Heat and mass transfer in evaporating twocomponent liquid film flow

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Abstract—Turbulent multicomponent gas flow with evaporation from a two-component liquid film is considered. To model the transport processes in detail special attention is drawn to the phase equilibrium of binary liquids and multicomponent thermodynamics. The numerical method applied solves the coupled governing equations together with the boundary and interfacial conditions. The solution technique is based upon a variational procedure for the determination of the temperature at the gas-liquid interface. The prediction for the evaporation of benzene-methanol mixtures into a hot tubular air stream clearly shows the influence of the phase equilibrium and its interaction with the local transport processes. Even small portions of a second component can lead to significant changes in the heat and mass transfer. This verifies the importance of detailed physical models and efficient solution procedures.

1. INTRODUCTION

GAS-LIQUID flow systems with coupled heat and mass transfer include a wide variety of processes such as boiling, condensation, film cooling or combustion premixing. Because of their widespread applications, evaporating liquid film flow and related problems have received considerable attention since Nusselt's early publications in 1916 [1].

Whereas a large number of investigations have been made concerning the evaporation of pure substances [2-10], the theoretical treatment of flows with multicomponent evaporation has not received adequate attention [11, 12]. Analysing the heat, mass, and momentum transfer mechanisms, especially for multicomponent flows with phase transition, is very important for practical applications since the phases involved in technical processes are nearly always mixtures of several components. Combustion premixing is just one such example since common fuels are a mixture of hydrocarbons. The individual components affect the local heat and mass transfer to varying degrees whereby the substances involved and the composition of the mixture play an important role [11, 12]. The phase equilibrium is determined by the behaviour of each substance in both of its phases, and mixtures with azeotrope formation or those with a miscibility gap, to name a few, are characteristic cases which frequently occur in engineering applications. For these reasons a multicomponent mixture exhibits a transfer behaviour which in most cases deviates

clearly from that of single component flow. Therefore, as a general rule it is necessary to develop a corresponding model.

In general, practical problems are much too complex to be treated theoretically. In order to analyse these problems, specific aspects are isolated or simplifications are made. Fully developed flow [4, 5] constant thermophysical properties [2, 4, 5], pure liquid phase, and single or two-component gas phases [2-10] are among the assumptions made. In some cases, integral balances have been combined with empirical correlations [5]. Such restrictions certainly are relevant to special flows, but these models and their results have limited practical use. Moreover, complex problems cannot be analysed simply by dividing the problem into several smaller more fundamental problems and by adding the results. Sometimes it seems that simplifications in the physical model have arisen not so much as a result of knowledge about the physico-chemical correlations but have arisen due to the necessity of making the physical model suit further theoretical developments.

In determining flow variables like evaporation velocity and wall temperature, either experimental investigations were to be made [6-8, 11] or numerical methods had to be implemented [6-12] in order to obtain the exact solutions to the transport equations. Because the crucial physical processes occur directly along the wall surface, the boundary-layer equations can be used as the governing equations. In the gas phase the complete boundary-layer equations must be

NOMENCLATURE	
c_k, c_1, c_2 concentration of component k, 1, 2; ρ_k/ρ c_p specific isobaric heat capacity	y wall distance [m] z axial coordinate [m].
g_n gravity constant [m s -] Δh_v latent heat of evaporation [kJ kg - 1] M, M_k molecular weight of mixture, component k [kmol kg - 1] m mass flux density [kg s - 1 m - 2] p pressure [bar] Pr, Pr_t Prandtl number, turbulent Prandtl number \mathring{q} heat flux density [kW m - 2] r radial coordinate [m] r_0 pipe radius [m]	Greek symbols δ_L film thickness [m] λ thermal conductivity [W m ⁻¹ K ⁻¹] μ dynamic viscosity [N s m ⁻²] ν kinematic viscosity [m ² s ⁻¹] ν_t eddy viscosity [m ² s ⁻¹] ν_t^+ ν_t/ν ρ density [kg m ⁻³] τ shear stress [N m ⁻²].
Re_0, Re_z Reynolds number based on r_0 , and on z Sc_k, Sc_1 Schmidt number of component k, turbulent Schmidt numberTtemperature [K]uaxial velocity [m s ⁻¹]vradial velocity [m s ⁻¹]xmole fraction in liquid phase	Subscripts e boundary-layer edge, centreline I gas-liquid interface k, 1, 2, 3 component k, 1, 2, 3 L liquid phase t turbulent w wall 0 inlet.

