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Fluid Mechanics of Distillation Trays (I): Depth-Averaged Theory and One-Dimensional Flows

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FLUID MECHANICS OF DISTILLATION TRAYS (I): DEPTH-AVERAGED THEORY AND ONE-DIMENSIONAL FLOWS†

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ABSTRACT

Rigorous design of a distillation column requires a better fundamental understanding of the fluid mechanics of bubble formation and global flows on trays than that currently available. To progress beyond the empirical- or correlation-based state of understanding that currently exists, a theoretical and computational framework is described here that is based on reducing the governing set of three-dimensional conservation equations to a two-dimensional set by averaging them across the depth of the fluid film flowing across the tray. In contrast to related previous works, realistic boundary conditions to the flow problem are provided in this paper by solving simultaneously for the flow on the tray and its inlet and outlet downcomers. In this first of a series of papers, attention is focused on situations in which the flow is invariant in the direction perpendicular to the main flow direction. By means of such a set of one-dimensional, depth-averaged equations, pre-

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dictions are made in several interesting and practically important situations in which the flow is either steady or time dependent.

INTRODUCTION

Separation processes account for 6% of the energy usage per annum in the United States (1). Among the various separation processes, distillation is the dominant separation process used in the petroleum and chemical industries (1). Moreover, distillation is more energy intensive than alternative means of separation and consumes 50% of the total energy used in separations (1). Massive scale of use plus energy intensiveness implies that small improvements can have significant impacts.

Between 1950 and the present, thermodynamic, or vapor-liquid equilibria, considerations and equilibrium stage models have dominated studies of distillation (see ref. 2). More recently, nonequilibrium stage models and accounting for mass-transfer resistances have been gaining popularity. However, inspection of recent treatises on distillation (see ref. 3) and conversations with industrial practitioners reveal that understanding of fluid mechanics — a subject that is equal in importance to thermodynamics in rational design of columns — has not progressed beyond the correlation stage. The goal of this research is to overcome this severely limiting aspect of the current *black-box approach* to distillation.

Eighty to eighty five percent of the distillation columns in practice are tray columns and such columns continue to be built despite advances in packed column design (4). In this paper, attention is focused on flows in tray columns. Figure 1 shows cross-sectional and top views of typical tray columns. As shown in Figure 1 and elsewhere (3), there are two main problems of interest in developing a better understanding of hydraulics of

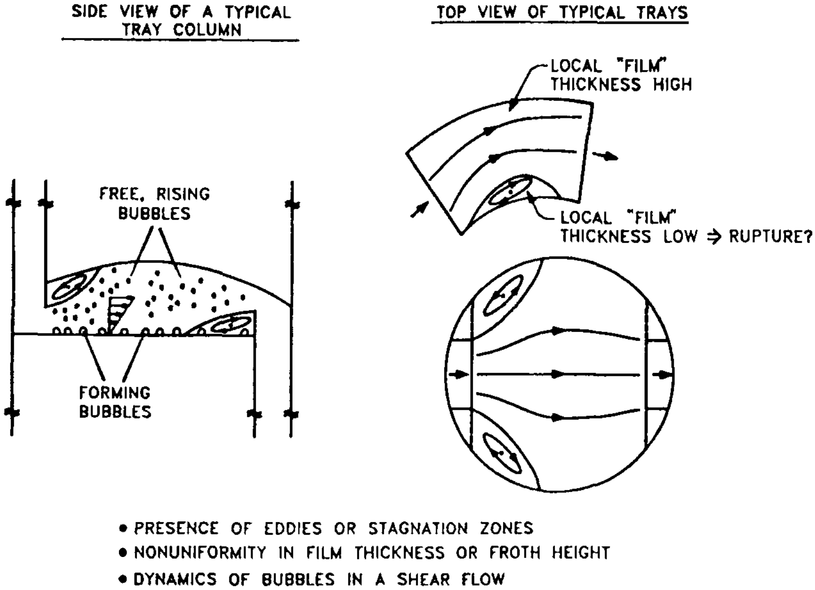

FIGURE 1. Schematic of opportunities for fundamental research in fluid mechanics of distillation columns: microhydrodynamics of bubbles, free surface flows of films and froths, and formation and growth of zones of fluid recirculation.

