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Dynamic model of a film absorber with coupled heat and mass transfer

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Abstract—The model describes the transient behaviour of a cooled film absorber with coupled heat and mass transfer, using a binary mixture with only one volatile component. The description consists of a set of seven coupled partial and ordinary differential equations for the temperature of a cooling medium, wall, mixture and vapour, for the film mass flow rate and concentration as well as for the vapour pressure. Output responses on a step change at the absorber inlet of the cooling water temperature, the vapour mass flow rate and the mixture mass fraction are shown. The model can be used in a general absorption cycle simulation program, to describe any film component (evaporator, condenser, heat exchanger, absorber, desorber).

INTRODUCTION

AN ABSORPTION cycle [1, 2] is a thermodynamic engine, driven by thermal energy, that transports heat from a certain temperature to a higher temperature. Absorption cycles form an alternative for the mechanically driven compression cycles. They can be used for heating and cooling purposes. When used as a heat pump, an absorption cycle is an alternative for a conventional boiler, with a higher energy efficiency. An absorption heat transformer is a means to upgrade waste heat without addition of extra thermal energy. A combination of the absorption and the compression cycle, the hybrid cycle, find increasing interest nowadays.

For the stationary situation general solutions for film absorption in laminar [3] or turbulent flow [4] have been published. The literature on the instationary state is scarce, although there are some good reasons to study the transient behaviour of an absorption cycle.

First, in the process industry a tendency is seen towards the use of more compact apparatus, with higher mass and energy flow densities. A means to establish this is by replacing the conventional shell and tube exchangers by more compact and efficient plate or plate-fin exchangers [5–7]. For absorption cycles it is expected that future machines are equipped with compact exchangers [8]. Also, to obtain higher energy efficiency, more complex cycles are developed like the double- and triple-effect cycle [9]. These developments lead to more severe requirements for control strategies and safety measures. Dynamic models are required to meet these demands in the design stage.

The sensitivity of the exergy efficiency of the absorber (and desorber) to variations in temperature difference over the component is a second reason to use dynamic models in the design stage: to estimate and minimize exergy losses under fluctuating conditions [10]. Fluctuating conditions are met when on/off control is utilized (e.g. hybrid cycle, gas-fired boiler), or when the heat demand or supply is not constant (e.g. absorption cycle coupled to a batch process, solar powered units).

A second application of our absorber model is found in parameter identification. We will show in this paper that, analogous to the transient determination of the heat transfer coefficient for compact heat exchangers [11], the mass transfer coefficient in the absorber can be determined from the transient behaviour. A straightforward determination of the mass transfer coefficient from stationary absorber input and output data is impossible when the heat and mass transfer are coupled.

In dynamic absorber models two extremes are possible. The first is the simple lumped parameter model [12, 13]: the absorber is considered as one lump and rigorous simplifications are made to deal with the vapour absorption. The second extreme describes the absorber with a set of coupled two-dimensional partial differential equations for film velocity, temperature and mass fraction. In ref. [14] this kind of description is used for a film evaporator. Because there are up till now no established models that are able to describe film flow characteristics over a large

NOMENCLATURE

A	coefficient in interface thermodynamic equilibrium relation $[\mathrm{K}]$
B	coefficient in interface thermodynamic equilibrium relation $[\mathrm{K\,m^2\,N^{-1}}]$
c_p	specific heat at constant pressure $[\mathrm{J\,kg^{-1}\,K^{-1}}]$
C	coefficient in interface thermodynamic equilibrium relation $[\mathrm{K}]$
D	mass diffusivity $[\mathrm{m^2\,s^{-1}}]$
E	factor in the equation of state, ZR/M_vV $[\mathrm{K^{-1}\,s^{-1}}]$
f	factor in film thickness relation, $(g/3\mu\rho_m)^{1/3}$ $[\mathrm{m^{1/3}\,s^{1/3}\,kg^{2/3}}]$
g	gravitational acceleration $[\mathrm{m\,s^{-2}}]$
G	factor in absorbed mass flow relation, $((1-w^*)A)/\rho_m k-(\Delta h/\alpha^*)$ $[\mathrm{K\,s\,m^2\,kg^{-1}}]$
h	enthalpy $[\mathrm{J\,kg^{-1}}]$
Δh	heat of absorption, $h^v-[h_m+(1-w)\phi_w]$ $[\mathrm{J\,kg^{-1}}]$
J	dimensionless mass flow rate per unit width, $\Gamma_m/\Gamma_{m,0}$
k	mass transfer coefficient $[\mathrm{m\,s^{-1}}]$
L	absorber length $[\mathrm{m}]$
m	mass per unit width $[\mathrm{kg\,m^{-1}}]$
m''_v	absorbed mass flow rate per unit width $[\mathrm{kg\,m^{-2}\,s^{-1}}]$
M_v	molar vapour mass $[\mathrm{kg\,mol^{-1}}]$
N	constant in dimensionless equations (1*)–(19*)
p	vapour pressure $[\mathrm{N\,m^{-2}}]$
P	dimensionless pressure, $(p-p_0)/(p_e-p_0)$
p_e	equilibrium pressure at T_0 and w_0, $(T_0-A_0w_0-C_0)/B_0$ $[\mathrm{N\,m^{-2}}]$
q	heat flow per unit width $[\mathrm{W\,m^{-1}}]$
R	universal gas constant $[\mathrm{J\,mol^{-1}\,K^{-1}}]$
t	time $[\mathrm{s}]$
T	temperature $[\mathrm{K}]$
T_e	equilibrium temperature at w_0 and p_0, $A_0w_0+B_0p_0+C_0$ $[\mathrm{K}]$
u	dimensionless velocity of propagation
v	dimensionless factor accounting for property variation with x and t
V	vapour volume per unit width $[\mathrm{m^3\,m^{-1}}]$
w	mass fraction of the volatile component $[\mathrm{kg\,kg^{-1}}]$
w_e	equilibrium mass fraction at T_0 and w_0, $(T_0-B_0p_0-C_0)/A_0$ $[\mathrm{kg\,kg^{-1}}]$
x	coordinate along the wall $[\mathrm{m}]$
X	dimensionless coordinate along the wall, x/L
y	coordinate perpendicular to the wall $[\mathrm{m}]$
z	arbitrary dimensionless quantity of state
Z	compressibility factor.

Greek symbols

α	heat transfer coefficient $[\mathrm{W\,m^{-2}\,K^{-1}}]$
γ	dimensionless mass fraction, $(w-w_0)/(w_e-w_0)$
Γ	mass flow rate per metre width $[\mathrm{kg\,m^{-1}\,s^{-1}}]$
δ	thickness $[\mathrm{m}]$
θ	dimensionless temperature, $(T-T_0)/(T_e-T_0)$
μ	dynamic viscosity $[\mathrm{kg\,m^{-1}\,s^{-1}}]$
ρ	density of the liquid $[\mathrm{kg\,m^{-3}}]$
τ	dimensionless time, $(t/L)(\Gamma_{m,0}/\rho_{m,0}\delta_{m,0})$
ϕ_w	derivative of h with respect to w at constant T, $\partial h/\partial w$ $[\mathrm{J\,kg^{-1}}]$
ϕ_p	derivative of h with respect to p at constant T, $\partial h/\partial p$ $[\mathrm{J\,kg^{-1}}]$.

Subscripts

0	reference quantity
1, 2	component 1 or 2
c	cooling medium
d	delay
i	inlet
j	position coordinate in computational grid
m	mixture
o	outlet
r	relaxation
v	vapour
w	wall.

Superscripts

n	time coordinate in computational grid
*	interface.

range of the flow rate, this kind of model also gives a failing description, despite its complexity. Our model falls in between these two extremes, it considers the film thickness averaged values of the velocity, temperature and concentration, leading to a description with a set of coupled one-dimensional partial differential equations. An advantage of our model over existing models like ref. [15], describing a complete NH_3/H_2O absorption heat pump, is that it also takes the dynamics of the system pressures and the film thickness or liquid mass at a certain position into account.