solved whereas in the liquid film phase, the convection terms can be dropped so that a Nusselt-type model can be applied [10, 12]. More elaborate models for evaporating liquid film flow were presented for both laminar [6, 8, 11] and turbulent [7-10, 12] gas flow, and in most cases the gas flow was modelled in detail [6-12]. In these models, however, the liquid film was at rest [6-9, 11]. A study concerning the evaporation of mixtures in laminar gas flow by Metz [11] expanded Splettstößer's model [6] to include binary liquid films and established for similarity solutions a constant wall temperature which strongly depends on the mixture composition. Similar results were found in Baumann [12], who investigated the evaporation of moving binary liquid films in turbulent gas flow. The change in composition due to different evaporation rates for the different components results in a change of wall temperature in the flow direction.

The aim of this work is to investigate the effect of the mixture upon the characteristic flow variables in tubular flow. The evaporation of hydrocarbon-alcohol mixtures into a gas phase consisting of hydrocarbon, alcohol, and air is numerically analysed. Emphasis is placed on the effects which result when the alcohol component is added to the pure hydrocarbon liquid. The model equations are solved by a solution procedure which consists of a combination of efficient numerical techniques.

2. PHYSICAL MODEL

2.1. Governing equations

The annular flow of a laminar two-component liquid film in a vertical tube with prescribed heat flux

through the wall is considered here. As shown in Fig. 1 the liquid evaporates into a hot turbulent air stream and forms a boundary layer along the film. The surface of the film is smooth, and secondary effects such



FIG. 1. Scheme of the boundary-layer flow along an evaporizing binary liquid film in a vertical tube.

as thermal diffusion, radiation, and surface tension are negligible. The turbulent flow of a ternary gas mixture is described in the (z, r)-coordinate system by the continuity equation and the balances for momentum, energy, and species concentrations

$$\frac{\partial}{\partial z}(r\rho u) + \frac{\partial}{\partial r}(r\rho v) = 0 \tag{1}$$

$$\rho\left(u\frac{\partial u}{\partial z} + v\frac{\partial u}{\partial r}\right) = -\frac{\mathrm{d}p_{\mathrm{e}}}{\mathrm{d}z} + \frac{1}{r}\frac{\partial}{\partial r}\left[r\mu(1+v_{\mathrm{t}}^{+})\frac{\partial u}{\partial r}\right]$$
(2)

$$\rho c_{p} \left(u \frac{\partial T}{\partial z} + v \frac{\partial T}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\mu c_{p}}{Pr} \left(1 + v_{t} + \frac{Pr}{Pr_{t}} \right) \frac{\partial T}{\partial r} \right] \\ + \left\{ \left[\frac{\mu c_{p1}}{Sc_{1}} \left(1 + v_{t}^{+} \frac{Sc_{1}}{Sc_{t}} \right) - \frac{\mu c_{p3}}{Sc_{3}} \left(1 + v_{t}^{+} \frac{Sc_{3}}{Sc_{t}} \right) \right] \frac{\partial c_{1}}{\partial r} \\ + \left[\frac{\mu c_{p2}}{Sc_{2}} \left(1 + v_{t}^{+} \frac{Sc_{2}}{Sc_{t}} \right) - \frac{\mu c_{p3}}{Sc_{3}} \left(1 + v_{t}^{+} \frac{Sc_{3}}{Sc_{t}} \right) \right] \frac{\partial c_{2}}{\partial r} \right\}$$
(3)

$$\rho\left(u\frac{\partial c_{k}}{\partial z} + v\frac{\partial c_{k}}{\partial r}\right) = \frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\mu}{Sc_{k}}\left(1 + v_{t}^{+}\frac{Sc_{k}}{Sc_{t}}\right) \times \frac{\partial c_{k}}{\partial r}\right], \quad k = 1, 2 \quad (4)$$