tray columns: (a) microscopic fluid mechanics of bubbles and (b) global or macroscopic flows on trays. The former problem is outside the scope of the present paper. An example of a study directed at developing a fundamental understanding of that problem can be found in (5), where tools from bifurcation theory are used to analyze shapes and stability of supported bubbles in a simple shear flow. The present paper is concerned with the latter problem. Thus, the primary goal of this paper is to develop a theoretical and computational framework that is capable of determining global flows on distillation trays and their inlet and outlet downcomers.

To our knowledge, there has been two papers (6, 7) to date which have attempted to model the flow across a distillation tray. However, these previous works suffer from two drawbacks. First, the algorithms developed in

(6) and (7) do not converge over certain portions of the parameter space, e.g. with respect to Reynolds number, that are typical of practical applications. Second, they only solve for the flow on a tray. Thus, by neglecting the downcomers, they assign physically unrealistic inlet and outlet boundary conditions to the flow problem on the tray.

As in (6) and (7), the method developed here is based on reducing the governing set of three-dimensional conservation equations to a two-dimensional set by averaging them across the depth of the fluid film flowing across the tray. However, in contrast to (4, 5), realistic boundary conditions to the flow problem are provided in this paper by solving simultaneously for the flow on the tray and its inlet and outlet downcomers. In this first of a series of papers, attention is focused on situations in which the flow is invariant in the direction perpendicular to the main flow direction. By means of such a set of one-dimensional, depth-averaged equations, predictions are made in several interesting and practically important situations in which the flow is either steady or time dependent.

THEORY AND COMPUTATIONAL ANALYSIS

Isothermal flow of a fluid on a distillation tray and its downcomers is governed by the continuity and momentum equations:

$$\nabla \cdot \underline{\mathbf{v}} = 0 \tag{1}$$

$$\rho\left(\frac{\partial \underline{\mathbf{v}}}{\partial t} + \underline{\mathbf{v}} \cdot \nabla \underline{\mathbf{v}}\right) = -\nabla p + \nabla \cdot \underline{\underline{\tau}} + \rho \underline{\underline{\mathbf{g}}}\,, \tag{2}$$

where $\underline{\mathbf{v}}$ is the velocity vector, ρ is density, t is time, p is the pressure, $\underline{\underline{\tau}}$ is the stress tensor, and $\underline{\underline{\mathbf{g}}}$ is the gravitational acceleration. The density ρ as well as the viscosity μ of the fluid are taken to be constants throughout this paper.

Because the local froth height h is much less than the lateral tray dimensions, say L, as depicted in Figure 2, the governing three-dimensional equations, Eqs. (1) and (2), can be averaged across the film depth to eliminate terms involving the vertical component of the velocity and derivatives with respect to the vertical direction, to give "averaged" two-dimensional equations (8). The resulting system of depth-averaged equations are akin to the celebrated shallow-water equations (9). If the asymptotic thickness of the film in the inlet downcomer sufficiently far upstream of the flat portion of the tray is h_o, then the condition for shallow flow is that $\epsilon \equiv h_o/L \ll 1$, as shown in Figure 2.

In the remainder of this paper, attention is focused on situations in which the flow is invariant in the direction perpendicular to the main flow direction along the tray, viz. the y-direction in Figure 2. In this case, the flow is determined by three dimensionless groups: a Reynolds number, Re, a capillary number, Ca, and the dimensionless asymptotic film thickness, ϵ. As usual, Re measures the relative importance of inertial forces to viscous forces and Ca measures the relative importance of viscous forces to surface tension forces.