In a simple absorption system heat is taken up from or released to the environment of the system at three temperature levels. A disturbance in the low temperature heat input is felt in the absorber as a change in the vapour mass flow rate. A change in the medium temperature heat output leads to a change in cooling medium input temperature. A disturbance in the high temperature heat input is transferred to the absorber as a change in the mixture input concentration (assuming the temperature change to be damped away by the mixture heat exchanger). The responses on step changes in these three inputs are shown. The simulations confirm that the transient behaviour of the pressure is an essential part of the description of the absorber. Because the transient behaviour of the film thickness is also part of the description, our model not only is fit to describe an absorber and a stripper, but also to describe a condenser and an evaporator [16, 17]. This means that the model can be used in a general absorption cycle simulation program as a basic subroutine, able to describe any film component (evaporator, condenser, heat exchanger, absorber, desorber).

MODEL

In Fig. 1 a schematic representation of the film absorber is given, showing the geometry, the input and output variables and the direction in which flows are taken as positive. In the absorber a mixture of two components flows down a flat plate as a thin liquid film. Only one of these components is present in the vapour phase. The mixture absorbs this volatile component. The heat of absorption released at the liquid–vapour interface is transported through the film and the wall towards a cooling medium flowing at the other side of the plate. Because of this the cooling medium leaves the absorber at a temperature $T_{c,o} > T_{c,i}$. At the exit, the mass fraction w_o of the volatile component in the mixture is larger than w_i.

Our model starts from the following assumptions.

(1) Heat conduction in the tangential direction in the cooling medium as well as in the wall is negligible.

(2) The mixture is a Newtonian fluid and flows under the influence of only gravity and friction at the wall.

(3) The fluid is a binary mixture of two components, only one of these components is present in the vapour phase.

(4) Heat and mass transfer in the film is only by heat and mass diffusion perpendicular to the direction of flow and by convection in the direction of flow.

(5) At the liquid–vapour interface thermo-dynamic equilibrium exists between liquid and vapour.

(6) All heat of absorption is released at the liquid–vapour interface.

(7) There is no heat transfer to the vapour. The vapour pressure does not vary within the absorber.

(8) Stationary state correlations for the film thickness (or velocity) and heat and mass transfer coefficients give valid results in transient responses.

Our model allows the thermodynamic and physical properties of the cooling medium, mixture and vapour, as well as the heat and mass transfer coefficients, to vary with space and time. This makes the model description valid over an arbitrary temperature, mass fraction and pressure range, as is desired to simulate start-up and shut-down behaviour. The variability of the properties leads to extra dimensionless terms in some of the equations. For reasons of clarity these terms are abbreviated to v_1, v_2, etc. In the Appendix these terms are worked out. If the properties are assumed constant all these v-terms vanish.

Under assumption (1) the heat balance for the cooling medium, flowing along a plate of unit width, is given by

$$\frac{\partial T_c}{\partial t} + \frac{v_1 \Gamma_c}{\rho_c \delta_c} \frac{\partial T_c}{\partial x} = \frac{v_1 \alpha_c}{\rho_c c_{p,c} \delta_c} (T_w - T_c). \quad (1)$$

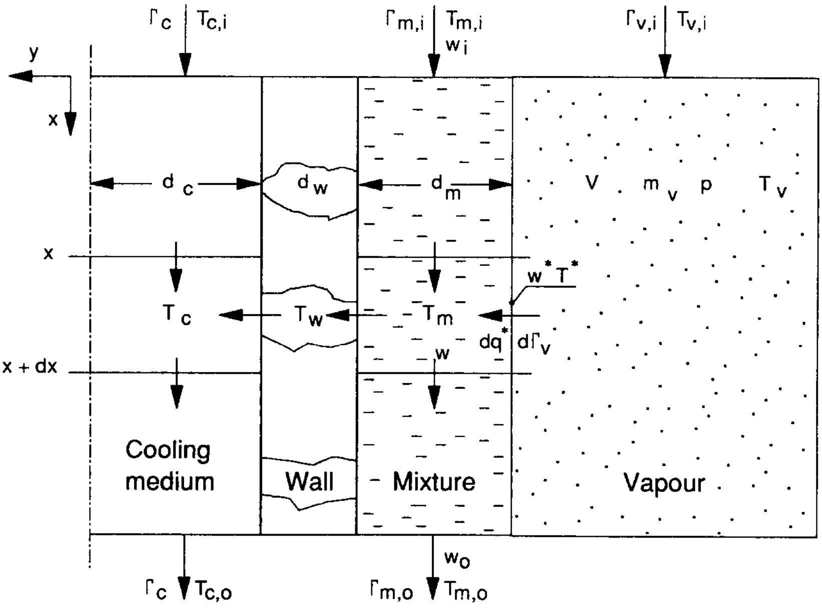

FIG. 1. Geometry of the film absorber, giving the directions in which the flows are taken positive.

This hyperbolic partial differential equation is an example of the transport equation. The velocity of propagation is given by $v_1\Gamma_c/(\rho_c\delta_c)$; the factor $\rho_c c_{p,c}\delta_c/(v_1\alpha_c)$ is a time constant, a kind of relaxation time. Under assumption (1) the heat balance for the wall is given by

$$\frac{\partial T_w}{\partial t}=\frac{\alpha_m}{\rho_w c_{p,w}\delta_w}(T_m-T_w)-\frac{\alpha_c}{\rho_w c_{p,w}\delta_w}(T_w-T_c). \tag{2}$$

The mass balance of the liquid film is expressed by

$$\frac{\partial(\mathrm{d}m_m)}{\partial t}=\mathrm{d}\Gamma_v-\frac{\partial\Gamma_m}{\partial x}\mathrm{d}x. \tag{3}$$

In our final description of the heat and mass transfer in the liquid film we only want the average values of film temperature and mass fraction to be explicitly present. Of course the temperature and mass fraction vary in the y-direction. The resulting heat and mass transfer across the film is described by transfer coefficients α and k. With the aid of equations (4)–(7), the interface conditions can be expressed in the mean film temperature T_m, the mean mass fraction w and the vapour pressure p

$$\mathrm{d}\Gamma_v=\frac{\rho_m k}{1-w^*}(w^*-w)\,\mathrm{d}x. \tag{4}$$

In the denominator of equation (4) a factor $1-w^*$ is present because at the film interface the diffusion is not equimolar [18]. If the mixture components are labelled 1 and 2, component 1 being the volatile component, then only component 1 can cross the interface according to assumption (3). For this reason from the general expression for the mass flow of component 1

$$\mathrm{d}\Gamma_1=-\rho D\frac{\partial w_1}{\partial y}+w_1(\mathrm{d}\Gamma_1+\mathrm{d}\Gamma_2)$$

a factor $1-w_1$ can be split off, because $\mathrm{d}\Gamma_2=0$ at the interface. According to assumption (6) the heat of absorption Δh is released at the interface

$$\mathrm{d}q^*=\mathrm{d}\Gamma_v\Delta h. \tag{5}$$

The heat flow from the interface to the bulk is described by

$$\mathrm{d}q^*=\alpha^*(T^*-T_m)\,\mathrm{d}x. \tag{6}$$

If the vapour pressure varies slow enough [19] to let assumption (5) be valid, the Clapeyron–Clausius equation describes the thermodynamic equilibrium between a liquid and its vapour phase. We linearize this equation to

$$T^*=Aw^*+Bp+C. \tag{7}$$

With equations (4)–(7) $\mathrm{d}m_v''$ can be expressed in T_m, w and p

$$\mathrm{d}m_v''=\frac{\mathrm{d}\Gamma_v}{\mathrm{d}x}=\frac{T_m-Aw-B\rho-C}{[(1-w^*)A/\rho_m k]-(\Delta h/\alpha^*)}=\frac{T_m-Aw-B\rho-C}{G}. \tag{8}$$

Mostly the value of G is not affected very much if w^* is replaced by w or even by w_0 (if the properties are assumed constant). Equation (8) is a crucial equation in our description. It couples the behaviour of the film and the vapour variables. The denominator of the equation reflects the coupling between heat and mass transfer in absorption: both the heat and the mass transfer coefficients are present in the expression.

