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MECHANISTIC AND LUMP APPROACH OF INTERNAL TRANSPORT
PHENOMENA DURING DRYING OF PAPER SHEET

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ABSTRACT

This paper is dealing with the mass and heat transport phenomena inside the paper sheet and shows how to deal with shrinkage during drying. The aim is identifying the intrinsic material properties being relevant for internal mass and heat transport. Two approaches will be followed. The first one is based on the description of microscopic mechanisms for mass and heat transport in a porous material, e.g. Darcy flow for liquid due to capillary forces and vapour diffusion due to a vapour pressure gradient, heat flow as a result of the mass flow and a temperature gradient. The contribution of each mechanism in the overall mass resp. heat fluxes is quantified by means of mechanistic transport parameters, such as vapour diffusivity, Darcy permeability, etc. In the second approach the heat and mass fluxes are related to both temperature and moisture gradients and the contribution of each driving force is weighed by a lump transport parameter. Finally, the coupling between the mechanistic and lump parameters is worked out.

INTRODUCTION

Transport phenomena in multi-cylinder paper dryers are rather complex by nature (1, 2). The paper sheet is submitted to alternating boundary conditions. The energy for drying is delivered mainly by steam condensation at the inner wall of the cylinder, where the shape and thickness of the condensate film depend on the revolution speed, siphon height, surface roughness etc. The conductive heat transfer via the cylinder wall to the papersheet may be hindered by a bad contact between paper sheet and cylinder wall. The convective mass and heat transfer at the drying interface depend on the air conditions and air flow patterns. As a result of these imposed boundary conditions complicated mass and heat transfer processes inside the paper sheet are initiated. A better description and understanding of the internal mass and heat transport phenomena are required for the reliable modelling of a multi-cylinder dryer.

Paper and cardboard are considered as non-homogeneous materials with a capillary-porous structure, in which three components (s=solid fibers, w=water and a=air) and three phases (s=solid, ℓ=liquid and g=gas) can be distinguished. According to Stanish et.al. (3) three types of water can be considered: free water, which is the liquid water within the pores of the paper, water vapour being present if the pores are partially saturated with liquid water and bound water that can be found within the paper fibers. Simular approaches for paper drying are given by Asensio & Yagoobi (4) and Harrmann & Schulz (5). Also an interesting overview of the physical mechanisms in drying of porous non-shrinking systems is given by Moyne et.al. (6).

Below mass and heat fluxes will be derived via a mechanistic and a lump approach and the coupling between both approaches will be worked out. The effects of shrinkage will be taken into account by defining solids based quantities for concentrations, fluxes and space coordinate and by introducing a shrinkage coefficient. First the mass and heat balances will be given.

MASS AND HEAT BALANCES

The mass balance over a small volume element with thickness ∂r is given by:

$$\left(\frac{\partial \rho_w}{\partial t}\right)_r = -\left(\frac{\partial n_w}{\partial r}\right)_t \tag{1}$$

and the heat balance:

$$\left(\frac{\partial(\rho_s h_s + \rho_w h_w)}{\partial t}\right)_r = -\left(\frac{\partial q}{\partial r}\right)_t \qquad (2)$$

Because water can be present in several states: $\rho_w h_w = \rho_\ell h_\ell + \rho_v h_v + \rho_b h_b$. These balances are given here in a fixed frame of coordinates. In case of shrinking systems, it is recommended to express these balances in terms of solid based quantities (7).

The solid based *mass concentration u* [in kg water/kg dry solid] is defined by:

$$u = \frac{\rho_w}{\rho_s} \qquad (3)$$

Thus:

$$\rho_w = \rho_s \cdot u \qquad (4)$$

The solids based *heat concentration H* [in Joule/kg dry solid] is given by:

$$H = h_s + u \cdot h_w \qquad (5)$$

Thus:

$$\rho_s h_s + \rho_w h_w = \rho_s H \qquad (6)$$

The *water flux* n_w can be split up into a convective and a diffusive part in several ways (8). By taking the solids velocity as a reference:

$$n_w = \rho_w v_w = \rho_w v_s + \rho_w (v_w - v_s) = \rho_w v_s + j_w^s \qquad (7)$$

in which j_w^s is the water diffusion flux with respect to the solids velocity. Because the solids mass flux $n_s = \rho_s v_s$ the water flux can be expressed as:

$$n_w = n_s \cdot u + j_w^s \qquad (8)$$

In an analog way the *heat flux q* consists of convective and conductive terms. By neglecting the contribution of the air, this flux can be formulated by:

$$q \approx n_s h_s + n_w h'_w - \lambda \frac{\partial T}{\partial r} = n_s H + j^s_w h''_w - \lambda \frac{\partial T}{\partial r} \tag{9}$$

in which h'_w and h''_w are flux averaged enthalpy concentrations,
e.g. $j^s_w h''_w = j^s_\ell h_\ell + j^s_v h_v + j^s_b h_b$. The heat flux with respect to the solids is defined by:

$$q^s = j^s_w h''_w - \lambda \frac{\partial T}{\partial r} \tag{10}$$

and the total heat flux can be written as:

$$q = n_s H + q^s \tag{11}$$

The solids *coordinate z* is defined as

$$dz = \rho_s dr \tag{12}$$

It should be realized that dz is expressed in kg solids/m^2.
The above mass and heat balances can now be transformed and expressed in terms of the solid based parameters u, H, j^s_w, q^s and z, according to:

$$\left(\frac{\partial u}{\partial t} \right)_z = - \left(\frac{\partial j^s_w}{\partial z} \right)_t \tag{13}$$

and

$$\left(\frac{\partial H}{\partial t} \right)_z = - \left(\frac{\partial q^s}{\partial z} \right)_t \tag{14}$$

