Analysis of Vapor and Liquid Flow in Packed Columns

Presented by
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1 Introduction

The problem described by the representative from BOC concerns the behavior of liquid and gas within a packed column used for distillation. The column is cylindrical in shape and contains layers of corrugated plates over which the liquid falls from input points, called *drip points*, from the top while gas flows up from the bottom. The aim of the work presented in this report is to provide mathematical models that describe the behavior of the liquid and gas flows. The analysis of these models provides information concerning the distribution of liquid and gas based on the geometry of the corrugated plates and the location of the drip points. This information is of interest to engineers at BOC.

Previous experience with such flows indicates that the two phases can be considered independently and thus the behavior of the liquid and gas flows are handled separately in the discussion below. The analysis of the liquid phase considers both the derivation of suitable model equations that describe the flow and possible techniques to solve the equations for the problems of interest. For the gas flow, the analysis centers on a systematic derivation of the relevant equations.

2 The Liquid Phase

The liquid in the system is injected from drip points at the top of the column and falls through the packed column. We first derive the governing equations, which are shown to be diffusive, and then give various suggestions for solving the equations subject to given locations of the drip points.

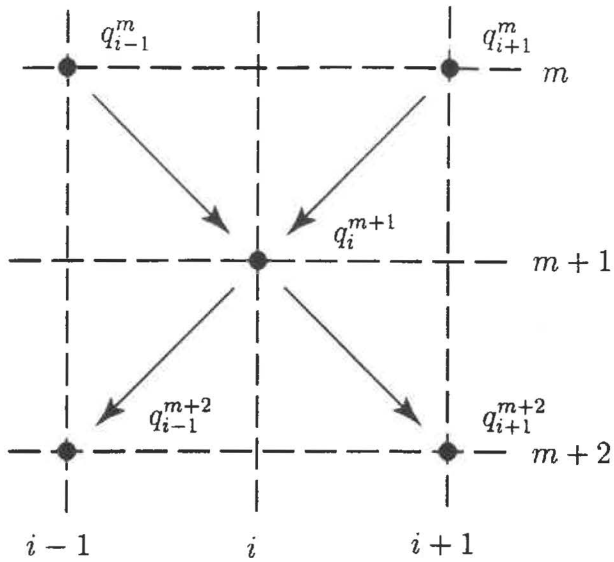

Figure 1: Lattice for liquid flow.

2.1 Model Equations

The flow of the liquid is dominated by gravity with the fluid traveling in a thin layer down the steep direction of the corrugated plates. As the fluid travels down it reaches points where corrugations of adjacent plates touch and at these points the fluid may be diverted in one direction or another.

There is some question regarding the form of the flow of the liquid. The main forces acting on the liquid within the layer are due to gravity and viscous drag, and as a result it is determined that the Reynolds number of the flow is a few hundred. Hence the flow remains laminar but inertial effects are important. Analysis of such behavior gives a relationship between the average downward velocity of the fluid u and the local thickness h of the fluid. In the slow flow case, when the Reynolds number is small, the velocity is proportional to the square of the thickness of the layer. Experimental evidence indicates that a linear relation might be appropriate but there is no further analysis available based on the discussion at the workshop.

The main modeling done for this aspect of the problem involves the spread of the fluid across a corrugated plate. This spreading is due mainly to the fluid impinging on the contact points between corrugations on adjacent plates. The intersection points are taken to be equally spaced with vertical separation Δz and horizontal separation Δx as indicated in figure 1. The intersection points $x_i = i\Delta x$ and $z_m = m\Delta z$ are staggered so that i only takes odd values when m is odd and only takes even values when m is even. The main problem is to determine the behavior of the volume flow rate (per unit length) given by uh within the lattice of intersection points. For simplicity of notation we introduce the variable $q = uh$ and use q_i^m to denote its value at the lattice point x_i, z_m. It is assumed that the flow arrives at each intersection point and then splits equally into streams that travel to the adjacent intersection points down the plate. This assumption together with conservation of mass gives

$$q_i^{m+1} = \frac{1}{2}\left(q_{i-1}^m + q_{i+1}^m\right) \tag{1}$$

for the flow about the point x_i, z_{m+1}. The macroscopic behavior of the packed column depends on a large number of interactions so that the appropriate limit to consider is $\Delta x \to 0$ and $\Delta z \to 0$. The relative size of the two limiting parameters will be considered shortly. Expanding (1) as a Taylor series about the central point x_i, z_m gives

$$q + \Delta z\frac{\partial q}{\partial z} + \ldots = \frac{1}{2}\left(q - \Delta x\frac{\partial q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 q}{\partial x^2} + \ldots + q + \Delta x\frac{\partial q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 q}{\partial x^2} + \ldots\right). \tag{2}$$