The mass $\mathrm{d}m_m$ in equation (3) can be expressed in terms of the film thickness δ_m

$$\mathrm{d}m_m=\rho_m\delta_m\,\mathrm{d}x. \tag{9}$$

Under assumption (2), ref. [20] gives a general relation between the film thickness and mass flow rate

$$\delta_m=a\left(\frac{v^2}{g}\right)^{1/3}\left(\frac{4\Gamma_m}{\rho_m v}\right)^b=\left(\frac{av^{2/3-b}4^b}{g^{1/3}\rho_m^{b-1}}\right)\frac{\Gamma_m^b}{\rho_m}=\frac{\Gamma_m^b}{\rho_m f} \tag{10}$$

together with experimental and theoretical values for a and b in the case of laminar, laminar-wavy and turbulent flow. The mass balance of the volatile component in the film is given by

$$\mathrm{d}m_m\frac{\partial w}{\partial t}+w\frac{\partial(\mathrm{d}m_m)}{\partial t}=\mathrm{d}\Gamma_v-\Gamma_m\frac{\partial w}{\partial x}\mathrm{d}x-w\frac{\partial\Gamma_m}{\partial x}\mathrm{d}x. \tag{11}$$

By elimination of $\mathrm{d}m_m$ with equations (3) and (9), of δ_m with equation (10) and by substitution of equation (8), equation (11) can be written as

$$\frac{\partial w}{\partial t}+f\Gamma_m^{1-b}\frac{\partial w}{\partial x}=\frac{(1-w)f}{\Gamma_m^b}\frac{T_m-Aw-Bp-C}{G}. \tag{12}$$

The thermodynamics of the liquid film can be described by an enthalpy balance. Under assumption (4) the enthalpy balance is given by

$$\mathrm{d}m_m\frac{\partial h_m}{\partial t}+h_m\frac{\partial(\mathrm{d}m_m)}{\partial t}=\mathrm{d}\Gamma_v h_v-\Gamma_m\frac{\partial h_m}{\partial x}\mathrm{d}x-h_m\frac{\partial\Gamma_m}{\partial x}\mathrm{d}x-\alpha_m(T_m-T_w)\,\mathrm{d}x. \tag{13}$$

The derivatives of h_m can be reduced to derivatives of the measurable quantities T_m, w and p, by taking the total derivative of h_m, and realizing that the partial derivatives are $c_{p,m}=\partial h_m/\partial T_m$ and $\phi_w=\partial h_m/\partial w$. The influence of the pressure on the mixture enthalpy is negligible under conditions met in absorption apparatus. For this reason $\partial h_m/\partial p$ terms are neglected in subsequent derivations. After elimination of $\mathrm{d}m_m$ with equations (9), (10) and (3), substitution of the total derivative of h_m and elimination of the derivatives of w with equation (12), using $\Delta h=h_v-h_m-(1-w)\phi_w$

and substituting equation (8), equation (13) transforms to

$$\frac{\partial T_{\mathrm{m}}}{\partial t}+f\Gamma_{\mathrm{m}}^{1-b}\frac{\partial T_{\mathrm{m}}}{\partial x}$$
$$=\frac{f}{c_{p,\mathrm{m}}\Gamma_{\mathrm{m}}^{b}}\left[\left(\frac{\Delta h}{G}T_{\mathrm{m}}-Aw-Bp-C\right)-\alpha_{\mathrm{m}}(T_{\mathrm{m}}-T_{\mathrm{w}})\right]. \tag{14}$$

Now we are going to rewrite the mass balance (equation (3)) in terms of the measurable quantities Γ_{m}, T_{m}, w and p. Using equations (9) and (10), the left-hand side of equation (3) can be developed to

$$\frac{\partial}{\partial t}\left(\frac{\Gamma_{\mathrm{m}}^{b}}{f}\right)\mathrm{d}x=\left(\frac{b}{f}\Gamma_{\mathrm{m}}^{b-1}\frac{\partial\Gamma_{\mathrm{m}}}{\partial t}-\frac{\Gamma_{\mathrm{m}}^{b}}{f^{2}}\frac{\partial f}{\partial t}\right)\mathrm{d}x. \tag{15}$$

Substitution of equations (15) and (8) in equation (3) finally gives as a film mass balance

$$\frac{\partial\Gamma_{\mathrm{m}}}{\partial t}+\frac{f}{b}\Gamma_{\mathrm{m}}^{1-b}\frac{\partial\Gamma_{\mathrm{m}}}{\partial x}$$
$$=\frac{f}{b}\Gamma_{\mathrm{m}}^{1-b}\frac{T_{\mathrm{m}}-Aw-Bp-C}{G}+v_{2}\frac{\Gamma_{\mathrm{m},0}^{2}}{\rho_{\mathrm{m},0}\delta_{\mathrm{m},0}L}. \tag{16}$$

The link between vapour pressure, vapour mass and vapour temperature is given by the following equation of state:

$$p=Z\frac{m_{\mathrm{v}}RT_{\mathrm{v}}}{M_{\mathrm{v}}V}=Em_{\mathrm{v}}T_{\mathrm{v}}. \tag{17}$$

The compressibility factor Z accounts for the deviation from ideal gas behaviour. If Z is computed from a correlation containing two parameters: reduced pressure and temperature, equation (17) is accurate within 4–6% for any vapour [21]. Assumption (7) allows us to represent the vapour phase by only one lump. The mass balance is given by

$$\frac{\partial m_{\mathrm{v}}}{\partial t}=\Gamma_{\mathrm{v,i}}-\int_{0}^{L}\mathrm{d}m_{\mathrm{v}}''\,\mathrm{d}x$$
$$=\Gamma_{\mathrm{v,i}}-\int_{0}^{L}\frac{T_{\mathrm{m}}-Aw-Bp-C}{G}\mathrm{d}x. \tag{18}$$

The enthalpy balance reads, accounting for assumption (7)

$$m_{\mathrm{v}}\frac{\partial h_{\mathrm{v}}}{\partial t}+h_{\mathrm{v}}\frac{\partial m_{\mathrm{v}}}{\partial t}=\Gamma_{\mathrm{v,i}}h(p,T_{\mathrm{v,i}})-h_{\mathrm{v}}\int_{0}^{L}\mathrm{d}m_{\mathrm{v}}''\,\mathrm{d}x. \tag{19}$$

The vapour enthalpy h_{v} is a function of pressure p and temperature T_{v}. Taking the total derivative, with $\partial h_{\mathrm{v}}/\partial p=\phi_{\mathrm{p}}$ and $\partial h/\partial T_{\mathrm{v}}=c_{p,\mathrm{v}}$, and using equations (17) and (18) to eliminate m_{v} and its derivative, equation (19) transforms to

$$\frac{\partial T_{\mathrm{v}}}{\partial t}=\frac{ET_{\mathrm{v}}\Gamma_{\mathrm{v,i}}}{p}v_{3}(T_{\mathrm{v,i}}-T_{\mathrm{v}})-\frac{\phi_{p}}{c_{p,\mathrm{v}}}\frac{\partial p}{\partial t}. \tag{20}$$

With the total derivative after t of equation (17) and using equation (20), from equation (18) an equation for p is derived

$$\frac{\partial p}{\partial t}=\frac{E}{\left(1+\dfrac{p\phi_{p}}{T_{\mathrm{v}}c_{p,\mathrm{v}}}\right)}\left\{\Gamma_{\mathrm{v,i}}[v_{3}(T_{\mathrm{v,i}}-T_{\mathrm{v}})+T_{\mathrm{v}}]\right.$$
$$\left.-T_{\mathrm{v}}\int_{0}^{L}\frac{T_{\mathrm{m}}-Aw-Bp-C}{G}\mathrm{d}x-v_{4}\right\}. \tag{21}$$

For an ideal gas, like water or methanol vapour approximately under common absorber conditions, the derivative $\partial h_{\mathrm{v}}/\partial p$ equals zero, and so the denominator of the factor in front of the right-hand side of equation (21) reduces to one.

