

**INVESTIGATION OF HYDRODYNAMICS, HEAT AND MASS TRANSFER
SIMULTANEOUSLY IN LIQUID FILM FLOW ON INCLINED PLATES USING CFD
APPLICATION****Mohammad Reza Khosravi Nikou¹, Mohammad Reza Ehsani^{1,*}**¹ Chemical Engineering Department, Isfahan University of Technology (IUT), 84155Isfahan, Iran**Abstract**

A two-phase flow CFD model using volume of fluid (VOF) method is presented for predicting the hydrodynamics, heat transfer and mass transfer of falling film flow on inclined plates, corresponding to the surface of texture of structured packing. Using the proposed CFD model the influence of solid surface microstructure, liquid properties and gas flow rate on flow behavior was investigated. From the simulated results it was shown that under the condition of no gas flow the liquid flow patterns are dependent on the microstructure of the plates, and proper micro structuring of the solid surface will improve the formation of a continuous liquid film. Increasing the wetted area results enhancement of heat and mass transfer from film. It was also found that liquid properties, especially surface tension, play an important role in determining the thin film pattern. However, there are very different liquid film patterns under the action of gas flow. Thinner liquid films break easily, but thicker liquid films remain continuous even at higher gas flow rate, which demonstrates that all factors affecting the liquid film thickness will affect the liquid film patterns under conditions of counter-current two-phase flow. Finally it was found that any changes in liquid film patterns influence too much on heat and mass transfer from the film.

Keywords: Structured packing, Hydrodynamics, Heat transfer, Mass transfer, CFD

1- Introduction

Liquid film flow can be found in many chemical and biochemical processes, such as distillation processes in packed columns and gas-liquid reaction processes in trickle bed reactors. The fluid dynamic behavior of this kind of flow is of great importance in determining process performance, and a better understanding of the hydrodynamics of this kind of flow allows us to predict process performance more accurately and to develop more effective and optimal equipment to improve the performance under the same operating condition. In the processes like reactive distillation, besides of hydrodynamics phenomena, it is too much important to understand heat and mass transfer phenomena, simultaneously.

Liquid film flow on the surface of inclined corrugated plates corresponding to structured packing has drawn great attention, and some experimental and theoretical research work has been carried out in recent years, but regarding heat and mass transfer there is no specific investigation on research papers. Among the hydrodynamics research, the group of Cerro et al. [1-5] carried out a number of experimental and theoretical studies into liquid film flow on solid surfaces with micro and micro-texture structures. In their studies a film evolution equation with an approximation of the viscose long-wave for the Navier-Stockes equations was presented. However, the inertia term was neglected, which is important to determine the stability of liquid film. The studies by Ataki and Bart [6] described rivulet flow on an inclined plate using experimental and CFD methods as a basis to understand the film flow on the surface of structured packing.

Soare et al. [7] proposed a simplified mathematical model for liquid flow on corrugated metal sheets in which the effect of surface tension was included by assuming that the force generated is uniformly distributed over entire flowing liquid film. Using analytical solutions the liquid film

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thickness, velocity and liquid flow rate can be calculated. Using FLUENT software package, Szulczewska et al. [8] simulated two-phase counter-current flow in a plate-type structured packing. The effect of the liquid flow rates on the interfacial area formed on the surface of the structured packing was investigated, but the effective wetted model can be unreliable.

The objective of the present work is to construct a two-phase CFD model using the VOF (volume of fluid) approach, which enables us to investigate the influence of the solid surface characteristics, liquid properties and gas flow rates on falling film flow, heat and mass transfer coefficients on inclined plates. The proposed model can also simulate the dynamic formation and breakdown of liquid film, enhancement in convection heat transfer and mass transfer increasing, which highlights the possibility of using CFD to predict the unsteady process of liquid film flow.

2- Theoretical and Numerical Methodology

Since the gas and liquid film on the plate do not inter-penetrate each other, a calculation using VOF [9] approach was chosen. This method is a surface-tracking technique applied to a fixed Eulerian mesh, which enables the computation of two-phase flow under the condition that phases do not mix, i.e., the gas liquid interface is clearly identified. The VOF allows the construction of the interface to become part of the solution based on the same grid system, which is a flexible and efficient method to describe the changes in topology of a gas-liquid interface [6, 8-13].

