

## MODELING OF MIXTURE SEPARATION IN A COLUMN WITH STRUCTURED PACKING. EFFECTS OF LIQUID MALDISTRIBUTION

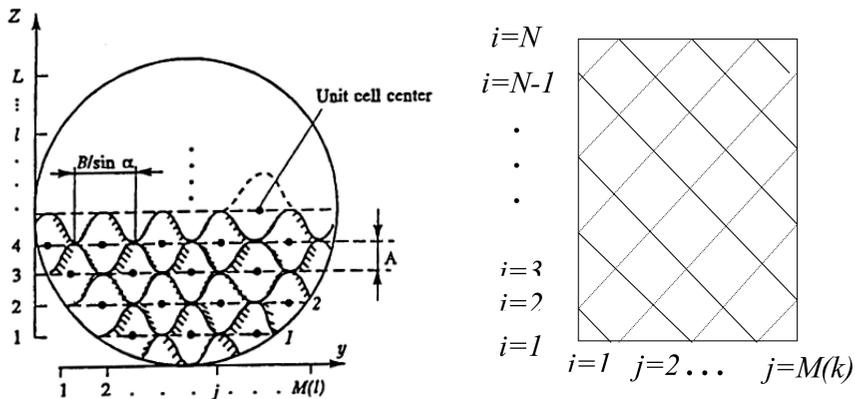
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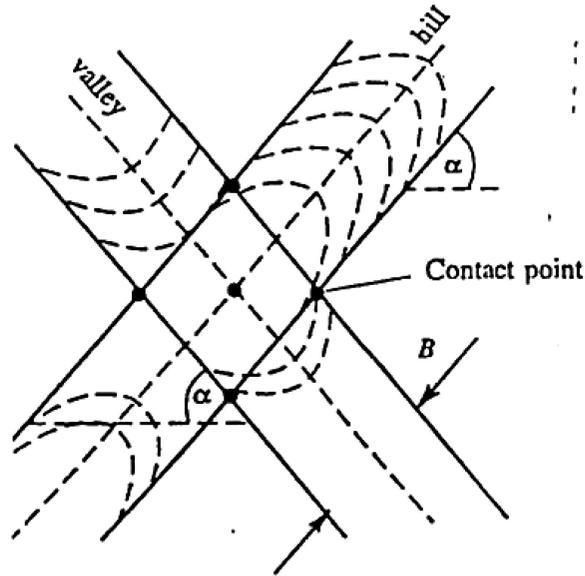
### INTRODUCTION

- What is the effect of maldistribution on the mass transfer efficiency of a distillation column containing structured packing?
- The column of structured packing is considered to consist of a set of unit cells
- Each pair of sheets gives a two-dimensional set of “elementary” cells:



### LIQUID SPREADING

- The “elementary” cells are used to calculate the liquid distribution over the column height and cross-section.
- Liquid distribution is calculated from top to bottom in every elementary cell based on a specified initial distribution
- Three parameters used to characterize liquid spreading:  $f_{ct}$ ,  $a_{ct}$ ,  $\varphi$



$a_{lg}$ ,  $a_{cr}$  – portions of the cell flow that goes along or across the corrugation  
 $a_{ct}$  – the cell flow that goes to the contact point

$$a_{lg} + a_{cr} + a_{ct} = 1,$$

$$a_{lg} = (1 - a_{ct}) \cos^2 \varphi,$$

$$a_{cr} = (1 - a_{ct}) \sin^2 \varphi.$$

$$Q_{i,j,1} = (a_{cr}Q)_{i+1,j,1} + (a_{lg}Q)_{i+1,j-1,1} + f_{ct}(a_{ct}Q)_{i+2,j,1} + (1 - f_{ct})(a_{ct}Q)_{i+2,j,2},$$

$$Q_{i,j,2} = (a_{cr}Q)_{i+1,j-1,2} + (a_{lg}Q)_{i+1,j,2} + (1 - f_{ct})(a_{ct}Q)_{i+2,j,1} + f_{ct}(a_{ct}Q)_{i+2,j,2},$$