For the sake of generality the equations are made dimensionless, with dimensionless variables

$$X=\frac{x}{L},\quad \tau=\frac{t}{L}\frac{\Gamma_{\mathrm{m},0}}{\rho_{\mathrm{m},0}\delta_{\mathrm{m},0}},$$
$$\theta=\frac{T-T_{0}}{T_{\mathrm{e}}-T_{0}},\quad \gamma=\frac{w-w_{0}}{w_{\mathrm{e}}-w_{0}},$$
$$P=\frac{p-p_{0}}{p_{\mathrm{e}}-p_{0}},\quad J=\frac{\Gamma}{\Gamma_{\mathrm{m},0}}$$

with

$$T_{\mathrm{e}}=A_{0}w_{0}+B_{0}p_{0}+C,$$
$$T_{0}=A_{0}w_{\mathrm{e}}+B_{0}p_{0}+C_{0},\quad T_{0}=A_{0}w_{0}+B_{0}p_{\mathrm{e}}+C_{0}.$$

The quantities with subscript 0 or e, like $\Gamma_{\mathrm{m},0}$, T_{0}, T_{e}, etc., relate to some reference state, e.g. the initial conditions at the mixture inlet for a required standard state. Now the following set of seven differential equations results :

$$\frac{\partial\theta_{\mathrm{c}}}{\partial\tau}+N_{1}\frac{\partial\theta_{\mathrm{c}}}{\partial X}=N_{2}(\theta_{\mathrm{w}}-\theta_{\mathrm{c}}) \tag{1*}$$

$$\frac{\partial\theta_{\mathrm{w}}}{\partial\tau}=N_{3}(\theta_{\mathrm{m}}-\theta_{\mathrm{w}})-N_{4}(\theta_{\mathrm{w}}-\theta_{\mathrm{c}}) \tag{2*}$$

$$\frac{\partial\gamma}{\partial\tau}+v_{5}J_{\mathrm{m}}^{1-b}\frac{\partial\gamma}{\partial X}$$
$$=-v_{5}\frac{N_{5}(\gamma-N_{6})}{J_{\mathrm{m}}^{b}}(\theta_{\mathrm{m}}+v_{6}\gamma+v_{7}P-v_{8}) \tag{12*}$$

$$\frac{\partial\theta_{\mathrm{m}}}{\theta\tau}+v_{5}J_{\mathrm{m}}^{1-b}\frac{\partial\theta_{\mathrm{m}}}{\partial X}=\frac{v_{5}N_{5}N_{7}}{J_{\mathrm{m}}^{b}}(\theta_{\mathrm{m}}+v_{6}\gamma+v_{7}P-v_{8})$$
$$-\frac{v_{5}N_{8}}{J_{\mathrm{m}}^{b}}(\theta_{\mathrm{m}}-\theta_{\mathrm{w}}) \tag{14*}$$

$$\frac{\partial J}{\partial\tau}+\frac{v_{5}}{b}J_{\mathrm{m}}^{1-b}\frac{\partial J}{\partial X}=\frac{v_{5}}{b}N_{5}J_{\mathrm{m}}^{1-b}[\theta_{\mathrm{m}}+v_{6}\gamma$$
$$+v_{7}P-v_{8}]+v_{2} \tag{16*}$$

$$\frac{\partial P}{\partial \tau}=\frac{-N_9[v_3(\theta_{\mathrm{v,i}}-\theta_{\mathrm{v}})+\theta_{\mathrm{v}}+N_{10}]}{1-N_{12}[(P+N_{11})/(\theta_{\mathrm{v}}+N_{10})]}J_{\mathrm{v,i}}$$

$$+\frac{N_5N_9(\theta_{\mathrm{v}}+N_{10})}{1-N_{12}[(P+N_{11})/(\theta_{\mathrm{v}}+N_{10})]}\left[\int_0^1(\theta_{\mathrm{m}}+v_6\gamma\right.$$

$$\left.+v_7P-v_8)\,\mathrm{d}X-v_4\right] \quad (21^*)$$

$$\frac{\partial \theta_{\mathrm{v}}}{\partial \tau}=-N_9v_3\frac{(\theta_{\mathrm{v}}+N_{10})}{(P+N_{11})}J_{\mathrm{v,i}}(\theta_{\mathrm{v,i}}-\theta_{\mathrm{v}})+N_{12}\frac{\partial P}{\partial \tau}. \quad (20^*)$$

In our transport equations we find two characteristic times: a delay time or residence time τ_{d} and a time constant or relaxation time τ_{r}. Therefore, many of the dimensionless groups in the equations before can be expressed as the inverse of a characteristic time scaled on the mixture residence time $\tau_{\mathrm{d,m}}$

$$N_1=\frac{v_1\Gamma_{\mathrm{c}}}{\rho_{\mathrm{c}}d_{\mathrm{c}}}\frac{\rho_{\mathrm{m,0}}\delta_{\mathrm{m,0}}}{\Gamma_{\mathrm{m,0}}}=\frac{\tau_{\mathrm{d,m}}}{\tau_{\mathrm{d,c}}},$$

$$N_2=\frac{v_1\alpha_{\mathrm{c}}}{\rho_{\mathrm{c}}c_{p,\mathrm{c}}d_{\mathrm{c}}}\frac{\rho_{\mathrm{m,0}}\delta_{\mathrm{m,0}}L}{\Gamma_{\mathrm{m,0}}}=\frac{\tau_{\mathrm{d,m}}}{\tau_{\mathrm{r,c}}},$$

$$N_3=\frac{\alpha_{\mathrm{m}}}{\rho_{\mathrm{w}}c_{p,\mathrm{w}}d_{\mathrm{w}}}\frac{\rho_{\mathrm{m,0}}\delta_{\mathrm{m,0}}L}{\Gamma_{\mathrm{m,0}}}=\frac{\tau_{\mathrm{d,m}}}{\tau_{\mathrm{r,w1}}},$$

$$N_4=\frac{\alpha_{\mathrm{c}}}{\rho_{\mathrm{w}}c_{p,\mathrm{w}}d_{\mathrm{w}}}\frac{\rho_{\mathrm{m,0}}\delta_{\mathrm{m,0}}L}{\Gamma_{\mathrm{m,0}}}=\frac{\tau_{\mathrm{d,m}}}{\tau_{\mathrm{r,w2}}},$$

$$N_5=\frac{L(T_{\mathrm{e}}-T_0)}{\Gamma_{\mathrm{m,0}}G}\propto\frac{\tau_{\mathrm{d,m}}}{\tau_{\mathrm{r},\gamma}},\quad N_6=\frac{(1-w_0)}{(w_{\mathrm{e}}-w_0)},$$

$$N_7=\frac{\Delta h}{c_{p,\mathrm{m}}(T_{\mathrm{e}}-T_0)},\quad N_{12}=\frac{\phi_p}{c_{p,\mathrm{v}}B_0},$$

$$N_8=\frac{L\alpha_{\mathrm{m}}}{c_{p,\mathrm{m}}\Gamma_{\mathrm{m,0}}}=\frac{\tau_{\mathrm{d,m}}}{\tau_{\mathrm{r},\theta\mathrm{m}}},\quad N_9=\rho_{\mathrm{m,0}}\delta_{\mathrm{m,0}}BEL,$$

$$N_{10}=\frac{T_0}{T_{\mathrm{e}}-T_0},\quad N_{11}=\frac{p_0}{p_{\mathrm{e}}-p_0}.$$

The dimensionless numbers are allowed to be a function of space and time. To find a solution of the set of differential equations boundary values and initial values have to be supplied.