2-1- Governing Equation

The mass, momentum and energy conservation equations for two-phase flow throughout the domain are:

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \vec{v}) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla P + \nabla \cdot [\mu(\nabla \vec{v} + \vec{v}^T)] + \rho \vec{g} + \vec{F} \quad (2)$$

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \vec{v} h) = \nabla \cdot (k \nabla T) + \frac{Dp}{Dt} - [\mu(\nabla \vec{v} + \nabla \vec{v}^T) : \nabla \vec{v}] - \nabla \cdot \left(\sum_k h_k j_k \right) \quad (3)$$

The equations given above are dependent on the volume fraction of all phases, expressed implicitly by the properties ρ and μ . In a two-phase system, for example, if the phases are represented by the subscripts 1 and 2 and the volume fraction of phase 2 is known, the density and viscosity in each cell are given by equations (4) and (5).

$$\rho = \alpha_2 \rho_2 + (1 - \alpha_2) \rho_1 \quad (4)$$

$$\mu = \alpha_2 \mu_2 + (1 - \alpha_2) \mu_1 \quad (5)$$

In the VOF model the movement of the phase interface is affected by the distribution of a_q , the volume fraction of q^{th} phase (secondary phase) in a computational cell. When in a particular computational cell $a_q=0$ the cell is empty of q^{th} fluid, and when $a_q=1$ the cell is full of q^{th} fluid. When $0 < a_q < 1$ the cell contains the interface between the q^{th} fluid and one or more other fluids [9]. Thus, the interface between two phases can be traced by solving the continuity equation for the volume fraction function:

$$\frac{\partial a_q}{\partial t} + \vec{v} \cdot \nabla a_q = 0 \quad (5)$$

The volume fraction for primary-phase in Eq. (5) will be obtained from the following equation:

$$\sum_{q=1}^n a_q = 1 \quad (6)$$

For thin liquid film flow, surface tension plays an important role. The surface tension model in CFX 11 is the continuum surface force model proposed by Brackbill et al. [14]. With this model the contribution of surface tension to the VOF calculation results in the source term of the momentum equation. In gas-liquid free surfaces, it has the following form for the two phases:

$$F = \sigma_{ij} \frac{\rho \kappa_i \nabla \alpha_i}{\frac{1}{2}(\rho_i + \rho_j)} \quad (7)$$

Where ρ is the volume-averaged density, σ is the surface tension coefficient, and κ is the free surface curvature defined in term of the divergence of the unit normal \hat{n} as:

$$\kappa = \nabla \cdot \hat{n} = \frac{1}{|n|} \left[\left(\frac{n}{|n|} \cdot \nabla \right) |n| - (\nabla \cdot n) \right] \quad (8)$$

Where:

$$\hat{n} = \frac{n}{|n|}, \quad n = \nabla a_q \quad (9)$$

The unit surface normal at the live cell next to the wall is replaced by the following equation, which is the so-called dynamic boundary condition, resulting in adjustment of the curvature of the surface near the wall:

$$\hat{n} = \hat{n}_w \cos \theta_w + \hat{m}_w \sin \theta_w \quad (10)$$

Where \hat{n}_w and \hat{m}_w , are the unit vectors normal to and tangential to the wall, respectively. The contact angle, θ_m is the angle between the wall and tangent to the interface at the wall.

2-2- Model Geometry and Boundary Conditions

All the model geometry and dimensions are given in Fig.1 and Tab.1.