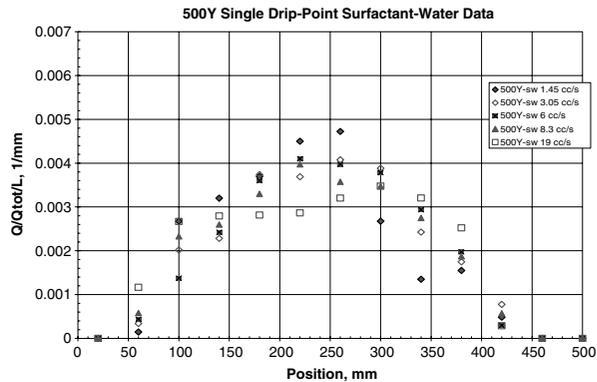
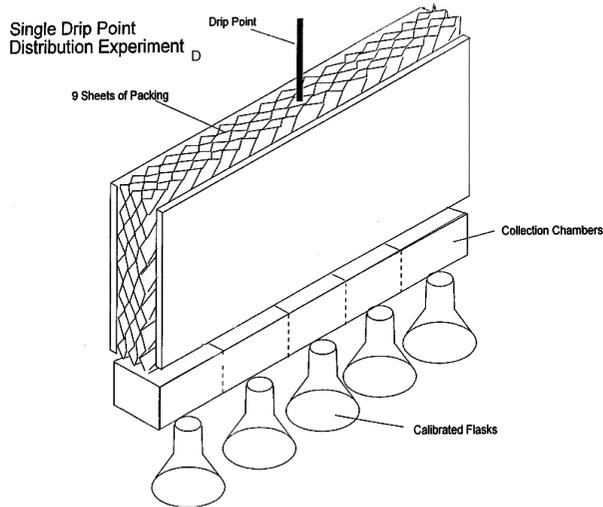
$$i = 1, 3, 5, \dots, N - 2; \quad j = 2, 3, 4, \dots, M - 1.$$

$f_{ct}$  – the contact point efficiency

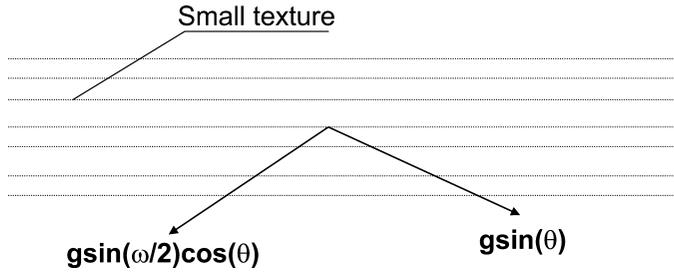
#### SPREADING COEFFICIENTS

- Coefficients ( $f_{ct}$ ,  $a_{ct}$ ,  $\varphi$ ) can be calculated from

- Single drip-point spreading experiments

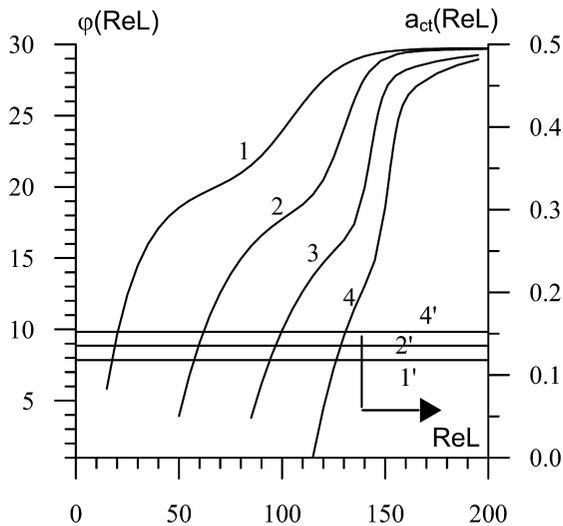


- Fundamental hydrodynamics
  - Shape of large ribs is considered as triangular
  - 3-D film flow for a single sheet of packing (without holes) can be reduced to 2-D Navier-Stokes equations
  - Spreading coefficient thus obtained ( $\varphi$ ) takes into account fundamental features of the film flow over corrugated sheets with both large ribs and small texture.

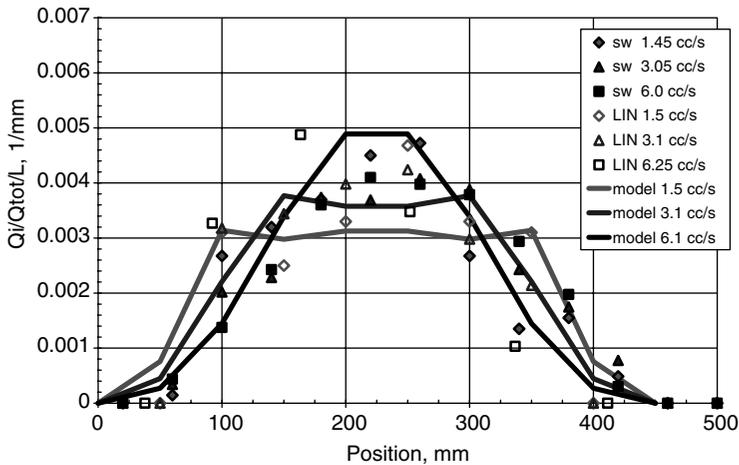


Amplitude of small texture is varied (0.1 mm – line 1, 0.15 mm – line 2, 0.2 mm – line 3, 0.25 mm – line 4).