SOLUTION METHOD

The equations are solved by an implicit method, using first-order backward discretization in space and time

$$\frac{\partial z}{\partial \tau}=\frac{z_j^{n+1}-z_j^n}{\Delta\tau}\quad\text{and}\quad\frac{\partial z}{\partial X}=\frac{z_j^{n+1}-z_{j-1}^{n+1}}{\Delta X}.$$

This means that the basic form of the transport equation

$$\frac{\partial z}{\partial \tau}+u\frac{\partial z}{\partial X}=c$$

transforms to

$$z_j^n=\left(1+u\frac{\Delta\tau}{\Delta X}\right)z_j^{n+1}-u\frac{\Delta\tau}{\Delta X}z_{j-1}^{n+1}-c\Delta\tau.$$

The truncation error

$$\frac{1}{2}\frac{\partial^2 z}{\partial \tau^2}\Delta\tau+\frac{u}{2}\frac{\partial^2 z}{\partial X^2}\Delta X+\cdots$$

is of order ΔX, $\Delta\tau$, respectively. The ΔX part gives rise to so-called numerical diffusion in the x-direction. For counterflow cooling ($u<0$) a forward discretization in space has to be used for the cooling water transport equation. The non-linear terms in the equations, like the second term on the left-hand side of (13*) are linearized with a truncation error of first-order in $\Delta\tau$

$$f(\tau+\Delta\tau)=f(\tau)+\Delta\tau\frac{\partial f}{\partial \tau}\approx f(\tau)$$

that is, these terms are substituted by their values in the preceding time step. If the properties are allowed to vary with space and time, the dimensionless N- and v-numbers are also computed in the preceding time step. Discretization of the set of equations leads to a matrix equation

$$\underline{z}^n=\underline{M}\underline{z}^{n+1}.$$

The matrix M is a profile matrix. The matrix equations are solved, using subroutines described in ref. [22], by LU-decomposition of the matrix followed by Gaussian elimination. To get a consistent set of initial values first the static solution of the equations (all time derivatives set zero) is computed. The values from the static solution are used as initial values in the dynamic solution.

MODEL VALIDITY

Our solution method is able to give results for counterflow as well as cocurrent flow cooling. Also by putting the appropriate N-values to zero, simpler subsystems of our physical system can be simulated, e.g. a film flow heat exchanger, an evaporator, a condenser or a stripping column (no heat of absorption).

In the introduction we already stated that a more detailed description of a film flow apparatus than this kind of model breaks down on the difficulty of finding a universal description of the film flow. In other words: a description like this is the best obtained so far. However, care should be taken of some of the limitations of the model.

First, the general expression (equation (10)) for the film thickness enables every kind of film thickness (laminar, wavy, turbulent) to be easily incorporated into the equations. However, the user of the model has to decide which kind of film thickness is valid for a certain flow rate (coefficients b and f) and which expressions for α and k are to be used.

Second, assumption (8) implicates that the form of the temperature and mass fraction profiles associated with a particular choice of α and k is not altered by any transient disturbance. This may be approximately valid for the temperature but for the mass fraction we can think of disturbances for which this is not valid.

Third, the expressions for δ, α and k implicitly assume profiles $u(y)$, $T(y)$ and $w(y)$. However, only the film thickness averaged quantities are present in the equations. Therefore, any change in temperature or composition travels with the mean velocity. For laminar films it is known that the interface velocity is 1.5 times the mean velocity. This means that changes in T and w start to arrive at the absorber exit already at 2/3 of the residence time $\tau_{d,m}$. This effect can be partly taken into account by choosing an appropriate numerical diffusion. In our simulations the chosen step size $\Delta X = 0.02$ and $\Delta\tau = 0.02$ not only appears to be a reasonable compromise between accuracy and computation time (approximately 4 min CPU time on an IBM AT3 computer for 1 unit of dimensionless time), but also gives the desired numerical diffusion.

RESULTS

For clearness of demonstration the simulations are given for a simple system with properties that are constant in space and time (v_1, v_3, v_5–$v_8 = 1$, $v_2 = v_4 = 0$), the vapour is an ideal gas ($N_{12} = 0$), the mixture film thickness follows the Nusselt equation ($a = 0.75^{1/3}$, $b = 1/3$). The dimensionless numbers and the boundary and initial conditions have values that give neat results. Still these values are realistic for common mixtures and absorber geometries under properly chosen operating conditions. The standard conditions for our simulations are: $\theta_{c,i} = \theta_w(0) = \theta_{m,i} = \gamma_i = P(0) = 0$, $J_{m,i} = 1$, $\theta_{v,i} = -2$, $J_{v,i} = 0.01$, $N_1 = N_2 = 1$, $N_3 = N_4 = 0.5$, $N_5 = -0.02$, $N_6 = N_7 = 50$, $N_8 = 1$, $N_9 = 1$, $N_{10} = 52$, $N_{11} = -50$. The time constant in an equation equals the inverse of minus one times the factor in front of the dependent variable on the right-hand side of the equation, e.g. in equation (14*) $J^b_m/(v_5(N_8 - N_5N_7))$. So all the time constants in equations (1*)–(20*) are equal to one except $\tau_{r,\theta m} = 0.5$. Also all the delay times are equal to one. In the simulations all the N-values are kept constant, except one that is varied in three steps over one decade. The input variables that are perturbed in the simulations are the cooling water temperature $\theta_{c,i}$, the vapour mass flow rate $J_{v,i}$ and the mixture mass fraction $\gamma_{m,i}$. In an absorption cycle these inputs form the link with the three heat reservoirs used in the cycle.

In Fig. 2 the output responses are shown of P and of θ_c, θ_w, θ_m and γ at the absorber outlet, on a step change at $\tau = 0$ in the inlet cooling water temperature $\theta_{c,i}$ from 0 to -1. The expected delay time in the responses equals 1, because of the N-values. Due to the numerical diffusion, the responses show a delay time of about 2/3, as would be found for laminar flow with a parabolic velocity profile. It appears that the response of θ_c is the fastest, followed by θ_w, θ_m, γ and P, as may be expected from the geometry. An increase in $P = (p-p_0)/(p_e-p_0)$ means that the vapour pressure p decreases (because $p_e < p_0$). To bring p down however, first the absorbed mass flow rate has to increase before it finally becomes equal to its original value again ($J_{v,i}$ is not altered). For this reason $\gamma(\tau)$ contains a maximum. In the case of condensation (equation (13*) is ruled out by making $N_6 = 1$ and $\gamma_i = \gamma(X) = 1$ for all X) the response of θ_m is faster because the chain of coupled phenomena now lacks one phenomenon: mass transfer in the film. Consequently for a film heat exchanger (equations (13*), (17*)–(20*) are ruled out with $N_5 = N_9 = 0$, $N_6 = 1 = \gamma_i = \gamma(X)$ for all X) the response is the fastest because now also the mass transfer from vapour to film has disappeared from one chain.

In Fig. 3 the effect of a variation of N_1 or $\tau_{d,m}/\tau_{d,c}$ from 1 to 0.1 on θ_m and γ appears to be smaller than a factor 10 in the characteristic time. The height of the response decreases with increasing $\tau_{d,c}$ (so decreasing Γ_c) because the cooling water warms up increasingly during its travel along the wall if Γ_c decreases.