$$c_1 + c_2 + c_3 = 1. \tag{5}$$

Dropping all convection terms in the equations for the shear stress and gravity driven laminar two-component film flow results in a Couette flow approximation. With the assumption of constant properties across the film the analytical solution for the film flow is given by

$$u_{\rm L}(y) = \frac{\rho_{\rm L}g_n\delta_{\rm L}}{\mu_{\rm L}} \left[-\frac{1}{2} \left(\frac{y}{\delta_{\rm L}} \right)^2 + \left(\frac{y}{\delta_{\rm L}} \right) \left(1 - \frac{\tau_{\rm I}}{\rho_{\rm L}g_n\delta_{\rm L}} \right) \right]$$
(6)

$$T_{\rm L}(y) = T_{\rm I} - \frac{\dot{q}_{\rm w} \delta_{\rm L}}{\lambda_{\rm L}} \left(1 - \frac{y}{\delta_{\rm L}}\right) \tag{7}$$

$$c_{1L}(y) = c_{1LI} = \text{const.}$$
(8)

These solutions contain the unknown interfacial values of temperature T_1 , species concentration c_{1L1} , and shear stress τ_1 . They result from the solution of the basic equations in the gas flow. The film thickness δ_L is calculated by integration of the velocity profile (6) using the continuity equation.

The turbulence model applied is an algebraic eddyviscosity model which accounts for interfacial mass transfer and pressure gradient. Following Cebeci and Chang [13] the model is used in its well-known formulation in the entrance region. Further downstream, Nikuradse's empirical mixing length expression together with van Driest's damping factor are applied. The transition from the boundary-layer interaction region to the fully developed region is covered by an empirical expression. For further details of the turbulence model the reader is referred to refs. [12, 13]. The turbulent Schmidt and Prandtl numbers used are $Sc_t = Pr_t = 0.9$.

2.2. Boundary conditions

The solution of the governing equations for the film flow, equations (6)-(8), already include the boundary conditions at the tube wall

$$y = 0(\triangleq r = r_0): \quad u_{\rm L} = 0, \quad v_{\rm L} = 0,$$
$$-\lambda_{\rm L} \frac{\partial T_{\rm L}}{\partial y} = \dot{q}_{\rm w}, \quad \frac{\partial c_{k\rm L}}{\partial y} = 0. \tag{9}$$

At the inlet the liquid has a prescribed mass flux \dot{m}_0^+ and concentration c_{1L0} . The temperature T_{L0} is set according to the thermal equilibrium at the inlet. Equation (6) with the condition of vanishing interfacial shear stress is used as the initial velocity profile in the liquid film. The gas flow is parallel with the given velocity, temperature, and species concentrations

$$x = 0: \quad u = u_0, \quad T = T_0, \quad c_k = c_{k0}, \quad k = 1, 2.$$
(10)

The unknowns at the gas-liquid interface, especially the temperature, vary in the streamwise direction. Since the film is very thin $(\delta_L/r_0 \ll 1)$ the displacement effect on the gas flow is neglected

$$r = r_0$$
: $u = u_1(z), v = v_1(z),$
 $T = T_1(z), c_k = c_{k1}(z), k = 1, 2.$ (11)

For the boundary conditions at the boundary-layer edge two regions are distinguished: the entrance region with a finite potential core, and the so-called developed region where the boundary layers have merged at the centreline. In the entrance region the values of temperature and species concentrations are those of the inlet. The velocity is constant across the potential core and for the present is an unknown function of the streamwise coordinate

$$0 \le r \le r_{e}: \quad u = u_{e}(z), \quad T = T_{0},$$

$$c_{k} = c_{k0}, \quad k = 1, 2. \tag{12}$$

In the developed region all unknowns vary in the streamwise direction. Because of symmetry it is required that

$$r = 0: \quad \frac{\partial u}{\partial r} = 0, \quad \frac{\partial T}{\partial r} = 0,$$
$$\frac{\partial c_k}{\partial r} = 0, \quad k = 1, 2, \quad u = u_e(z). \tag{13}$$

The centreline velocity u_e is determined by integration of the continuity equation over the gas flow which results in

$$\int_{0}^{r_{0}} r\rho u \, \mathrm{d}r - \frac{r_{0}^{2}}{2} \rho_{0} u_{0} + \int_{0}^{z} r\rho_{1} v_{1} \, \mathrm{d}z = 0.$$
 (14)

