mathrm{cm/s}$. **Figure 6** shows the relationship between X and ϕ with k_1 as parameter. It can be seen from these two figures that when k_1 is 0.1, X and ϕ in the fluidized-bed reactor are approximately equal to those in the plug-flow reactor. When k_1 becomes large, these two values are appreciably smaller than those for the plug flow. When the reaction with the higher rate constant takes place in a fluidized bed, the reaction rates of reactant gas A and intermediate B in the emulsion phase are considerably higher than the mass transfer rate between the two phases. Hence, the conversion and the yield in a fluidized bed are both much lower than those in a plug-flow reactor.

In this calculation, the reaction characteristics in a fluidized bed are strongly affected by the rate constants k_1, k_2 and the minimum fluidizing gas velocity U_{mf}. When the size of fluidized particles and the individual rate constants are small, the reactant conversion and the yield of the intermediate in a fluidized-bed reactor closely approach the values for an ideal plug-flow reactor. If the following relationship between the rate constants k_1, k_2 and U_{mf} are obtained, the reactant conversion and the yield of the intermediate in a fluidized-bed reactor can be approximately equal to those in a plug-flow reactor.

$$(k_1+k_2)U_{mf} \leqq 0.2 \tag{13}$$

The application range of Eq. (13) is as follows:

$$k_1 \quad \text{or} \quad k_2 \leqq 5\,l/\mathrm{s}$$

$$U_{mf} \leqq 15\,\mathrm{cm/s}$$

The reactant conversion and the yield of intermediate calculated by this model under the above conditions agreed with those in an ideal plug-flow reactor within an error of 5%.

3. Conclusion

The reaction characteristics of a parallel consecutive reaction in a fluidized bed were analyzed on the basis of the "Bubble Assemblage Model". The following results were obtained.

(1) When the size of fluidized particles and the individual reaction rate constants are small, the reactant conversion and the yield of intermediate for a fluidized-bed reactor closely approach the corresponding values for the ideal plug-flow reactor.

(2) When the size of fluidized particles is small, the effects of reactor diameter upon reactant conversion and yield of intermediate are small, and scale-up of the fluidized-bed reactor becomes easy.

(3) To produce the intermediate in high yield, it is necessary to develop a catalyst which has a favorable selectivity toward the reaction intermediate, but a catalyst with high activity is not the prime requirement.

Appendix

The B. A. model involves the following assumptions.

(1) A fluidized bed is represented by n compartments in series. The height of each compartment is equal to the size of each bubble at the corresponding bed height.

(2) Each compartment is considered to consist of the bubble phase and the emulsion phases.

(3) The bubble phase is assumed to consist of spherical bubbles surrounded by spherical clouds. The diameter of the bubbles and that of the cloud are given by Davidson[1] as

$$\left(\frac{Rc}{Rb}\right)^3=\frac{U_b+2U_{mf}/\varepsilon_{mf}}{U_b-U_{mf}/\varepsilon_{mf}} \tag{A-1}$$

(4) The total volume of the gas bubbles within the bed may be expressed as $(L-L_{mf})S$.

(5) Gas interchange takes place between the two phases. The interchange coefficient per unit volume of bubbles is given by Kobayashi *et al.*[3]

$$Fo=\frac{11}{D_B} \tag{A-2}$$

(6) The bubbles are considered to grow until they reach the maximum stable size. The maximum stable bubble diameter D_T is calculated from

$$D_T=\left(\frac{Ut}{0.71}\right)^2\frac{1}{g} \tag{A-3}$$

Bubble size in the bed and bubble rising velocity are respectively expressed as

$$D_B=1.4\rho_s d_p\left(\frac{U}{U_{mf}}\right)h+Do \tag{A-4}$$

$$U_b=0.71(gD_B)^{1/2} \tag{A-5}$$

The bed expansion ratio is calculated from

$$R=1+\frac{U-U_{mf}}{0.71(g\bar{D}_B)^{1/2}} \tag{A-5}$$

where $\bar{D}_B$ is the average bubble diameter in the bed. From the above assumptions, the height of the n-th compartment becomes

$$\Delta hn=2Do\frac{(2+m)^{n-1}}{(2-m)^n} \tag{A-6}$$

where

$$m=1.4\rho_s d_p\left(\frac{U}{U_{mf}}\right)$$

The number of bubbles in the n-th compartment becomes

$$N=\frac{6S(R-1)}{\pi R(\Delta hn)^2} \tag{A-7}$$

The volumes of the cloud, the bubble phase and the emulsion phase in the n-th compartment are expressed as

$$V_{cn}=\frac{N\pi(\Delta hn)^3}{6}\left(\frac{3U_{mf}/\varepsilon_{mf}}{U_b-U_{mf}/\varepsilon_{mf}}\right) \tag{A-8}$$

$$V_{bn}=\frac{N\pi(\Delta hn)^3}{6}\left(\frac{U_b+2U_{mf}/\varepsilon_{mf}}{U_b-U_{mf}/\varepsilon_{mf}}\right) \tag{A-9}$$

$$V_{en}=S\Delta hn-V_{bn} \tag{A-10}$$

If particle size, particle density, distributor arrangement, bed diameter and superficial gas velocity are known, V_{cn}, V_{bn} and V_{en} in Eq. (4)–(9) are calculated from (A-8). (A-9) and (A-10).