In Fig. 4 the effect of the variation of N_2 or $\tau_{d,m}/\tau_{r,c}$ is shown. An increase of $\tau_{r,c}$ leads to an increase of the height of the response because of an increase of the heat capacity of the cooling water flow. It appears that along with this increase also the response of θ_m and γ becomes quicker.

In Fig. 5 the responses for varying N_3 and N_4 are given. As may be expected the influence of $\tau_{d,m}/\tau_{r,w}$ is very pronounced. Of course the final value of the response equals that of the standard simulation in Fig. 1.

In Fig. 6 the output responses on a step change in the inlet vapour mass flow rate $J_{v,i}$ from 0.01 to 0.02 are given. The response of P is the fastest, followed by γ, θ_m, θ_w and θ_c. Because $\gamma_o - \gamma_i = N_6J_{v,i}/J_m = 50J_{v,i}$, γ will rise from 0.5 to 1. For the same reasons as mentioned with Fig. 2 the responses for pure condensation and absorption are faster than for coupled heat and mass transfer. Pure absorption (no heat effect) is effectuated by deleting equation (14*): $N_7 = N_8 = 0 = \theta_{m,i} = \theta_m(X)$ for all X.

Figure 7 contains the responses of θ_m and γ for three values of N_5. These values lead to $\tau_{r,p} = 1, 3.3, 10$ and $\tau_{r,\theta m} = 0.5, 0.77, 0.91$. It appears that the pressure time constant is dominant: γ and θ_m follow the response in P, although the responses are becoming increasingly smoother. Figure 7 demonstrates that, as already stated in the introduction, our model is suited for a second application : parameter identification, especially the determination of the mass transfer coefficient k. Due to the coupling between heat and mass transfer, it is not possible to determine the mass transfer coefficient k directly from stationary experimental results, because the driving force $w^* - w$ cannot be computed in a straightforward way from the measured input and output values. This means that, because N_5 strongly depends on the mass transfer

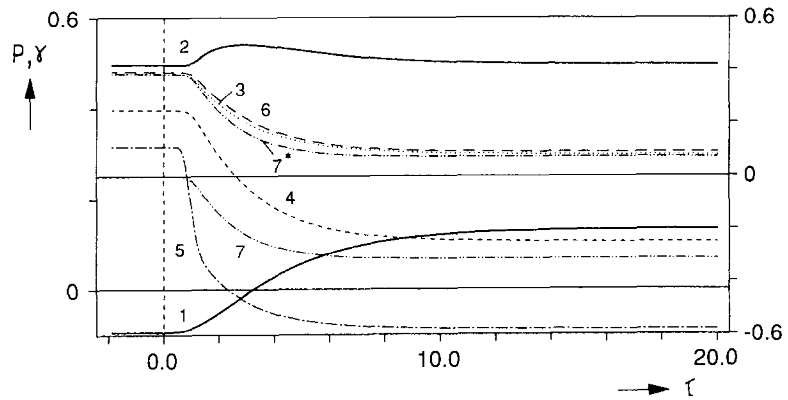

FIG. 2. Response at the absorber outlet on a step change of $\theta_{c,i}$. Standard conditions: 1, P; 2, γ; 3, θ_m; 4, θ_w; 5, θ_c; 6, θ_m for a condenser; 7, θ_m for a film heat exchanger; 7*, id. shifted upwards to the position of θ_m.

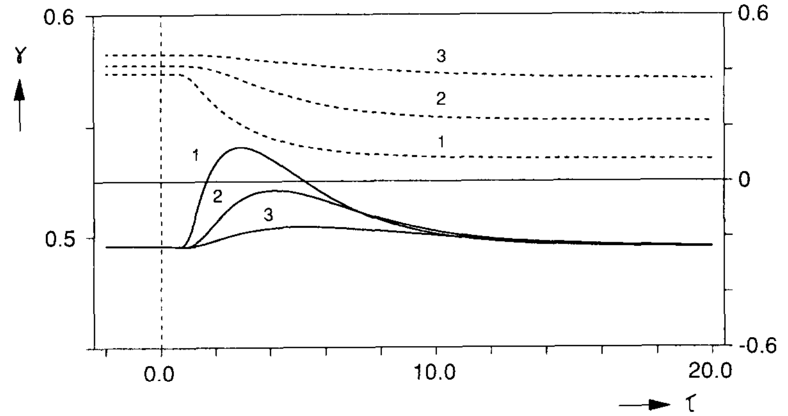

FIG. 3. Response at the absorber outlet on a step change of $\theta_{c,i}$. Solid lines describe γ, broken lines describe θ_m: 1, $N_1 = 1$; 2, $N_1 = 0.3$; 3, $N_1 = 0.1$.

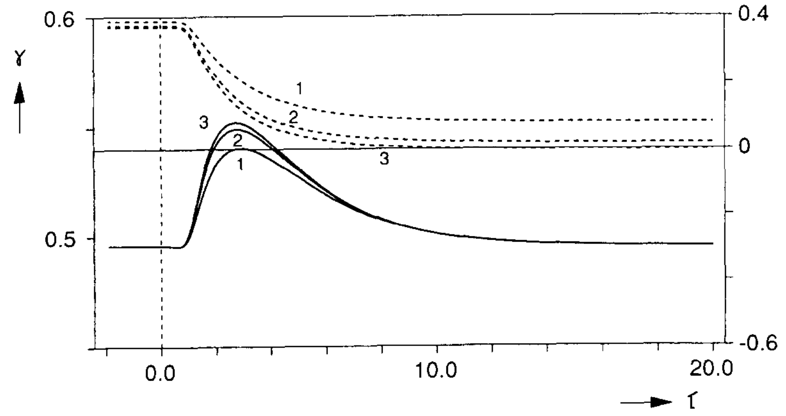

FIG. 4. Response at the absorber outlet on a step change of $\theta_{c,i}$. Solid lines describe γ, broken lines describe θ_m: 1, $N_2 = 1$; 2, $N_2 = 0.3$; 3, $N_2 = 0.1$.

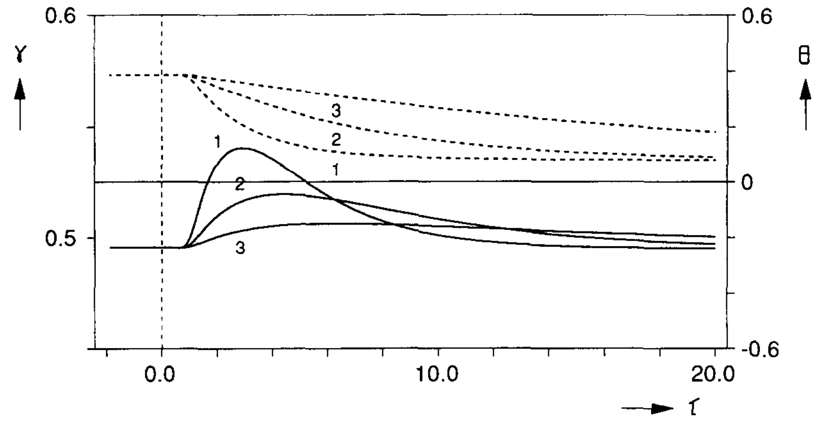

FIG. 5. Response at the absorber outlet on a step change of $\theta_{c,i}$. Solid lines describe γ, broken lines describe θ_m: 1, $N_3 = N_4 = 0.5$; 2, $N_3 = N_4 = 0.15$; 3, $N_3 = N_4 = 0.05$.