The interfacial balances for the unknown values of velocities u_1 , v_1 , temperature T_1 , and species concentrations c_{k1} are given by the continuity of mass flux, heat flux, and momentum flux

$$(\rho v)_1 + \left[\frac{\mu}{Sc_3(1-c_1-c_2)}\left(\frac{\partial c_1}{\partial r} + \frac{\partial c_2}{\partial r}\right)\right]_1 = 0 \quad (15)$$

$$(\mathring{m}_{11} + \mathring{m}_{21})\Delta h_{\rm v} - \left[\lambda \frac{\partial T}{\partial r}\right]_{\rm I} - \mathring{q}_{\rm w} = 0 \qquad (16)$$

$$\tau_{\rm L} = \mu \frac{\partial u}{\partial r} = \tau_{\rm I}. \tag{17}$$

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Here \dot{m}_{k1} denotes the mass flux density of component k

$$\hat{m}_{k1} = -\left(\frac{\mu}{Sc_k}\frac{\hat{c}c_k}{\hat{c}r}\right)_{l} + (\rho_k v)_{l}, \quad k = 1, 2.$$
 (18)

The mass balances in the liquid for the evaporating components k together with mass flux conservation across the interface $d\vec{m}_k^+/dz = \vec{m}_{k1}$ yield the current liquid composition

$$c_{k \perp I} = \dot{m}_{k}^{+} / (\dot{m}_{1}^{+} + \dot{m}_{2}^{+}); \quad x_{k \perp I} = c_{k \perp I} \frac{M}{M_{k}};$$
$$\frac{1}{M} = \frac{c_{1 \perp I}}{M_{1}} + \frac{c_{2 \perp I}}{M_{2}}.$$
(19)

The interfacial concentrations c_{k1} in the gas phase are calculated from the phase equilibrium at the interface $p_{k1} = p_{k1}(x_{k11}, T_1)$ according to

$$c_{11} = \frac{p_{11}}{p_{11} + p_{21} \frac{M_2}{M_1} + (p_e - p_{11} - p_{21}) \frac{M_3}{M_1}}.$$
 (20)

A similar relationship holds for the second component.

In the post-dryout region where the film is completely evaporated the boundary conditions (9) at the tube wall apply for the gas flow.

2.3. Thermophysical properties

The thermophysical properties of the ternary ideal gas mixture and the binary liquid mixture depend on temperature and concentrations. They are calculated from the pure component data by means of mixing rules applicable to any multicomponent mixture. The pure component and phase equilibrium data are taken from various data compilations and are approximated by polynomials in terms of temperature for a fixed pressure of p = 1 bar. For further details of the thermophysical properties see ref. [12].

2.4. Numerical solution procedure

In the solution method a coordinate transformation and a stream function are applied. A marching procedure in the streamwise direction leads to a set of coupled ordinary differential equations which are subject to a set of strongly coupled interfacial balances and unknown boundary conditions. Starting with first estimates for the boundary conditions, the overall solution method corrects these values until all balances are fulfilled. The most important feature of this iterative method is an efficient Newton-Chord variational procedure for the determination of the temperature at the gas-liquid interface. For a detailed description of the numerical approach the reader is referred to ref. [12].

3. RESULTS

In order to show the influence of liquid mixtures on the characteristics of heat and mass transfer in twophase multicomponent film flow, the evaporation of fuel-like liquid benzene-methyl alcohol mixtures into a hot air stream is investigated. The following sets of initial conditions are chosen:

inlet temperature	$T_0 = 373$ and 573 K, resp.
Reynolds number	$Re_0 = 64240$ and 31020 ,
	resp.
liquid feed	$m_0^+ = 100 \text{ g m}^{-1} \text{ s}^{-1}$
feed concentration	$c_{1L0} = 0.70, \ldots, 1.00$
wall heat flux	$\dot{q}_{u} = 0$
transition to turbulence	$\xi_{\rm tr} = 0.06$ and 0.16, resp.

