A note on the composition-dependency of the density within the mass transfer layer

Mohammad Ali Aroon 1, Milad Asgarpour Khansary 2

1-Membrane Research Lab., Caspian Faculty of Engineering, College of Engineering, University of Tehran, Iran; 2-Confirm Smart Manufacturing, University of Limerick, Limerick, Ireland

**Abstract**

In the conventional mass transfer analysis in binary mixtures, a constant total mass concentration (or density) in the mass transfer layer has been assumed. This assumption is valid only once the concentration of diffusing component in the mixture is very low. Here, an explicit ***composition-dependency*** is introduced for the density within the mass transfer layer in order to see what happens when the conventional composition-independency assumption for the density within the mass transfer layer is relaxed. The governing equations are derived analytically and solved numerically. It was found that the conventional approach is a special case of our newly proposed composition-dependent density profile. While application of conventional approach is limited to very dilute binary mixtures, newly approach is applicable to general binary mixtures.

**Keywords**: binary mass transfer; density; composition dependency; mass flux;

# Problem definition

Conventionally, a constant total density in the mass transfer layer of binary mixture has been assumed [[1](#_ENREF_1)]. However, this assumption can be valid only when diffusing component in the mixture (hereafter *A*) is very dilute [[1](#_ENREF_1)]. In this case, when considering the one dimensional mass transfer as shown in Fig. 1 under steady state condition with no homogeneous reaction conditions, one may obtain the mass balance of the diffusing component *A* in the binary mixture as [[2](#_ENREF_2)]. Here, *z is* mass transfer direction and is the diffusional mass transfer contribution, is the density of diffusing component *A* and is the mass average velocity in *z*-direction. The diffusional mass transfer contribution () can be given by the Fick’s first law i.e. ) [[2](#_ENREF_2)], where is the total density which is assumed constant at any positions. is the binary diffusivity and is the weight fraction of diffusing component *A*. The governing differential equation simplifies as given by Eq. 1.

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The solution to the differential equation Eq. 1 is given in literature as in Eq. 2-3 [[1](#_ENREF_1)], where subscripts 1 and 2 indicate boundary 1 (*z*=0) and boundary 2 (*z*=) of the mass transfer layer respectively, is the thickness of the mass transfer layer, and are the mass and molar fluxes of the diffusing component *A* (with respect to stationary coordinate) from boundary 1 (*z*=0) to boundary 2 (*z*=) respectively. Here and *c* are the total concentration in the mass transfer layer. In this case, the density at boundary 1 and boundary 2 is equal due to composition-independent assumption, however for clarity, we kept in Eq. 2.

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However, the total concentration in the mass transfer layer of a binary mixture cannot be assumed constant unless diffusing component *A* is very dilute. This is because, alongside the mass transfer direction, the mass transfer alters the composition profile and therefore total concentration. This in turn means that density within the mass transfer layer varies alongside the mass transfer direction. It can be concluded that a composition-dependent density profile within the mass transfer layer exists, which is in contrast to the conventional composition-independent density profile within the mass transfer layer as illustrated in Fig. 1.

***boundary 1***

***boundary 2***

**, the conventional approach**

**The new approach**

Fig. 1. Schematic demonstration of the composition dependency of density in the conventional and new approaches

This letter addresses the introduction of a composition-dependent density within the mass transfer layer in a binary mass transfer condition and illustrates how it affects the mass transfer properties, particularly the mass fluxes.

# Applying the composition-dependency of the density in the mass transfer layer

In order to explicitly introduce the composition-dependency of the density in Eq. 1, we replace the density by its equivalent tailor series approximation up to the second term i.e. . Here, subscript *z* shows that the density is varying alongside *z* direction. In this context, subscript 1 corresponds to , or boundary 1. This approximation implies a linear profile for the composition-dependency of density, which can be descending or ascending, depending on value. While this linear profile is the simplest form of such dependency [[3](#_ENREF_3)], it avoids exhaustive mathematical manipulation [[4](#_ENREF_4)] and keeps the context concise on the considered concept i.e. the composition-dependency of density. The proposed approach provides a straightforward opportunity to see what happens when we relax the composition-independency of density. Showing term as , then can be written as at any position in *z* direction.

In Eq. 1, it would be much helpful and interesting to find an alternative relationship for the mass velocity in *z*-direction () under variable density assumption. For this purpose, we employed the continuity equation under aforementioned conditions, i.e. . By inserting the composition-dependent density profile and performing required integrations, the mass velocity in *z*-direction () can be obtained as given in Eq. 4. In which, is mass average velocity corresponding to .

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Noting that at any position in *z* direction we may write , then by inserting Eq. 4 in Eq. 1 and performing required mathematical manipulations, we obtained Eq. 5 where .

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It is worthy to mention that when the density is constant and independent of the composition in the mass transfer direction i.e. , one can readily realize that . This implies that Eq. 5 simplifies to Eq. 2 which can be found in literature [[1](#_ENREF_1)] or in alternative forms such as given in Eq. 3.

In order to examine how the mass flux () is affected by composition-dependent density in the mass transfer layer, in comparison to the mass flux () with the composition-independent density in the mass transfer layer, we defined as in Eq. 6, which measures the relative magnitude of the fluxes in the two approaches.