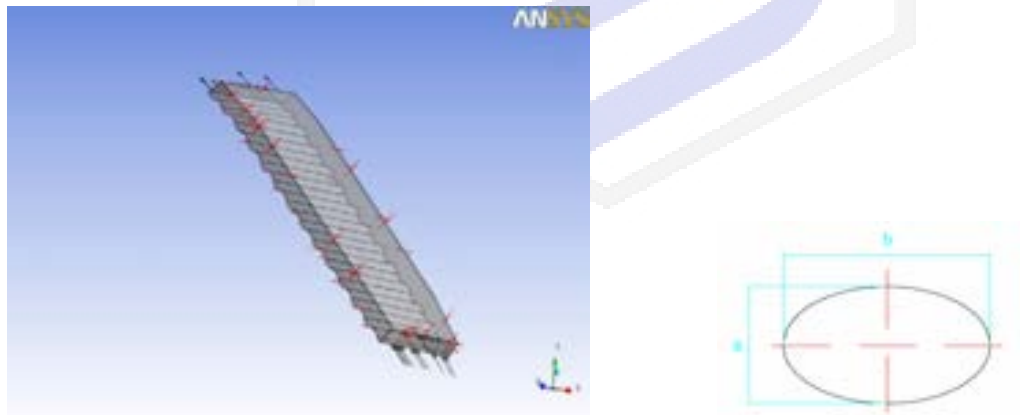


Figure.1 The model geometry

Table.1 Structural parameters of various geometries

Type	Design parameters		Plate dimensions	Plate inclination angle	Mesh statistics
	a(mm)	b(mm)	H×L×t (mm)	degree	-
Flat plate			53×20×3	45	3051
Corrugated plate1	0.25	4	53×20×3	45	1067375
Corrugated plate2	0.5	8	53×20×3	45	618278
Corrugated plate3	0.5	4	53×20×3	45	679716
Corrugated plate4	1	8	53×20×3	45	30664

Three-dimensional coordinate system is used for computation. No slip boundary condition is provided at the wall. All the boundary conditions are specified in the following table.

Table.2 Boundary conditions

Location	Boundary condition types
Inlet	Velocity, Volume fractions, mass fraction of methanol, Temperature
Outlet	Velocity
Wall	No-slip, Temperature

2-3- Simulation Scheme

The CFD software, ANSYS-CFX version 11, is used to simulate the motion of gas-liquid two-phase flow on structured packing. A high resolution was chosen as the solution of the momentum and energy equations. The SIMPLEC algorithm is used to solve the pressure field.

3- Results and Discussion

3-1- Influence of Plate Structure

Influence of corrugated plate structure on hydrodynamic, heat and mass transfer of two-phase flow of Methanol-Isopropanol mixture on smooth and four types of plates, whose structural parameters are listed in Tab.1, has been referred in Figures 2-4.

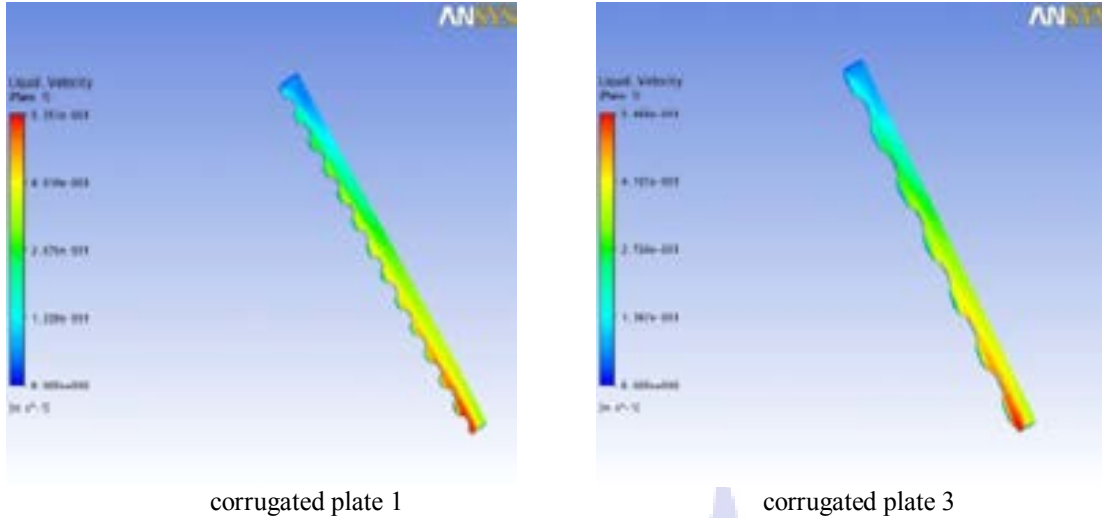
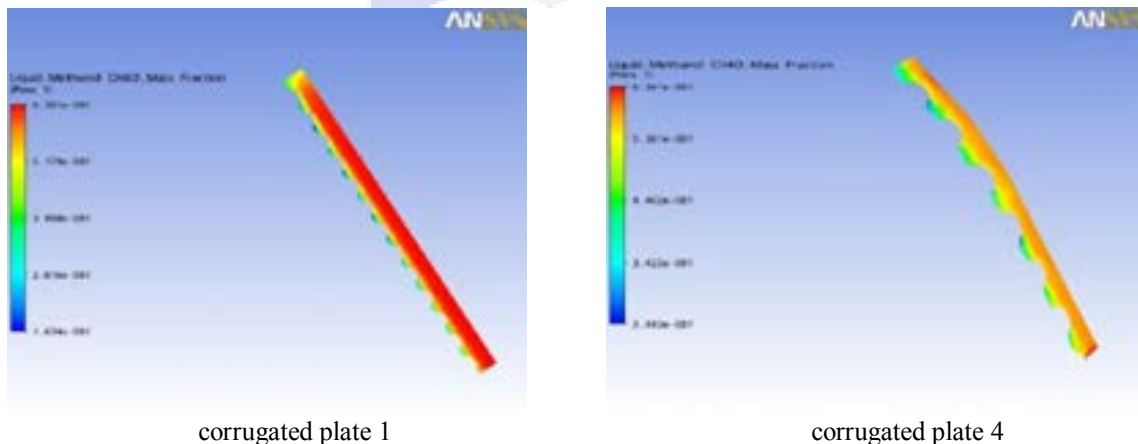