The resulting one-dimensional, depth-averaged, shallow flow equations are nonlinear. The steady version of these equations is solved by Galerkin/finite element analysis (10). The transient version of these equations is solved by a method of lines with a finite element discretization in space and a finite difference discretization in time. To account for rapid variations in film height along the tray, the locations of mesh or nodal points are

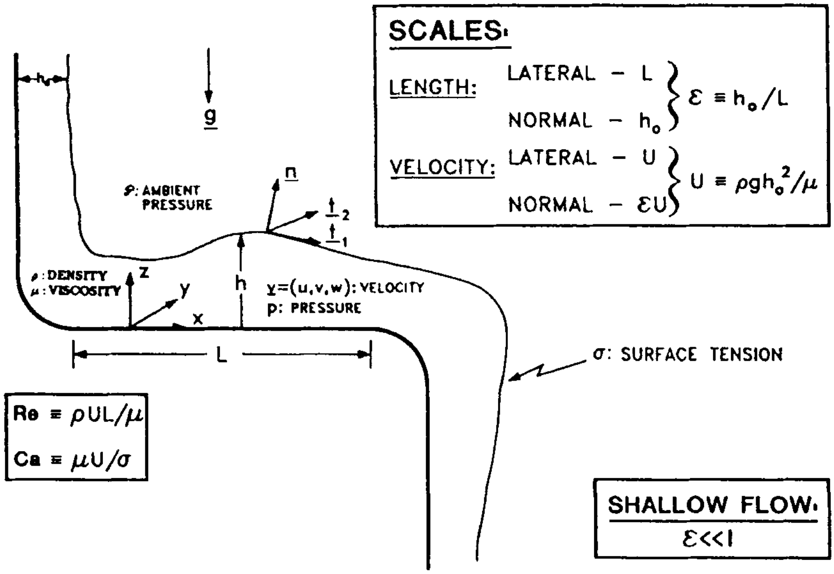

FIGURE 2. Problem statement: characteristic scales and conditions for shallow flow.

adaptively determined by means of a moving finite element algorithm due to Benner *et al.* (11).

RESULTS

Figure 3 shows the variation of the film height on the tray and its inlet and outlet downcomers, and also the locations of mesh points as determined adaptively by the moving element algorithm for the situation in which the flow is steady, $Re = 700$, and $\epsilon = 0.1$. Figure 3 makes plain that the nodes are deployed where they are most needed, i.e. at the location on the tray where the froth height is varying most rapidly.

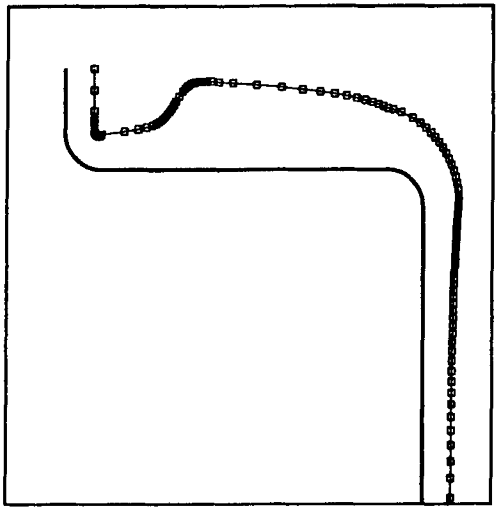

FIGURE 3. Locations of mesh points or nodes determined by the moving finite element algorithm. Here $Re = 700$, $Ca = 0$, and $\epsilon = 0.1$.

Figure 4 shows the evolution of film profiles with the dimensionless asymptotic film thickness ϵ when the flow is steady and $Re = 1,000$. The situation in which $\epsilon = 0.1$ is readily understood if one realizes that as the fluid traverses the tray, it is decelerated by the action of tray friction. Thus, the film must rise as the tray is traversed to conserve mass. As ϵ decreases, the importance of frictional forces increases, which causes the location on the tray where the froth height is a maximum to shift toward the inlet downcomer. When the fluid that exits the inlet downcomer and enters the flat portion of the tray suffers a sudden increase in film thickness, the film profile closely resembles the celebrated hydraulic jump (12).