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Eq. 6 shows that is a function of the expansion coefficient (), the ratio of diffusive fluxes () and the weight fractions of diffusing component “*A*” in the mass transfer boundaries (, ), where subscript *1* and *2* indicates each mass transfer boundaries. The expansion coefficient, , can be rewritten as . Therefore, Eq. 6 can be rewritten as Eq. 7.

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# Discussion on the composition-dependency of the density in the mass transfer layer

An interesting practice for the examination of proposed approach is pure liquid evaporation from a container into the ambient air, which is experimentally used to determine the mass transfer coefficients. For such a process, it can be readily seen that as only one of components (evaporating liquid) is diffusing in a stagnant film. Indeed, it always can be assumed that the concentration of the evaporating liquid at *boundary 2* is zero () as it would be stripped away due to the ventilation. In this case, Eq. 7 reads Eq. 8, noting that .

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We evaluated Eq. 8 for 0*<ωA1<*0.7, 0.5*< ρ*1/*ρ*2 *<*5 and -1*< β* *<*1 in order to get an overall understanding of a composition-dependency profile for density (see supplementary file *SI1*). We also examined it for some specific liquids including water, methanol, ethanol, ethyl glycol, tetrahydrofuran, benzene, N-methyl-2-pyrrolidone, chloroform and hexadecane, which can be found in supplementary file *SI2*. The values of *Rn* against *ωA1* at different *β* are shown in Fig. 2. It can be concluded that as the difference in densities increases (as reflected by *β* and *ωA1* ), the deviation in mass flux calculated by composition-independent density increases from those calculated by composition-dependent density as seen in Fig. 2. It is very interesting that, in all values of *β*, all mass flux profiles approach to when *ωA1* goes to zero*.* This phenomenon confirms that constant density assumption is applicable only when component *A* in a binary mixture is very dilute. Therefore composition-dependent density should be used for mass flux calculation. It is noted that the composition-independent density assumption predicts lower mass flux when density at boundary 2 is lower than density at boundary 1 i.e. *ρ*1 < *ρ*2 (*β*<0). Similarly, the calculated mass fluxes using the composition-independent density assumption are higher than those predicted by composition-dependent density when density at boundary 1 is lower than density at boundary 2 i.e. *ρ*1 > *ρ*2 (*β*>0).

Fig. 2. Values of *Rn* against *ωA1* at different *β* values, demonstration of systematic deviation of predicted mass flux due to the composition-independent density assumption

The logarithmic values of *Rn* (for better visibility) against *ωA1* at different *ρ*1/*ρ*2 are shown in Fig. 3. It can be seen that when density is constant within mass transfer layer i.e. *ρ*1=*ρ*2, the newly proposed composition-dependent density profile reads the conventional composition-independent density profile. When density at boundary 1 is higher than density at boundary 2 i.e. *ρ*1>*ρ*2, the mass flux predicted by conventional composition-independent density profile is always higher than the mass flux predicted by the newly proposed composition-dependent density profile as *Rn* *<* 1. This means using the mass flux predicted by conventional method for calculation of mass transfer coefficients would result in larger values. Similarly, when density at boundary 1 is lower than density at boundary 2 i.e. *ρ*1<*ρ*2, the mass flux predicted by conventional composition-independent density profile is always lower than the mass flux predicted by the newly proposed composition-dependent density profile as *Rn* *>* 1.

Fig. 3. Logarithmic values of *Rn* against *ωA1* at different *ρ*1/*ρ*2 values, demonstration of systematic deviation of predicted mass flux due to the composition-independent density assumption

The values of *Rn* against *ρ*1/*ρ*2 at different *β* are shown in Fig. 4. The special case of *β*=0 implies that density is constant throughout the mass transfer layer from boundary 1 to boundary 2 i.e. *ρ*1=*ρ*2=*ρ* and in this case, the newly proposed composition-dependent density profile reads the conventional composition-independent density profile as indicated in Fig. 4 by the open circle. At any *β* when *ρ*1=*ρ*2, the newly proposed composition-dependent density profile reads the conventional composition-independent density profile. It is worthy to note that any *β* shows the slop of linear approximation that we applied to density profile (see section 2).

Fig. 4. Values of *Rn* against *ρ*1/*ρ*2 at different *β* values, demonstration of systematic deviation of predicted of mass flux due to the composition-independent density assumption

# Concluding remark

By introducing a composition-dependent density profile, we improved the accuracy of mass flux calculations in comparison to the conventional composition-independent density profile. It was shown that the conventional composition-independent density profile is a special case of our newly proposed composition-dependent density profile when *β=0* or component “*A*” in a binary mixture is very dilute. Therefore*,* the application of conventional approach is limited to binary mixtures where one component in the mixture (generally diffusing component) is very dilute. But the newly approach is applicable to whole composition range. Indeed, our analysis dealt with real mixtures, then the present work covers the results presented by Hanna [[5](#_ENREF_5), [6](#_ENREF_6)] who studied mass fluxes within mass transfer layer considering variable density approach in ideal gas mixtures.

# Data availability

The supplementary information (python scripts and raw data) can be found on:

<https://sites.google.com/site/miladasgarpour/Posts/Completed/varRho>.

# Conflict of interest

There’s no conflict of interest to declare.

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