Figure.2 Liquid velocity profile on corrugated plates no. 1 and 3($Re_l= 835$, $Re_g= 1685$)

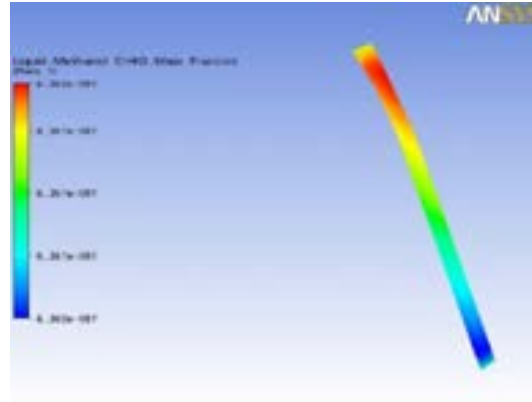
As liquid moves over the solid surface the film breaks randomly, and breaking points of film occurs at the neighboring regions of the transition points from convexities to concavities. When changing the texture or structural parameters of the wavy plates the flow pattern of liquid films will change accordingly. It is found that for wavy plates with small waves the liquid film breaks up at many points and no continuous film forms. By contrast, continuous films can form easily on the plates with large waves.

It is expected that when there is continuous film over structured packing, heat and mass transfer enhanced by increasing turbulence on the film. From Fig.3 it can be distinguished that, when flat plate structure becomes wavy, methanol concentration gradient between inlet and outlet increased. It means interfacial area will be increased by waviness. Heat and mass transfer enhancement are increased by increasing waviness on plate till to reach to maximum and after that starts to decrease. By increasing too much waviness amplitude on corrugated plate, continuous film is broken and results to decrease transport phenomena drastically. It can be explained by this reason, increasing the value of waviness amplitude will increase the amount of stagnant points in liquid concaves. If the eddies inside stagnates could be replaced by passing the flow over structured packing, the amount of decrease is not significant (Fig.4) but when stagnant pool is big enough, it effects on transfer process too much.