Retaining the dominant terms in both Δx and Δz gives

$$\Delta z\frac{\partial q}{\partial z} = \frac{\Delta x^2}{2}\frac{\partial^2 q}{\partial x^2}. \tag{3}$$

This equation indicates that the volume flow, or momentum, $q = uh$ is governed by the steady-state, advection-diffusion equation

$$\frac{\partial q}{\partial z} = D\frac{\partial^2 q}{\partial x^2}, \tag{4}$$

where the diffusion coefficient is

$$D = \frac{\Delta x^2}{2\Delta z}, \tag{5}$$

which, unusually, has the units of length.

The basic model as described by (4) does not include transient effects or any motion of the liquid normal to the plates, which occurs due to small holes drilled in the plates. The analysis given above can be extended to include these effects. The extended equation takes the form

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial z} = D\frac{\partial^2 q}{\partial x^2} + D_y\frac{\partial^2 q}{\partial y^2}, \tag{6}$$

where y measures distance normal to the plates and D_y is the coefficient of diffusion in that direction. The value of D_y depends on the density of holes and could be found experimentally. The transient behavior is of little physical interest as the packed columns are typically running for very long periods of time and hence in steady state. Of greater interest is the extension to more dimensions and the value of D_y. While no specific modeling is given to determine its value, some of the ideas described later in the section on gas flow may be relevant to estimating this coefficient from the geometry of the corrugations and the drilled holes.

2.2 Methods of Solution

The problem to be solved involves the behavior of the liquid subject to a given number and location of point sources at $z = 0$ representing the drip points and subject to an impermeable outer cylinder of radius R representing the outer surface of the packed column. In practice, the drip points are arranged on a regular rectangular array at the top of the cylinder. Engineers at BOC are interested in finding out whether a few additional drip points should be added or existing drip points blocked in order to create a uniform distribution of liquid at the bottom of the column. For simplicity it is assumed that the packing in the cylinder extends to the outer boundary and that there is no special streaming of fluid down the outer boundary. In a typical column, the packing is oriented in one of two perpendicular directions with a change of direction at vertical intervals of approximately 20 cm. Hence there is a periodic variation in the z direction of the diffusion coefficients. There are three other important length scales within the problem; these are:

1. $d \simeq 10\,\text{cm}$, the typical horizontal distance between drip points,
2. $d^2/D \simeq 2.5\,\text{m}$, the typical vertical distance down the packed column for the diffusion to get each drip point to spread to near its neighbor, and
3. $R^2/D \simeq 1000\,\text{m}$, the typical vertical distance for a drip point near the middle to spread to the outer cylinder.

The height of the packed column, H, is around 10 m which gives a distance over which the required transfer processes can occur.

Two methods of solution are discussed below. First, because the change in the packing direction occurs on a relatively small scale, the diffusion can be averaged to give an effective isotropic spread of the fluid governed by the equation

$$\frac{\partial q}{\partial z} = D_e \left(\frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} \right), \tag{7}$$

where an effective diffusity, D_e, is found by averaging the horizontal diffusion lengths in both directions. These are proportional to $\sqrt{D}$ and $\sqrt{D_y}$, respectively, so that

$$D_e = \frac{1}{2}\left(\sqrt{D} + \sqrt{D_y}\right)^2 . \tag{8}$$

The problem can now be solved using analytical methods. The second approach is to attack the problem directly using numerical methods.