The quantities of interest in film evaporation applications are heat and mass transfer rates as well as wall temperature levels. The present investigation clearly indicates the strong influence of the mixture composition. The phase equilibrium of the azeotropic benzene-methyl alcohol mixture plays a major role in the immediate vicinity of the gas-liquid interface. Figure 2 shows the vapour pressure of the mixture as a function of the liquid composition for a fixed interfacial temperature T_1 of 293 K. For various inlet



FIG. 2. Vapour pressure of components and mixture for benzene (1) and methanol (2) at 293 K and 1 bar.



FIG. 3. Interfacial temperature vs liquid composition for various inlet temperatures, adiabatic wall condition, and laminar flow (similarity solutions).

temperatures T_0 , Fig. 3 depicts the influence of c_{1L0} on T_1 which results from the solution of the coupled system of equations for fixed mixture composition, adiabatic wall condition, and laminar flow. Similarity solutions exist for this case, where the liquid film is at rest, and the results agree with those of Metz [11]. Two effects are evident. The first is the strong influence that small portions of the second component have on the phase equilibrium. The vapour pressure nearly doubles when adding about 10% alcohol to pure benzene. The second is the major decrease in temperature at the interface by about 15 K for the same case. Likewise T_0 directly affects T_1 , and to achieve the same temperature change, $\Delta T_{\rm I} = 15$ K, T_0 must change by about 150 K. Therefore, mixtures with a vapour pressure maximum such as benzene-methyl alcohol, or others with a vapour pressure minimum are well suited for controlling evaporation processes which rely on exact temperature levels as in the case of evaporation cooling.

Figures 4 and 5 show the interfacial heat and mass flux, respectively, as functions of the mixture com-



FIG. 5. Interfacial mass flux vs liquid composition for different inlet temperatures, adiabatic wall condition, and laminar gas flow (similarity solutions).

position for various temperatures T_0 . For similarity solutions these values are independent of the position along the tube when multiplied by $Re_2^{0.5}$. Both fluxes increase as expected with increasing temperature of the inlet flow although the Reynolds number weakens this tendency in these particular figures. With higher alcohol concentration c_{1L0} , the heat flux increases only slightly and the mass flux decreases significantly such that its change is about 50% for methanol concentrations up to 30% ($c_{1L0} = 0.70$). One factor involved here is the improved heat conductivity of the gas due to the presence of alcohol. Another point is the high amount of heat required to evaporate the alcohol due to its much larger heat of evaporation.

Figures 6 and 7 show the heat flux and mass flux rates in turbulent gas flow for the evaporation of a liquid mixture having a composition which changes in the axial direction due to the transport processes. All curves terminate at the end of the liquid film. Starting for example with a mixture of 20% methanol, the more volatile alcohol evaporates more predominantly such that the benzene concentration in



FIG. 4. Interfacial heat flux vs liquid composition for different inlet temperatures, adiabatic wall condition, and laminar gas flow (similarity solutions).



FIG. 6. Local interfacial heat flux for various liquid feed compositions and inlet temperatures for adiabatic evaporation in turbulent gas flow.



FIG. 7. Local interfacial mass flux for various liquid feed compositions and inlet temperatures for adiabatic evaporation in turbulent gas flow.

the film increases. The state of the mixture is shown in the phase equilibrium diagram and changes as indicated by the arrow (Fig. 2). In the region where the film consists of about 90% benzene, the partial pressure of the methanol decreases significantly causing a corresponding decrease in the total vapor pressure. As can be seen by the results of the interfacial heat flux along the tube axis (Fig. 6), the mixture composition influences the heat transfer only slightly. This was already evident in Fig. 4. This means that more benzene evaporates for about the same heat flux. Due to the large differences in the heats of evaporation of the two components, the benzene mass flux increases comparatively much more than the alcohol concentration decreases (see Fig. 5). This is manifested by a local maximum in the plot of the total mass flux at the interface in Fig. 7. Similar plots result when starting with other mixture compositions. With a higher alcohol concentration, the resulting peak shifts further downstream and becomes more prominent, and the wetted length of the tube is increased. In the regions approaching the dryout point all curves in Figs. 6 and 7 asymptotically tend towards that of pure benzene. The local effects described clearly indicate the distinction between the evaporation of a mixture and that of pure benzene, and these effects are not limited to just the substances investigated here. They also affect the mass flux averaged across the tube length because even this value increases near the peak. This is again in contrast to the behaviour of pure benzene.