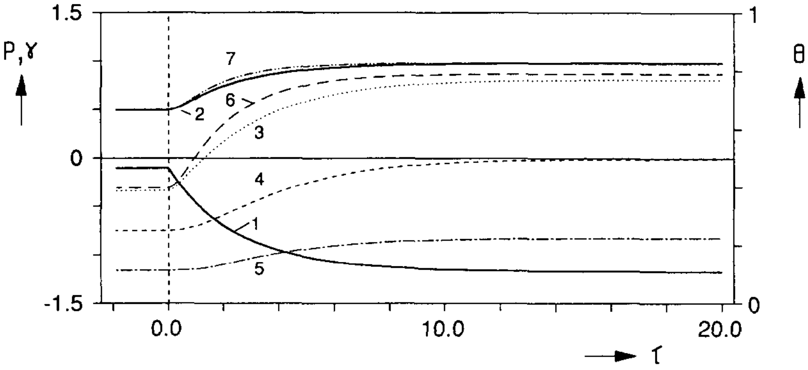

FIG. 6. Response at the absorber outlet on a step change of $J_{v,i}$. Standard conditions: 1, P; 2, γ; 3, θ_m; 4, θ_w; 5, θ_c; 6, θ_m for a condenser; 7, θ_m for a stripper.

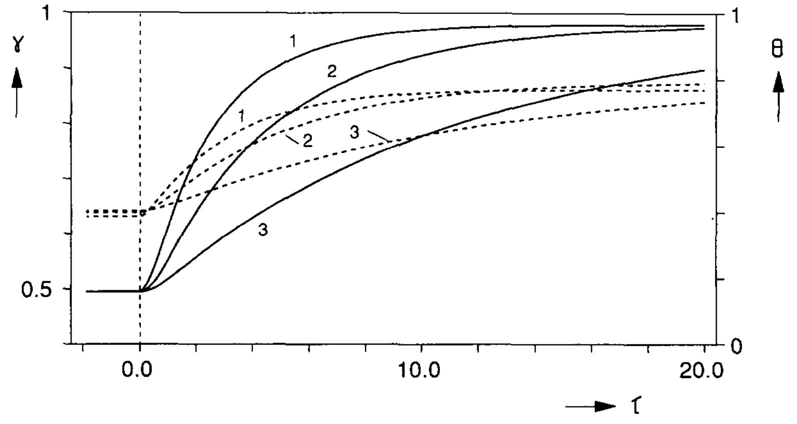

FIG. 7. Response at the absorber outlet on a step change of $J_{v,i}$. Solid lines describe γ, broken lines describe θ_m: 1, $N_5 = -0.02$; 2, $N_5 = -0.006$; 3, $N_1 = -0.002$.

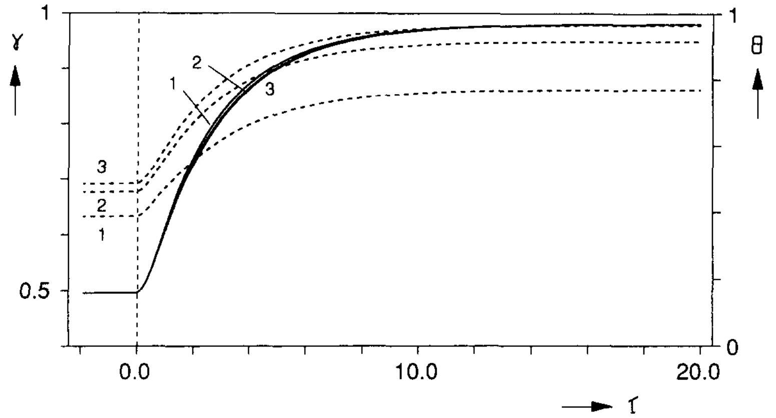

FIG. 8. Response at the absorber outlet on a step change of $J_{v,i}$. Solid lines describe γ, broken lines describe θ_m: 1, $N_8 = 1$; 2, $N_8 = 0.3$; 3, $N_8 = 0.1$.

coefficient k, the response of P on $J_{v,i}$ gives an alternative means to compute the mass transfer coefficient directly. A necessary condition is that $\Delta h/\alpha^*$ in the expression for G is either negligible (very short flow length) or α^* is known, which is mostly true for moderate or large flow lengths (linear temperature profile).

Figure 8 illustrates the effect of varying N_8 so that $\tau_{r,\theta m} = 0.5, 0.77, 0.91$. Again the response of P is dominant and θ_m is hardly affected by the value of $\tau_{r,\theta m}$.

Figure 9 gives the result of a variation in N_9 such that $\tau_{r,P} = 1, 3.3, 10$. It appears that the time constant of the response of P and so of θ_m is twice as high as the value of $\tau_{r,P}$. This must be due to the coupling of θ_m, γ and P. If only θ_m and P (condensation) or γ and P (absorption) are coupled, the time constants are only 1.5 times as high as $\tau_{r,P}$.

Figure 10 gives the responses on a step change in the inlet mass fraction $\gamma_{m,i}$ from 0 to -1. The response of P is immediate, the exit γ, θ_m, θ_w and θ_c follow with increasing delay. Because $J_{v,i}$ does not change, the final values of θ_m, θ_w, θ_c and $\gamma_o - \gamma_i$ equal the initial values. Because P rises immediately, $\theta_{m,o}$ first decreases (desorption) until $\tau = 0.6$ and then increases until $\tau = 1.4$ because of the extra absorption necessary to bring P up (and so p down), at constant $J_{v,i}$, to its new final value. Also shown are the responses of P and γ for a stripper. These responses are a little bit faster for the same reason as in Fig. 6.

Figures 11 and 12 give an idea of the propagation of the disturbances in θ_m and γ along the film. Close inspection shows that for $\tau = 0.3$ or 0.6 at the bottom of the absorber γ already decreases before the disturbance has reached this part of the film (desorption because of decreasing p). Consequently θ_m also decreases below its initial value.

CONCLUSION

The advantage of our model above existing published models is that it also describes the transient behaviour of the film flow rate and the vapour pressure. The formulation of the equations is in such a form that they can be considered as a module. This module can easily be made fit to describe other film

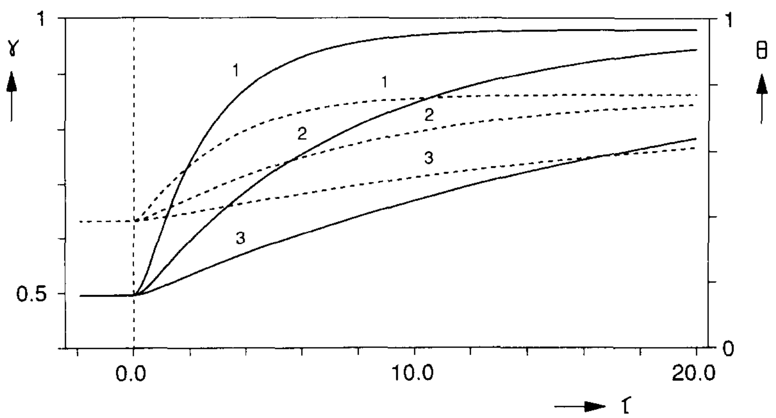

FIG. 9. Response at the absorber outlet on a step change of $J_{v,i}$. Solid lines describe γ, broken lines describe θ_m: 1, $N_9 = 1$; 2, $N_9 = 0.3$; 3, $N_9 = 0.1$.

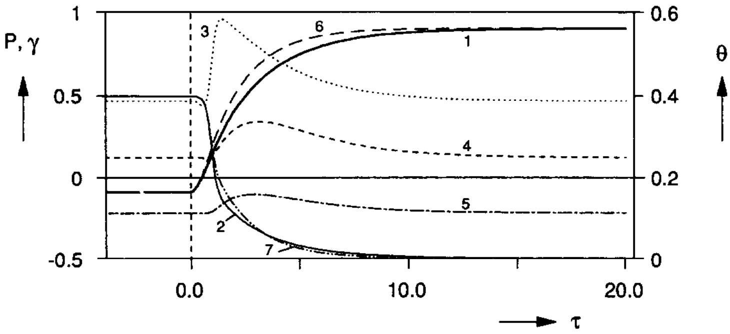

FIG. 10. Response at the absorber outlet on a step change of γ_i. Standard conditions: 1, P; 2, γ; 3, θ_m; 4, θ_w; 5, θ_c; 6, P for a stripper; 7, γ for a stripper.