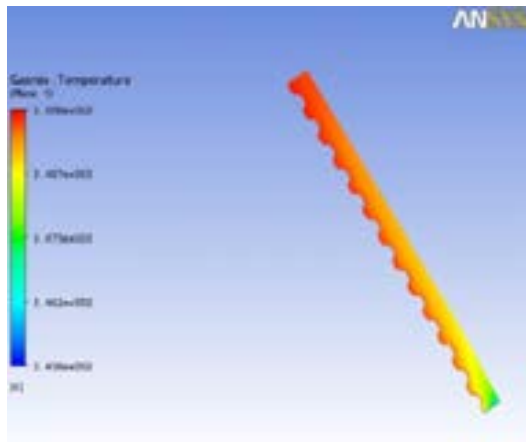
corrugated plate 1

corrugated plate 4

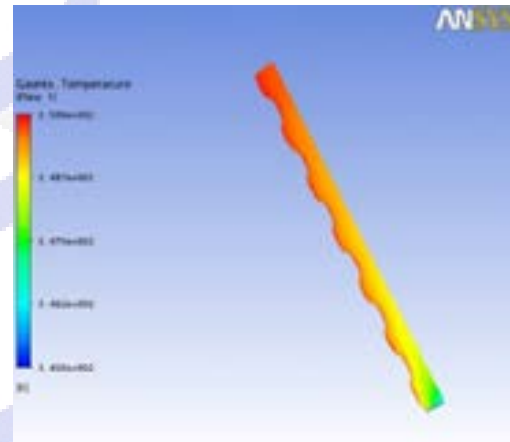


flat plate

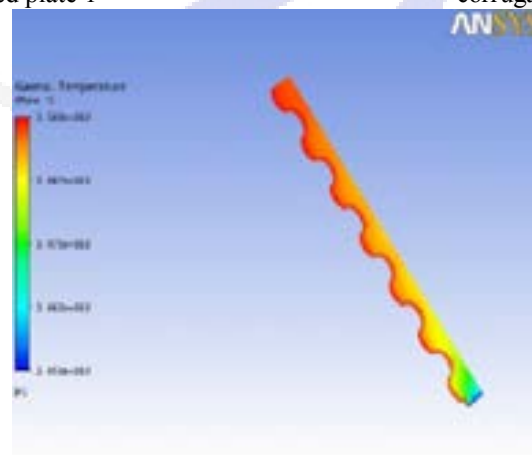
Figure.3 Methanol concentration profile in liquid phase over corrugated plates no. 1 and 4 and flat plate ($Re_l=835$, $Re_g=1685$)



corrugated plate 1



corrugated plate 3



corrugated plate 4

Figure.4 Temperature profile in gas phase over corrugated plates no. 1, 3 and 4 ($Re_l=835$, $Re_g=1685$)

3-2- Influence of Liquid Properties

To investigate the effect of liquid properties on the flow behavior, Water-Air mixture, Glycerol-Air mixture and Methanol-Isopropanol mixture (properties are listed in Tab.3) were selected to cover a range of surface tension, viscosity, and contact angles etc. Fig.5,6 shows liquid profile

and liquid temperature for these two mixture. It was found that by increasing liquid viscosity, film thickness increased and film will be continuous.

Besides liquid viscosity, surface tension plays a very important role in liquid stability. In general, low surface tension systems tend to yield low contact angles which favor complete wetting of surface structure. This means that, for a given solid surface, one may expect better wetting for lower surface tension liquids. To investigate the influence surface tension on the film flow, systems of methanol-isopropanol mixture was simulated.

Table.3 Mixture properties

Mixture	ρ (kg/m ³)	μ (kg/m s)	σ (N/m)	θ (degree)
Water-Air	998.2	0.001003	0.0722	57
Glycerol-Air	1262	1.495	0.0727	56
Methanol-Isopropanol	776.2	0.00776	0.02776	40