Nomenclature

A	= reactant gas	[—]
B	= intermediate product	[—]
C_A	= concentration of A	[mol/cm³]
C_{Ao}	= concentration of A at reactor inlet	[mol/cm³]
$C_{A\,out}$	= concentration of A at reactor outlet	[mol/cm³]
C_B	= concentration of B	[mol/cm³]
$C_{B\,out}$	= concentration of B at reactor outlet	[mol/cm³]
C_b	= concentration in bubble phase	[mol/cm³]
C_{bA}	= concentration of A in bubble phase	[mol/cm³]
C_{bB}	= concentration of B in bubble phase	[mol/cm³]
C_{bE}	= concentration of E in bubble phase	[mol/cm³]
C_e	= concentration in emulsion phase	[mol/cm³]
C_{eA}	= concentration of A in emulsion phase	[mol/cm³]
C_{eB}	= concentration of B in emulsion phase	[mol/cm³]
C_{eE}	= concentration of E in emulsion phase	[mol/cm³]
D_B	= bubble diameter	[cm]
$\bar{D}_B$	= average bubble diameter	[cm]
Do	= bubble diameter at surface of distributor	[cm]
D_R	= reactor diameter	[cm]
d_p	= diameter of fluidized particles	[cm]
E	= final product	[—]
Fo	= gas interchange coefficient per unit volume of bubble	[l/s]
$F'o$	= gas interchange coefficient per unit volume of bubble phase	[l/s]
g	= gravitational acceleration	[cm/s²]
h	= distance from distributor	[cm]
Δhn	= length of n-th compartment	[cm]
k_1	= reaction rate constant from A to B	[l/s]
k_2	= reaction rate constant from A to E	[l/s]
k_3	= reaction rate constant from B to E	[l/s]
L	= bed height	[cm]
L_{mf}	= bed height at minimum fluidized gas velocity	[cm]
N	= number of bubbles in n-th compartment	[—]
n	= number of compartments	[—]
R	= bed expansion ratio	[—]
Rb	= radius of bubble	[cm]
Rc	= radius of cloud	[cm]
r_A	= reaction rate of A	[mol/cm³·s]
r_B	= formation rate of B	[mol/cm³·s]
r_E	= formation rate of E	[mol/cm³·s]
S	= cross-sectional area	[cm²]
U	= superficial gas velocity	[cm/s]
U_b	= bubble rising velocity	[cm/s]
U_{mf}	= minimum fluidized gas velocity	[cm/s]
U_T	= terminal velocity of fluidized particles	[cm/s]

V_{bn}	=	volume of bubble phase in n-th compartment	[cm^3]
V_{cn}	=	volume of cloud in n-th compartment	[cm^3]
V_{en}	=	volume of emulsion phase in n-th compartment	[cm^3]
X	=	conversion of reactant A	[—]
ϕ	=	yield of intermediate	[—]
ρ_s	=	particle density	[g/cm^3]
ε_{mf}	=	void fraction at U_{mf}	[—]

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HEAT AND MASS TRANSFER DURING EVAPORATION FROM A FREE SURFACE OF WATER FLOWING THROUGH FIBROUS SHEET IN AN INCLINED ENCLOSURE

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Key Words: Desalination, Enclosure, Surface Evaporation, Thermal Convection, Solar Energy, Capillary Flow

The simultaneous phenomena of heat and mass transfer from water flowing through a fibrous sheet attached below the upper boundary of an inclined enclosure have been studied as a fundamental work for developing a new type of solar still.

Experimental work was carried out with two kinds of fibres, two angles of inclination, and different feed rates at various heat inputs.

The maximum temperature at the upper wall of the enclosure increased linearly with applied heat flux and was almost independent of the feed rate and the kind of fibre.

Experiments with high-permeability sheet showed an increase in evaporation rate of about 16% at a 10-degree angle and 30% at a 36-degree angle. Thermal convection in the enclosure became evident at a low feed rate and declined with increase in feed rate.

A mathematical model for the temperature distribution in the preheating zone was formulated and the heat transfer properties were studied by curve-fitting with the experimental data. The result provides useful data for designing the new type of solar still.

Introduction

A multistage thermal-diffusion solar still has been developed in Japan.[7] The authors have conducted a series of studies to support the project and have presented static[5] and dynamic[6] simulations of the process with a simplified mathematical model. However, heat and mass transfer in the still are not so simple if the phenomena are observed in detail. Its main part is composed of several enclosures of which the upper boundary is a fibrous sheet attached below a waterproof partition. Liquid is allowed to flow through the fibrous sheet and part of it evaporates from the free surface, condensing on the upper side of the lower partition. The heat due to condensation is mainly utilized as heat input to the next stage.

Published works[1] related to thermal convection in such an enclosure have mostly dealt with isothermal wall conditions. Sparrow and Prakash[3] recently studied this phenomena simultaneously with internal and external convection at one side wall and it was

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