2.2.1 Analytical Methods

The method of solution presented at the workshop initially was an analytical one involving the solution of (7) for a single point source which takes the form of an infinite sum of Bessel functions. The solution to the problem is the sum of point-source solutions for each drip point. While this solution is available, it is not useful for practical computations because the number of drip points is large (approximately 1000) and the number of terms in each series needed for an accurate approximation is moderately large (around 20 depending on the position of the drip point relative to the cylindrical boundary). An alternate representation of the solution for practical computations is desired or some sufficiently accurate approximate solution.

The length scales within the problem indicate that, because the cylinder is only ten meters high, the majority of drip points will induce flows that do not interact with the outer cylinder to any significant degree. Hence these points can be taken as producing a simple cylindrical Gaussian distributed flow. The more difficult points are those near the outer surface, specifically those within $O(H^2/D_e)$, which do interact with the outer cylinder. To a first approximation these points see the outer cylinder as flat and hence an approximate solution can be found simply by solving the diffusion equation in all space but including an image source outside the cylinder for each of these "near boundary" sources. Such an approximation has been considered already by BOC and is not sufficiently accurate. Evidently, a next correction to this approximation is needed which would include the curvature of the boundary. This could be handled by an analysis of the rescaled problem

$$\frac{\partial q}{\partial z} = \frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2}, \tag{9}$$

with a drip point source at $x = -1$, $y = 0$ so that

$$q = \delta(x+1, y) \qquad \text{on } z = 0,$$

and with a zero flux condition on the impermeable boundary so that

$$\frac{\partial q}{\partial n} = 0 \qquad \text{on } \left(x + \frac{1}{\epsilon}\right)^2 + y^2 = \frac{1}{\epsilon^2}.$$

Here n is the normal to the surface and the goal is to find an asymptotic solution in the limit $H^2/D_e = \epsilon \to 0$. The first term in this solution would involve the point source and an image. The next term, which is yet to be found, may provide a correction which would yield the desired accuracy with a reduced computational effort.

There are other possible approaches to finding suitable approximate solutions for drip points near the boundary. One approach would be to consider the exact solution involving the infinite sum of Bessel functions and expanding the terms asymptotically for the case when the drip point source is near the boundary. An approximate solution would result by truncating this asymptotic expansion at some desired order of accuracy. Another possible approach is to use approximations for the higher terms in the Bessel series expansion and hence approximating the sum of these higher order terms. Finally it may be possible to analytically "re-sum" the series into an alternative form with better convergence properties.

2.2.2 Numerical Methods

The most computationally efficient method of obtaining an approximate solution to the problem is thought to be by direct solution of the underlying problem using a finite difference or finite volume technique. Such a procedure allows such approximations as the effective diffusion, D_e rather than the periodic vertical variations in diffusion to be removed and gives the distribution of liquid throughout the packed bed not just at the required z position. The main discussion at the workshop centered on ensuring that the solution is sufficiently accurate.

There are three main aspects of the problem that must be considered when considering accuracy. First, there is the accuracy of the numerical discretization of the diffusion equation and with central differences in the horizontal direction and Crank-Nicholson in the vertical this should not pose a problem. Second, the method must accurately describe the position of the drip points. It is known that the fluid will spread from each drip point to a distance of order $\sqrt{HD_e}$ and so the drip point position must be at least this accurate. This distance is in fact very large and a grid with around 10000 points in the horizontal plane will give significantly greater accuracy that required by this criteria and actually allows accurate positioning of the drip points to within a few cm which is more than necessary while allowing computations to be performed in a reasonable time on a PC. For faster calculations a horizontal grid involving 1000 points is believed to still be sufficiently accurate. The third accuracy consideration involves the description of the outer cylindrical boundary. If a single grid is used than a radial grid will provide a good definition of the boundary but there will be computational problems associated with the close packing of grid points near the center of the cylinder. The alternative of a Cartesian grid will not allow the outer boundary to be described with sufficient accuracy. The alternatives of using a hybrid mesh with a cylindrical outer region and a Cartesian inner region with either overlapping or mesh interpolation is possible and expected to give good results. These suggestions were not attempted during the workshop.