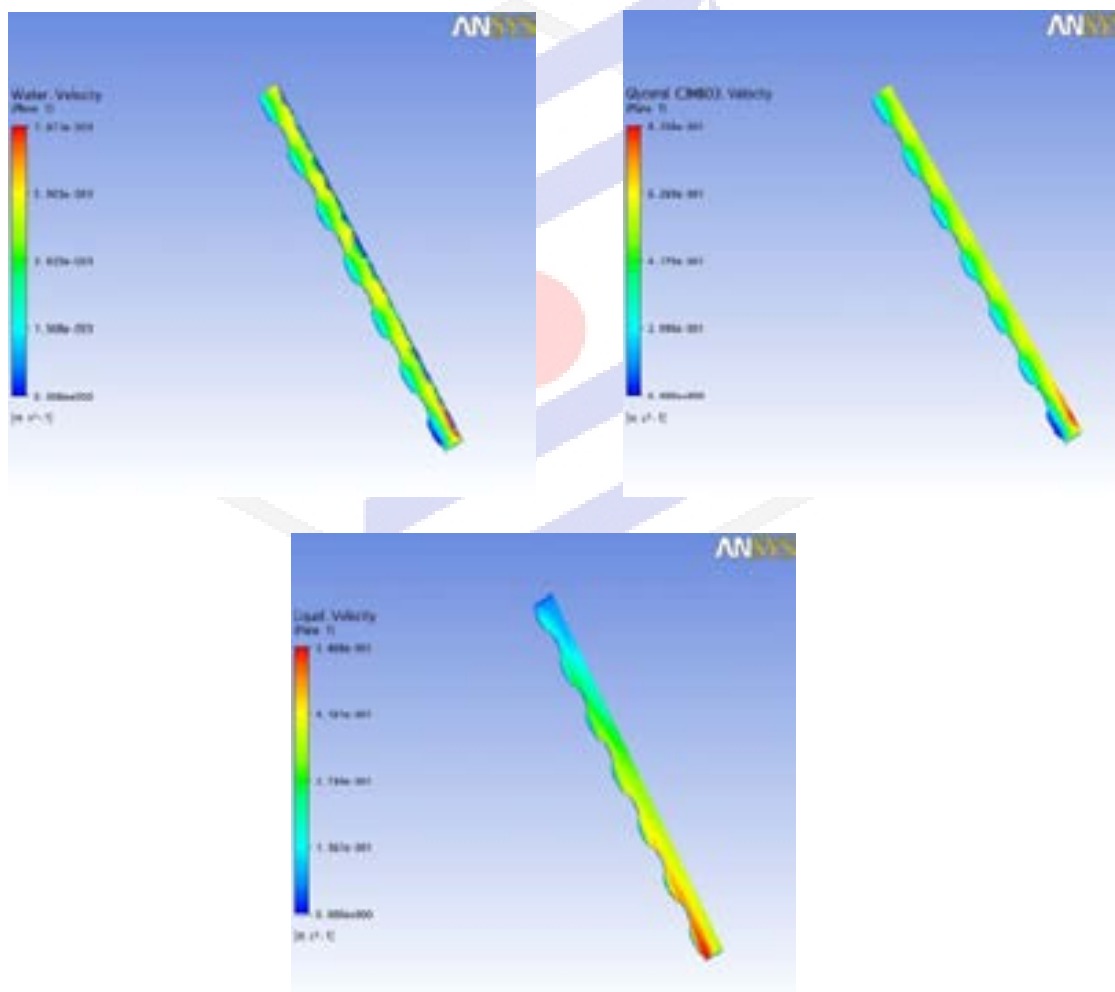


Figure.5 Liquid velocity profile for Water-Air, Glycerol-Air and Methanol-Isopropanol