The spreading behavior of surfactant+ water and LIN is similar despite relatively large differences in physical properties (surface tension, viscosity, etc.).



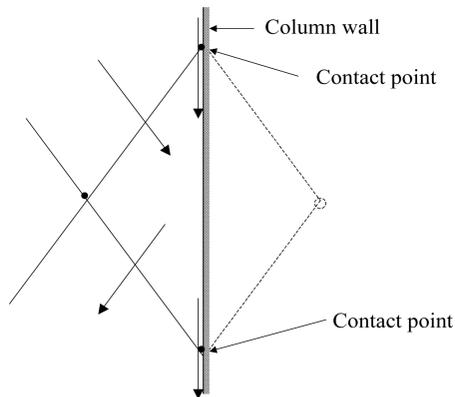
**Figure 1.** Hydrodynamics calculations of  $\phi(\text{ReL})$  based on the Navier-Stokes equations. Sulzer 500Y, LIN



**Figure 2.** Liquid distribution over a set of burettes. Sulzer 500Y, LIN & Surfactant-Water (sw)

#### EDGE BOUNDARY CONDITIONS

- The edge cell contact point “efficiency”  $f_{ct}^{edge}$  is different from the bulk contact point “efficiency”  $f_{ct}$
- There are two ways for liquid to leave the edge cell
  - Along/across the large ribs inclined from the wall.
  - Down the wall to the edge cells below.
- Above a critical liquid Reynolds number the dimensional flow rate away from the edge remains constant.



### MASS TRANSFER

- Mass transfer takes place in the elementary cells between counter-current flows of vapor and liquid

$$Q_2 \frac{dy}{dz} = \beta_2(y^* - y), \quad \beta_2 = \frac{a_w Sh_2}{Sc_2} \frac{1}{\varepsilon_0(1-\gamma)} \frac{a_p \Delta z}{Re_V \sin \theta}$$

$$Q_1 \frac{dx}{dz} = \beta_1(x - x^*), \quad \beta_1 = \frac{a_w Sh_1}{Sc_1} \frac{1}{\varepsilon_0 \gamma Re_L \sin \theta} \sqrt{u^*},$$

$$(y^* - y) = \chi(x - x^*), \quad \chi = \frac{4Sh_1 Sc_2}{Sh_2 Sc_1} \left( \frac{v_1 C_1}{v_2 C_2} \right) \frac{(1-\gamma)}{\gamma} \sqrt{u}$$

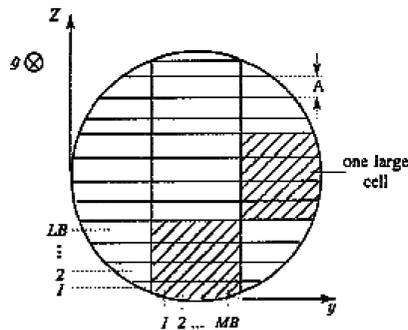
$$y^* = \frac{\alpha x^*}{1 - x^* + \alpha x^*}, \quad y|_{z=0} = y^{in}, \quad x|_{z=1} = x^{in}.$$

Non-dimensional local flow rates  $Q_1$  and  $Q_2$  are varied from unit cell to unit cell.

$$Sh_1 = Sh_1(Sc_1, Q_1 Re_L), \quad Sh_2 = Sh_2(Sc_2, Q_2 Re_V), \quad a_w = a_w(Q_1 Re_L).$$

### ELEMENTARY CELL "LUMPING"

- Mass transfer calculations cannot be done on the elementary cell level because the number of cells is too large
  - A single 900 mm diameter plug contains  $\sim 162000$  elementary cells
- "Large cells" are created by lumping 12–15 elementary cells together in the same horizontal slice
- No new parameters added