3 The Gas Phase

In generating a model for the motion of the gas recall that we are considering it to act in complete isolation to the liquid flow. The gas flow is significantly different from the liquid flow, particularly because if fills the space within the packed bed. In addition the density is so small that gravity has a negligible effect on the flow and hence the gas density is nearly constant throughout the packed bed. The Reynolds number of the flow is typically several thousand so that the flow is dominated by inertia and the flow tends to follow the corrugated channels formed in each plate and only have a small interaction with the gas flow in the adjacent channels. The work presented here centers around a development of a model of the gas flow and a model for the movement of a dilute species within the gas phase. These two aspects of the gas phase are discussed separately below.

3.1 Gas Flow

Because the gas flow is effectively high Reynolds number flow in a porous media the equations governing the flow are expected to be, from mass conservation,

$$\nabla \cdot \mathbf{u} = 0, \tag{10}$$

where $\mathbf{u}$ is the average volume flow of the gas within the pores, and from momentum balance,

$$-\nabla p = k|\mathbf{u}|\mathbf{u}, \tag{11}$$

where k is the permeability tensor. (This form is often ascribed to Ergun [1] who looked at flow in porous media over a range of Reynolds numbers and extended Darcy's law for slow flow to the form $-\nabla p = k_1 \mathbf{u} + k_2 |\mathbf{u}|\mathbf{u}$.) An appropriate form for k is related to the geometry of the packed column. It is noted that the packed bed has several symmetries due to the repeating planar structure. In particular the corrugations in the plates are at right angles and hence there are three principle directions. The first of these is the direction normal to the plate and the other two are mutually orthogonal and lie in the plane of the plate. Let us define y to be the direction normal to the plate, as before, and let x and z lie in the plane of the plate. The permeability in the y direction is expected to be different from that in the other two directions, the permeability in the latter two directions being isotropic. Given these observations, an appropriate form is given by

$$k = \begin{pmatrix} k_p & 0 & 0 \\ 0 & k_n & 0 \\ 0 & 0 & k_p \end{pmatrix} \tag{12}$$

where k_p and k_n are constants. These two constants can be determined by considering the packed bed with unidirectional flow in it. For example, the pressure drop created by uniform flow across the plates gives k_p. Measurements from these flows can be obtained experimentally or theoretically using a CFD package on a single "unit cell" of the packed material.

3.2 Species Transport by the Gas

As a final topic, we consider the movement of a dilute species within the gas phase. Such transport is important in determining where the transfer between the liquid and gas occurs.

The distribution of the species cannot be described simply by a variable representing the average concentration. This is because the underlying gas flow is primarily restricted to the two sets of orthogonal corrugations. Hence, to describe the distribution we must consider the concentration in each of the sets of corrugations. To generate the model of the process, we consider the case where the two sets of corrugations are at 45° angles to a uniform gas flow u in the vertical z direction (now measuring distance up the column). CFD calculations done at BOC on transport within a single unit cell indicate that a certain fraction of the incoming flow of species in each set of corrugations transfers to the other set. This transfer fraction appears to be independent of the average flow velocity. We therefore assume that the fraction transferred is $1 - f$ where f is constant. In practice the transfer is very small (values of f near 0.9 are calculated) and thus we take $f = 1 - \epsilon$, where the smallness of ϵ will be exploited in deriving a suitable limiting form of the equations. The lattice of flows

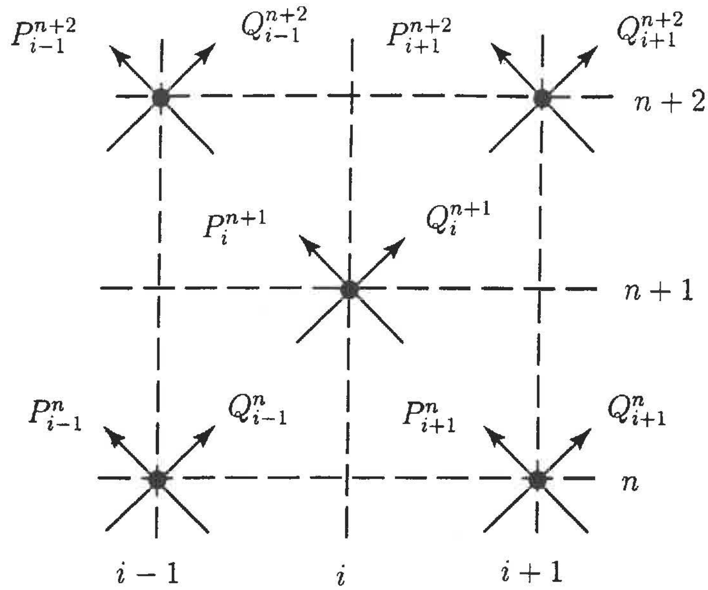

Figure 2: Lattice for gas species flow.