Rosen and Krylov (13), for example, have reported a large effect on column efficiency when trays are not perfectly flat. Figure 5 shows the effect

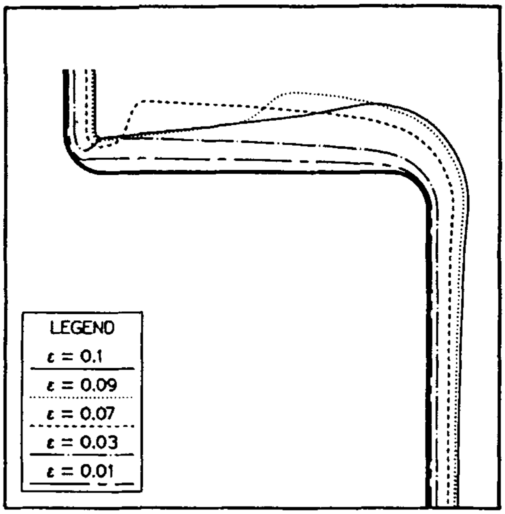

FIGURE 4. Effect of asymptotic film thickness ϵ on film profiles. Here $Re = 1{,}000$ and $Ca = 0$.

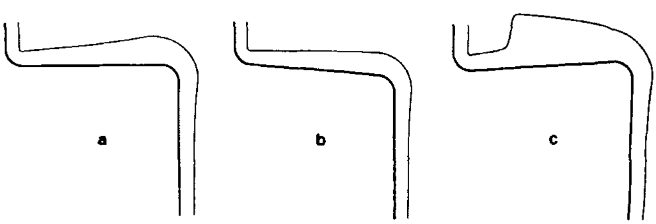

FIGURE 5. Effect of tilting a tray from the horizontal on film profiles: (a) $\theta = 0^o$, horizontal tray; (b) $\theta = 5^o$, downward-tilted tray; and (c) $\theta = -4.75^o$, upward-tilted tray. Here $Re = 1{,}000$, $Ca = 0$, and $\epsilon = 0.1$.

of tilting a tray from the horizontal. Evidently, whereas tilting a tray slightly downward has little effect on the height profile on the tray, tilting it upward by about the same amount can drastically change the height profile on it.

Understanding the effects of process upsets on flows in tray columns is sometimes equally important as understanding steady flows. Figure 6 shows the response of the froth on a level tray when the column is subjected to a step change in liquid flow rate by decreasing the Reynolds number from 1,000 to 700. Whereas the position on the tray where the froth height is a maximum is located near the outlet downcomer when $Re = 1,000$, it is located near the inlet downcomer when $Re = 700$. Remarkably, the froth height smoothly changes from the profile that it has when $Re = 1,000$ to the profile that is has when $Re = 700$ without oscillations. This fact stands in direct contrast to a simple leveling flow (14) where there is no net flow from left to right and the domain is blocked at the locations where the tray meets the downcomers.

Figure 7 shows the effect of sinusoidally perturbing the liquid flow rate on the tray by varying Re sinusoidally in time. The consequence of such transient forcing of the flow rate is generation of capillary waves on the film surface that travel between the intlet and outlet downcomers.

CONCLUSIONS

According to the foregoing results, the one-dimensional set of depth-averaged equations can provide valuable insights into various situations that are encountered in practical applications, e.g. hydraulic jumps on trays that are observed in experiments and consequences of installing trays