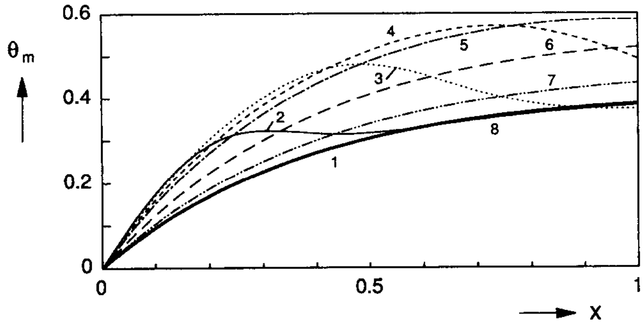

FIG. 11. Temperature as a function of position at distinct times. Conditions identical to Fig. 10: 1, $\tau = -0.02$; 2, $\tau = 0.3$; 3, $\tau = 0.6$; 4, $\tau = 1$; 5, $\tau = 1.4$; 6, $\tau = 3$; 7, $\tau = 6$; 8, $\tau = 20$.

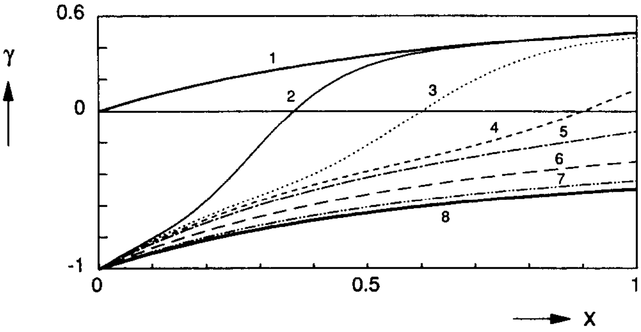

FIG. 12. Mass fraction as a function of position at distinct times. Conditions identical to Fig. 10: 1, $\tau = -0.02$; 2, $\tau = 0.3$; 3, $\tau = 0.6$; 4, $\tau = 1$; 5, $\tau = 1.4$; 6, $\tau = 3$; 7, $\tau = 6$; 8, $\tau = 20$.

components like a stripper, a condenser, an evaporator or a film heat exchanger, just by changing some of the dimensionless numbers and the entrance or boundary conditions. The responses at the absorber outlet are shown on a step change at the absorber inlet in the cooling water temperature, the vapour mass flow rate and the mixture mass fraction. Clearly delay times and time constants can be identified from the responses. Also the propagation of the disturbance along the film is shown. The time constants that can be determined from the responses do not always equal the expected values because of the coupling of the equations. Therefore, the pressure time constant determines the relaxation time of the responses on a step change of $J_{v,i}$ and γ_i. This again underlines that a description of the transient behaviour of the vapour pressure is an essential part of the dynamic absorber model. The pressure response gives an alternative means to determine the mass transfer coefficient.

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APPENDIX

The following dimensionless quantities account for the variation of the thermodynamic and physical properties in space and time. If the properties may be considered as constant, which is the case for mixtures like $H_2O/LiBr$ or $CH_3OH/LiBr/ZnBr_2$ for T, w, p combinations associated with realistic absorber operating conditions, the v-variables equal one, except v_2 and v_4 that equal zero in this case. Meaning of the v-variables

$$v_1 = \left(1 + \frac{h_c}{\rho_c c_{p,c}} \frac{\partial \rho_c}{\partial T_c}\right)^{-1},$$

$$v_2 = \frac{J_m}{b}\left(\frac{1}{f}\frac{\partial f}{\partial \gamma}\frac{\partial \gamma}{\partial \tau} + \frac{1}{f}\frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial \tau}\right),$$

$$v_3 = \frac{[h_v(p, T_{v,i}) - h_v(p, T_v)]}{c_{p,v}(T_{v,i} - T_v)}, \quad v_4 = \frac{[P + N_{11}]}{E}\frac{\partial E}{\partial \tau},$$

$$v_5 = \frac{f}{f_0}, \quad v_6 = \frac{A}{A_0}, \quad v_7 = \frac{B}{B_0}, \quad v_8 = 1 + C - C_0.$$

COMPORTEMENT TRANSITOIRE D'UN ABSORBEUR A FILM AVEC TRANSFERTS DE MASSE ET DE CHALEUR COUPLE

Résumé—Le modèle décrit le comportement transitoire d'un absorbeur à film, refroidi. Les transferts de masse et de chaleur sont couplés et on utilise un mélange binaire dans lequel un seul des components est volatile. Le système est décrit par 7 equations differentielles partielles ou ordinaires couplées pour les températures du fluide froid, du mur, du mélange et de la vapeur, ainsi que les débits et concentration massiques dans le film et la pression de vapeur. On donne les résultats de modifications par sauts de la température de l'eau de refroidissement, du débit-masse de vapeur et de la concentration massique à l'entrée. Ces réponses en palier montrent que la description de comportement transitoire de la pression de vapeur est essentielle pour le développement d'un modèle dynamique de l'absorbeur. Ce modèle peut etre utilisé dans la simulation d'un cycle d'absorption général pour décrire tout les composants à film tombant (evaporateur, condenseur, echangeur de chaleur, absorbeur, desorbeur).

DYNAMISCHES VERHALTEN EINER RIESELFILMABSORBER MIT GEKOPPELTEN WARME- UND STOFFUBERTRAGUNG

Zusammenfassung—Das Modell beschreibt das dynamische Verhalten einer gekühlten Rieselfilmabsorber mit gekoppelten Wärme- und Stoffübertragung an einem binären Gemisch dass nur eine flüchtige Komponente enthaltet. Ins Gesamt 7 partielle und gewöhnliche Differentialgleichungen beschreiben das Verhalten der Temperature des Kühlmediums, der Wand, des Gemisches und der Dampf, sowie des Massenstroms und der Konzentration des Films und der Druck. Die Ergebnisse einer sprungartigen Anderung der Eintrittswert der Kühlmediumtemperatur, des Dampfmassenstroms oder der Filmkonzentration werden gezeigt. In ein algemeines Simulationsprogram einer Absorptionsanlage ist das Modell benutzbar zur Beschreibung des Verhaltens jeder Rieselfilmkomponent (Verdampfer, Verflüssiger, Wärmeaustauscher, Absorber, Austreiber).

ДИНАМИЧЕСКАЯ МОДЕЛЬ ПЛЕНОЧНОГО АБСОРБЕРА ПРИ НАЛИЧИИ ВЗАИМОСВЯЗАННОГО ТЕПЛО- И МАССОПЕРЕНОСА

Аннотация—Представлена модель, описывающая переходный режим работы охлаждаемого пленочного абсорбера при наличии взаимосвязанного тепло- и массопереноса с использованием бинарной смеси, содержащей только один летучий компонент. Модель представлена системой из семи взаимосвязанных дифференциальных уравнений, как обыкновенных, так и в частных производных, для температуры охлаждающей среды, стенки, смеси и пара, для массового расхода пленки и концентрации, а также для давления пара. Показано влияние скачкообразного изменения на входе в абсорбер температуры охлаждающей воды, массового расхода пара и массовой доли смеси на режим его работы. Модель может использоваться для описания любого пленочного компонента (в испарителе, конденсаторе, теплообменнике, абсорбере, десорбере) при моделировании полного цикла поглощения.