and interactions is shown in figure 2. We take the mass flow of the species in corrugations running from right to left up the column as P_i^n and the mass flow in the corrugations running from left to right up the column as Q_i^n. Note that the points z_n, x_i correspond to the places where the two flow interact.

To generate the model we consider a single cell as before. The discrete equations are

$$P_i^{n+1} = (1-\epsilon)P_{i+1}^n + \epsilon Q_{i-1}^n$$

$$Q_i^{n+1} = (1-\epsilon)Q_{i-1}^n + \epsilon P_{i+1}^n$$

This discrete system is expanded in powers of Δx and Δz to give

$$\Delta z\frac{\partial P}{\partial z} = -\epsilon P + \Delta x(1-\epsilon)\frac{\partial P}{\partial x} + \frac{1}{2}(1-\epsilon)\Delta x^2\frac{\partial^2 P}{\partial x^2} + \epsilon Q - \epsilon\Delta x\frac{\partial Q}{\partial x}\dots \tag{13}$$

$$\Delta z\frac{\partial Q}{\partial z} = -\epsilon Q - \Delta x(1-\epsilon)\frac{\partial Q}{\partial x} + \frac{1}{2}(1-\epsilon)\Delta x^2\frac{\partial^2 Q}{\partial x^2} + \epsilon P + \epsilon\Delta x\frac{\partial P}{\partial x} + \dots \tag{14}$$

where we have retained some terms of higher order as there is cancellation of certain terms in the subsequent analysis. To get the problem into a usable form we note that there are two other natural variables to use to describe the flow, namely

$$A = P + Q \qquad \text{and} \qquad D = P - Q,$$

where A is the average mass flow in the system (equal to uC where C is the average concentration) and D is the difference between the mass flows in the two directions. Adding and subtracting (13) and (14) gives the system

$$\Delta z\frac{\partial A}{\partial z} = \Delta x\frac{\partial D}{\partial x} + \frac{1}{2}(1-\epsilon)\Delta x^2\frac{\partial^2 A}{\partial x^2} + \ldots \tag{15}$$

$$\Delta z\frac{\partial D}{\partial z} = -2\epsilon D - \Delta x(1-2\epsilon)\frac{\partial A}{\partial x} + \frac{1}{2}(1-\epsilon)\Delta x^2\frac{\partial^2 D}{\partial x^2} + \ldots \tag{16}$$

This system has numerous limits. The main observation made is that (16) implies that the difference, D, must decay relatively quickly up the column. This observation suggests that shortly after the species are injected in the flow the mass flows in the two directions will become nearly equal. Hence in the limit $\Delta x \to 0$ and $\Delta z \to 0$, we expect that $D \to 0$ such that the lowest order balance in (16) is

$$0 = -2\epsilon D - \Delta x(1-2\epsilon)\frac{\partial A}{\partial x} \tag{17}$$

This balance can be used in (15) to give

$$\Delta z\frac{\partial A}{\partial z} = \frac{1-2\epsilon}{2\epsilon}\Delta x^2\frac{\partial^2 A}{\partial x^2} \tag{18}$$

This is a diffusion equation for the average flow of species in the system and can be written in the form

$$\frac{\partial A}{\partial z} = \alpha\frac{\partial^2 A}{\partial x^2}, \tag{19}$$

where

$$\alpha = \frac{1-2\epsilon}{2\epsilon}\frac{\Delta x^2}{\Delta z} \tag{20}$$

This model now allows the diffusion parameter within the species transport model to be estimated from information about the distance between intersection points of the corrugations and from CFD calculations used to determine the transfer coefficient ϵ at each intersection.

References

[1] Ergun, S., (1949) Ind. Eng. Chem., **41**, p1179