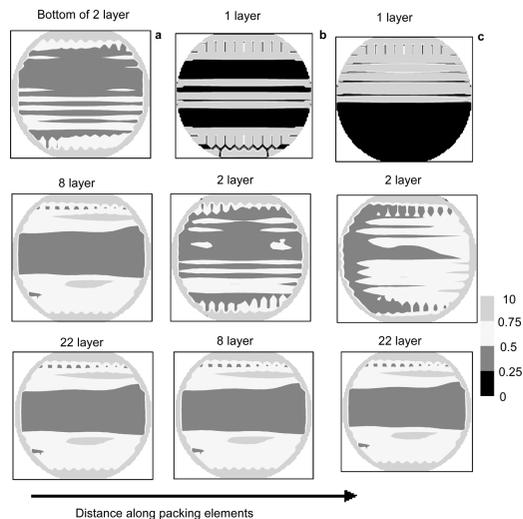
### MASS TRANSFER SOLUTION

- Liquid and vapor flow rate known in every cell
  - Vapor flow assumed constant

- An asymptotic analytical solution to the mass transfer problem connects the input and output compositions for the cell
- Newton's method is used to solve the resulting non-linear system of equations
- Sparse matrix algebra is used to invert the corresponding Jacobian matrix at every iteration

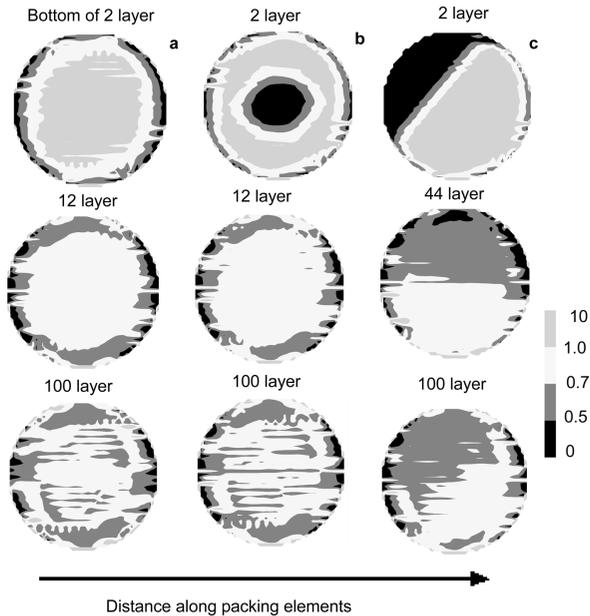
**EVOLUTION OF LIQUID DISTRIBUTION**  
 COLUMN DIAMETER 200 MM, R114/R21, 500Y  
 Three initial irrigations:

- “regular” (100% of drip points)
- 50% of the drip points blocked in the center
- 50% of drip points blocked (which are parallel to the top layer elements)



**EVOLUTION OF LIQUID DISTRIBUTION**  
 COLUMN DIAMETER 900 MM, R114/R21, 500Y  
 Three initial irrigations:

- “regular” (100% of drip points)
- 15% of the drip points blocked in the center
- 30% of drip points blocked (which are parallel to the top layer elements)



## MASS TRANSFER RESULTS

200 & 900 MM, R114/R21, 500Y

- Line 0 corresponds to the case of uniform distribution of the liquid and vapor
- Line 1 corresponds to the “normal” distributor (case (a) in figure 3). Black triangular symbol corresponds to experiment with such initial irrigation (6 layers column of  $D = 200$  mm).
- Line 2 corresponds to the initially maldistributed irrigation when 50% of the drip points were blocked in the center (case (b) in figure 3). Red circle symbol corresponds to experiment with such distributor at 6 layers.
- Line 3 corresponds to very strong initial maldistribution (case (c) in figure 3) when a half of the packing elements are not irrigated on the top. Red square symbol corresponds to experiment with 6 layers ( $D = 200$  mm).
- The experiments and calculations are at total reflux with bottom composition of  $R114 = 6\%$ .
- Lines 4–6 give the effects of initial maldistribution for a larger diameter column of  $D = 900$  mm (cases (a-c) in figure 4, respectively). Blue diamond symbols corre-

spond to experiments with 6 and 11-layers (“normal” distributor). The experiments and calculations are at total reflux with bottom composition of  $R_{114} = 0.3\%$ .

### CONCLUSIONS

- A “many-cell” approach is developed to analyze the effects of the liquid maldistribution over the cross section and height of distillation columns with structured packing.
- The liquid spreading coefficients used in the model are obtained by use of both the hydrodynamics calculations and the simple “single drip-point” experiments.
- Evolution of the different initial maldistribution over the column height is calculated for small and large diameters. It is shown that the evolution results in “unique steady state liquid distribution over the layer”. The amount of layers needed to reach this state depends on the column diameter and on the initial distribution.
- The corresponding mass transfer calculations compare the separation efficiency of a column where the liquid phase is distributed initially uniformly in some pattern of drip points to the efficiency of a column with maldistribution. It is shown that the maldistribution effects are strongly dependent on the column diameter.