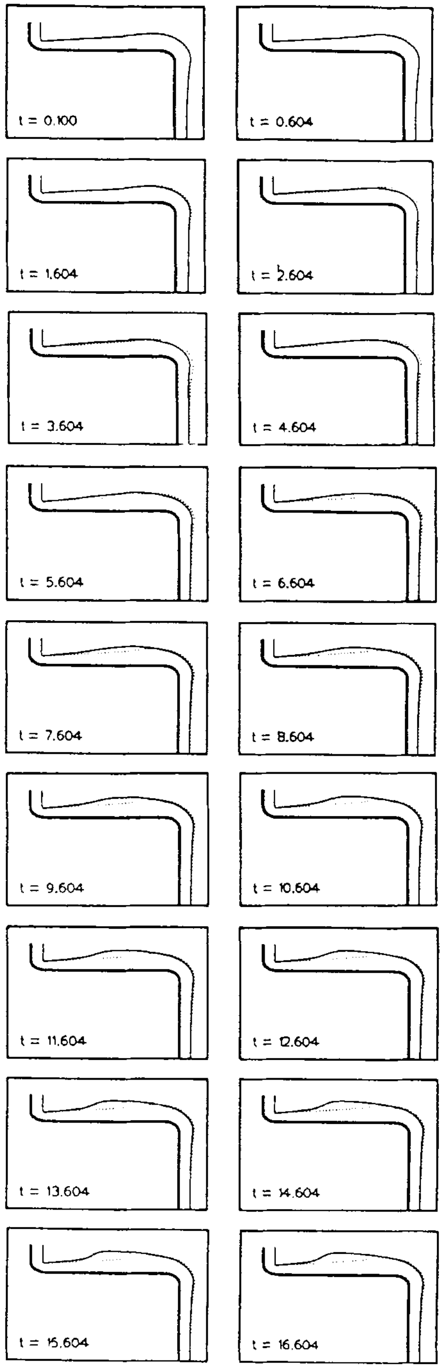

FIGURE 6. Dynamic response of a film to a step change in flow rate. At time $t = 0$, the Reynolds number is changed from 1,000 to 700. Here $Ca = 0$ and $\epsilon = 0.1$. This figure continues onto the next page.

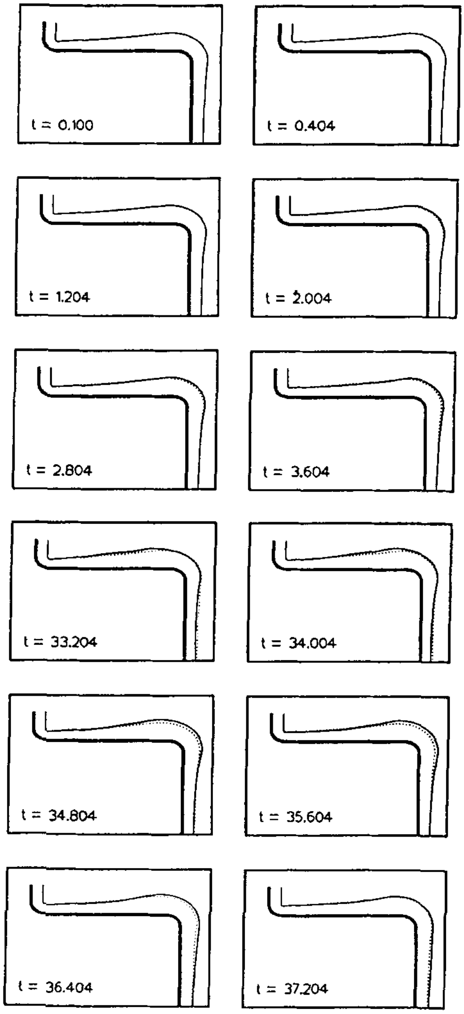

FIGURE 7. Dynamic response of a film to periodic forcing of the flow rate. For times $t > 0$, the Reynolds number is varied sinusoidally as $Re = 1{,}000 + 300\sin(\pi t/4)$. Here $Ca = 0$ and $\epsilon = 0.1$. This figure continues onto the next page.

that are not perfectly level. Moreover, the finite element-based methodologies developed in this paper do not suffer from the limitations encountered by numerical methods advanced by previous investigators. By way of example, whereas the calculations of McDermott *et al.* (6) were restricted to Reynolds numbers less than 0.3, the present method is capable of determining the flow on a tray at any value of Re.

Understanding of variations in froth height caused by actual tray shapes and other fluid mechanical details that can limit tray performance, such as formation of zones of fluid recirculation, are also important. Numerical prediction of flows on some practically important types of trays is considered in the sequel to this paper (15).

Further extensions of the single-phase fluid mechanical models presented here and in (15) are also needed to incorporate multi-phase, hole activity, and mass transfer effects, among others. Prado and Fair (16) have already considered these realistic complications in the modeling of the performance of distillation trays albeit taking a more empirical approach than those presented here and in (15) for describing the fluid mechanics.

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