mixture over corrugated plate 2

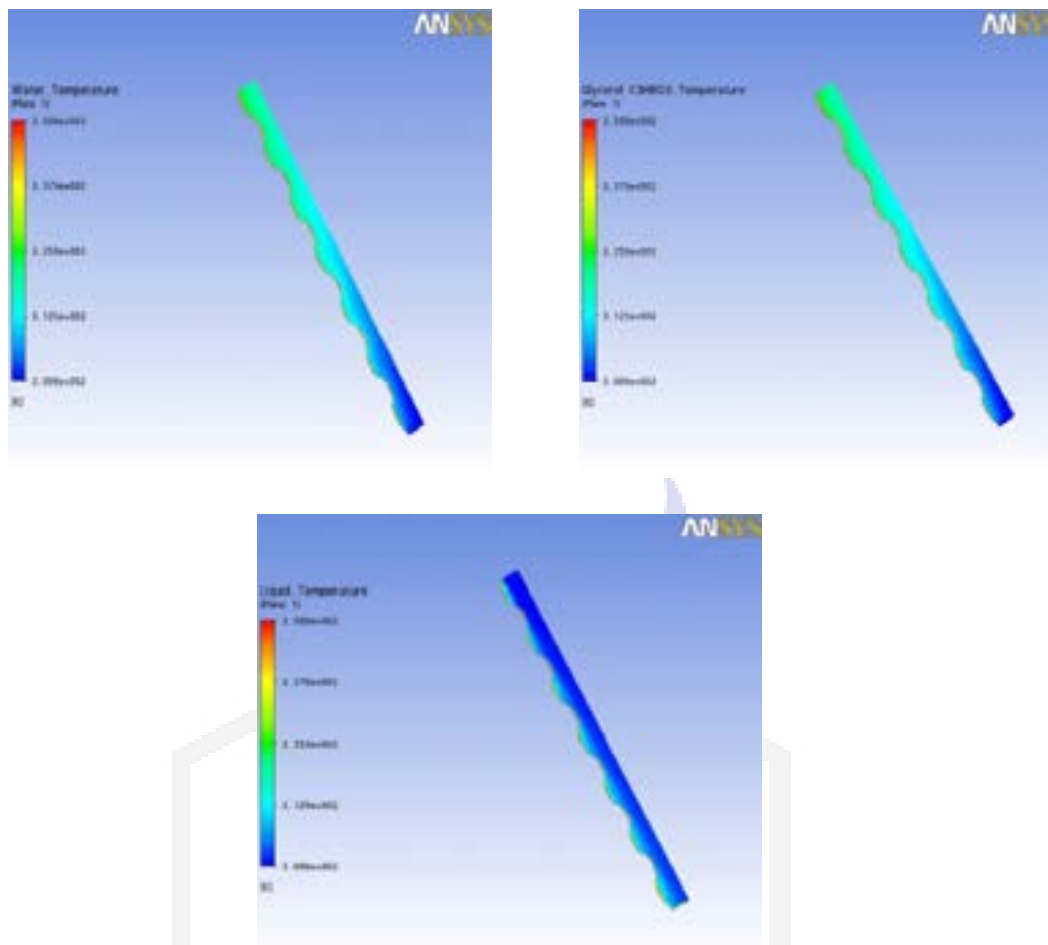
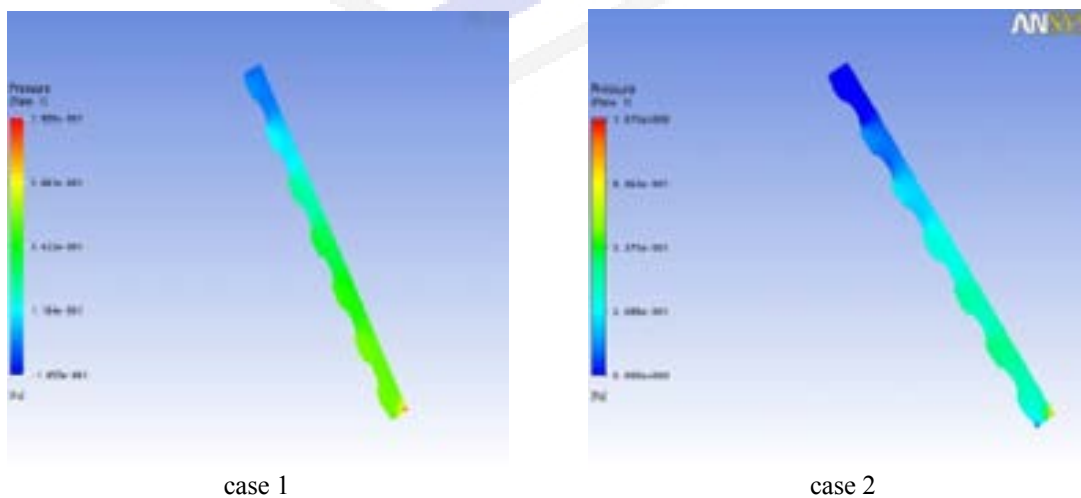