Subsequently, it is very important to pay attention to the real behaviour of two-phase multicomponent flows and to model them properly, especially regarding the design, computation, and optimization of practical flow problems.

4. CONCLUDING REMARKS

For the two-phase multicomponent flow in twocomponent liquid film evaporation a physical model has been proposed. It especially accounts for the phase equilibrium of binary liquids and for multicomponent thermodynamics. The model is evaluated by means of an efficient numerical procedure with the Newton– Chord variational method being the most valuable technique. The application to the annular flow of evaporating liquid benzene–methanol mixtures clearly demonstrates that small portions of a second component in the liquid film can create significant changes in the temperature levels as well as in the heat and mass transfer. The results indicate that detailed physical models and efficient solution procedures are important for the investigation of such complex flows.

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TRANSFERT DE MASSE ET DE CHALEUR DANS UN ECOULEMENT AVEC EVAPORATION D'UN FILM LIQUIDE A DEUX COMPOSANTES

Résumé—On considère l'écoulement gazeux turbulent à plusieurs composantes avec évaporation d'un film liquide à deux composantes. Pour modéliser en détail les processus de transport, on étudie particulièrement l'équilibre de phase des liquides binaires et des multicomposantes thermodynamiques. La méthode numérique pour résoudre les équations couplées de bilan reliées avec les conditions limites et les conditions d'interface, est basée sur une procédure de variation pour la détermination de la température à l'interface gaz-liquide. Le calcul de l'évaporation de mélanges benzène-méthanol dans un écoulement tubulaire d'air chaud montre clairement l'influence de l'équilibre de phase et son interaction avec le processus de transport local. Même des petites parties d'une seconde composante peuvent conduire à des changements significatifs dans le transfert de masse et de chaleur. Cela souligne l'importance de modèles physiques détaillés et des procédés de résolution efficaces.

WÄRME- UND STOFFÜBERGANG BEI DER VERDUNSTUNGSSTRÖMUNG VON BINÄREN FLÜSSIGKEITEN

Zusammenfassung—Es wird die turbulente Mehrkomponenten-Gasströmung mit Verdunstung eines binären Flüssigkeitsfilms betrachtet. Bei der detaillierten Modellierung der Transportprozesse werden insbesondere das Phasengleichgewicht binärer Flüssigkeiten und die Mehrkomponenten-Thermodynamik berücksichtigt. Das numerische Verfahren zur Lösung der gekoppelten Bilanzgleichungen in Verbindung mit den Phasengrenzflächen- und Randbedingungen basiert auf einem Variationsverfahren zur Bestimmung der Temperatur an der Phasengrenze. Die Berechnung der Verdunstung von Benzol-Methanol-Mischungen in eine Heißluft-Rohrströmung zeigt deutlich den Einfluß des Phasengleichgewichts und seines Zusammenwirkens mit den lokalen Transportvorgängen. Selbst geringe Anteile einer zweiten Komponente können beträchtliche Änderungen im Wärme- und Stoffübergang bewirken. Dies unterstreicht die Bedeutung von detaillierten physikalischen Modellen und effizienten Lösungsverfahren.

тепло- и массоперенос при пленочном течении испаряющейся бинарной жидкости

Авиотация — Исследуется турбулентное течение многокомпонентного газа при испарении пленки двухкомпонентной хидкости. При моделировании процессов переноса особое внимание уделяется фазовому равновесию бинарных жидкостей и термодинамике многокомпонентных систем. Применяющийся численный метод позволяет решить систему уравнений с соответствующими граничными условиями, в том числе и с условиями на межфазной границе. Способ решения основан на вариационном методе. Вычисления, проведенные для испарения смесей бензола и метанола при течении воздуха в цилиндре, ясно иллюстрируют эффект фазового равновесия и его взаимодействие с процессами локального переноса. Существование даже малых долей второго компонента может привести к значительным изменениям тепло- и массопереноса, что подтверждает важность детальных физических моделей и эффективных методов решения.