Figure.6 Temperature profile of liquid phase for Water-Air, Glycerol-Air and Methanol-Isopropanol mixture over corrugated plate 2

3.3 Influence of Gas Flow

The counter-current flow behavior and heat and mass transfer changes were simulated, and are shown in Fig.7



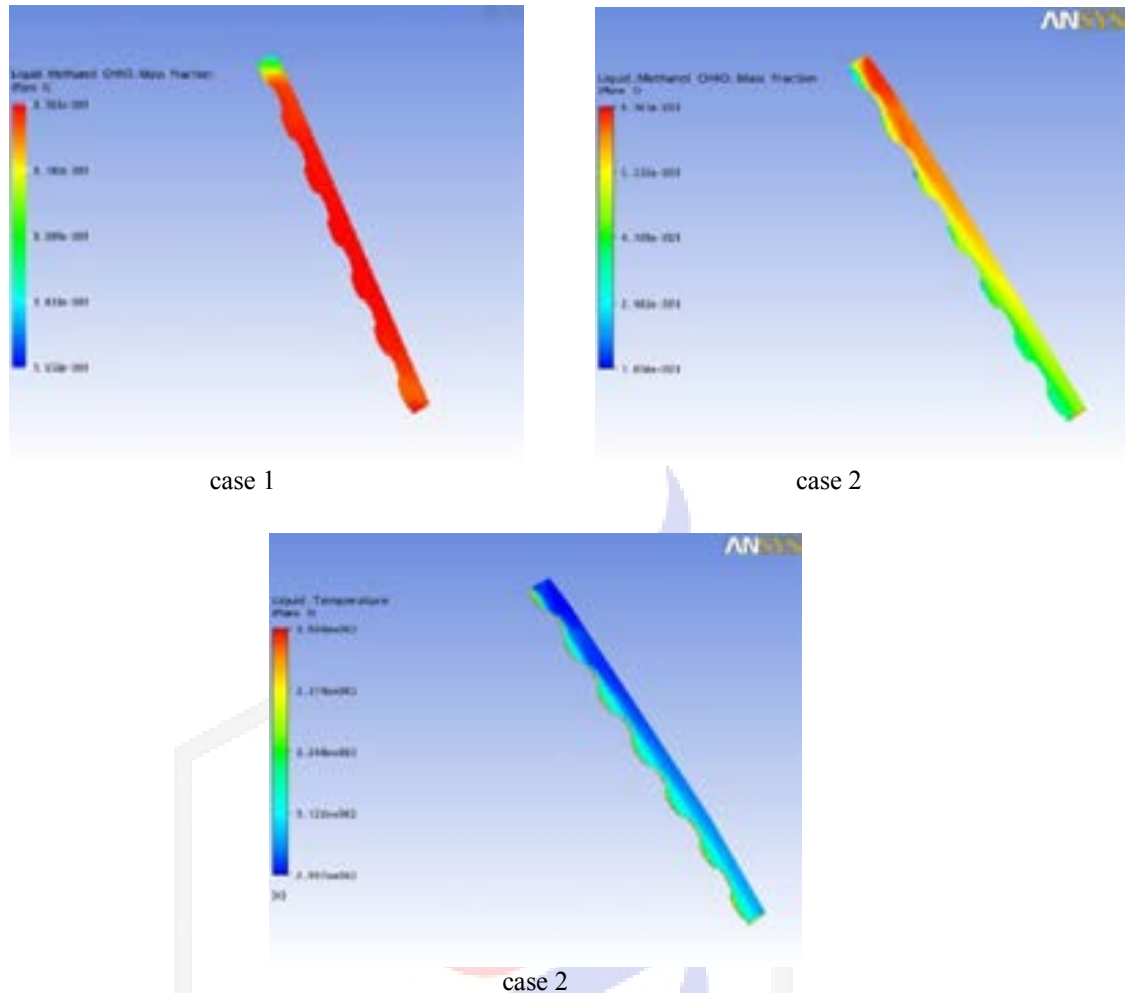


Figure.7 Gas flow rate effects on pressure drop, methanol concentration and temperature profile of liquid phase for Methanol-Isopropanol mixture over corrugated plate 2
(Case1: $u_g=0.36\text{m/s}$ and Case2: $u_g=0.72\text{m/s}$)

The simulation results in this figure demonstrate that the flow behavior of two-phase flow and transfer processes on structured packing is greatly influenced by film thickness. Thus, all effects increasing the film thickness will be of advantage in forming a continuous film. Once the film breaks down a number of dry patches come into being, which are extremely disadvantageous to heat and mass transfer processes.

4- Conclusion

A numerical method for simulation of coupling of hydrodynamic and heat and mass transfer for two-phase flow inside smooth and four types of geometry of structured packing has been presented.

It has been shown that adding waviness structure to smooth plates could increase heat and mass transfer phenomena but when concavity and convexity increase too much, because of generating stagnant point, this enhancement will be reversed and decrease transfer drastically.

The fluid properties, especially the liquid surface tension, play an important role in determining the flow hydrodynamic. The simulated results indicate that under counter-current two-phase flow, measures to increase continuity of film to reduce occurrence of dry patches.

Gas flow has positive effects because of turbulence but when discontinuity is generated on structured packing, transport phenomena decreased rapidly.

Appendix

A. Nomenclature

Arabic symbols

A	[m]	Amplitude of the solid surface
F	[kg/m ³ s ²]	Source term in the momentum equation
G	[m/s]	Gas flow rate
g	[m/s ²]	Acceleration of gravity
h	[kj/kg]	Enthalpy
L	[m ³ /m ² h]	Liquid flow rate
m	[-]	Surface tangential
n	[-]	Surface normal
P	[Pa]	Pressure
Re _L	[-]	Reynolds number of liquid
		phase = $\frac{4\Gamma}{\mu}$
T	^o C	Degree of centigrade
t	s	Time

Greek symbols

α	[-]	The volume fraction of phases
β	[degree]	Inclined angle of plate
θ	[degree]	Contact angle
κ	[-]	Curvature of free surface
λ	[m]	Wave length of solid surface
μ	[kg/ms]	Dynamic viscosity
ρ	[kg/m ³]	Density
σ	[N/m]	Surface tension
v	[m/s]	Velocity vector
Γ	[kg/ms]	Mass flow rate unit perimeter

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