Before working out expressions for j^s_w and q^s first attention will be paid to how to describe shrinkage behaviour.
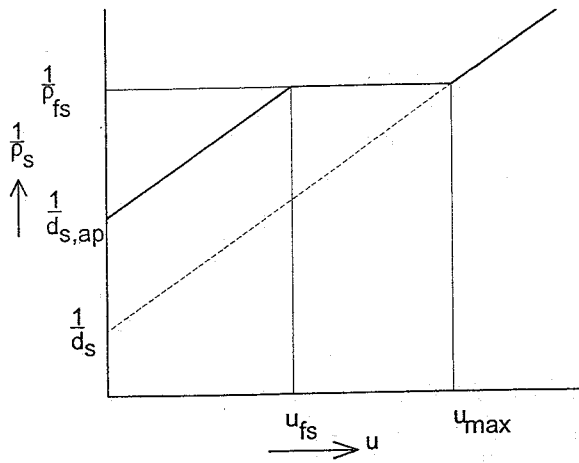
FIGURE 1. Schematic representation of shrinkage behaviour of paper sheet. Specific volume (m^3/kg dry solid) versus moisture concentration (kg water/kg dry solid).

SHRINKAGE

In general the shrinkage of a paper sheet is uni-directional, which means that shrinkage takes only place in the same direction as the uni-directional mass and heat fluxes. It appears to be very handy to describe shrinkage behaviour in terms of solids based parameters u en the specific volume $/\rho_s$ (see Figure 1). A local shrinkage coefficient σ is introduced according to (7):

$$\partial\left(\frac{1}{\rho_s}\right) = \sigma \cdot \partial\left(\frac{u}{d_w}\right) \tag{15}$$

The shrinkage function $\sigma = \sigma(u)$ has to be determined experimentally. For a paper sheet it generally holds that:

$$
\begin{aligned}
&\sigma = 1 \quad \text{for} \quad && o \leq u \leq u_{fs} \\
&\sigma = 0 \quad \text{for} \quad && u_{fs} < u \leq u_{max} \\
&\sigma = 1 \quad \text{for} \quad && u_{max} < u < \infty
\end{aligned}
\tag{16}
$$

With the aid of these equations the solids concentration ρ_s and porosity of the papersheet can be calculated straight forward as functions of the moisture concentration. For the uni-directional shrinking paper sheet the introduction of the solids based coordinate z changes a moving external boundary at r=R(t) into a fixed one at z=z$_{max}$. It can be shown that by using the shrinkage coefficient the solids flux n$_s$ can be related to water flux n$_w$ as follows:

$$n_s = -\frac{\dfrac{d_{s,ap}}{d_w}\sigma}{1-\dfrac{d_{s,ap}}{d_w}(\sigma-\overline{\sigma})u}\cdot n_w \qquad (17)$$

In modelling shrinking systems also the solids mass balance should be included. However, this balance can be eliminated by applying the above relation.

MECHANISTIC MODEL

It has already been mentioned that three types of water can be distinguished, and therefore the total water flux can be splitted up according to:

$$j_w^s = j_\ell^s + j_v^s + j_b^s \qquad (18)$$

Equations for the mass transport of liquid, vapour and bound water will now be given.

Transport of Free Water

In a shrinking system the solid is moving. The mass flux of liquid water, with respect to the solid velocity, can be described by means of Darcy's law:

$$j_\ell^s = \rho_\ell(v_\ell - v_s) = -d_w \frac{K_\ell}{\eta_\ell}\frac{\partial P_\ell}{\partial r} \qquad (19)$$

This equation also holds for non-shrinking systems by taking v$_s$=0. The liquid pressure P$_\ell$ depends on the overall pressure P and the capillary pressure P$_{cap}$ according to P$_\ell$=P-P$_{cap}$ and Equation (19) becomes:

$$j_\ell^s = -d_w \frac{K_\ell}{\eta_\ell}\left[\frac{\partial P}{\partial r} - \frac{\partial P_{cap}}{\partial u}\frac{\partial u}{\partial r} - \frac{\partial P_{cap}}{\partial T}\frac{\partial T}{\partial r}\right] \tag{20}$$

Transport of Water Vapour

The gas phase inside the paper sheet consists of water vapour and air and can be considered as a binary system. Departing form the basic equation for mass transfer in such systems, as given by Bird et.al. (8), it can be derived that:

$$j_v^s = j_{v,conv}^s + j_{v,diff}^s \tag{21}$$

in which the convective vapour flux is given by

$$j_{v,conv}^s = (j_v^s + j_a^s)\omega_v \tag{22}$$

and the diffusive vapour flux by

$$j_{v,diff}^s = -D_{eff}\frac{\rho_v + \rho_a}{\varepsilon}\frac{\partial \omega_v}{\partial r} \tag{23}$$

It should be remarked, that in these equations the fluxes and concentrations are expressed as bulk quantities. D_{eff} is the binary vapour-air diffusion coefficient in a porous and tortuous phase.

The convective vapour flux can again be described with Darcy's law for gas flow in porous medium:

$$j_{v,conv}^s = -\rho_v' \frac{K_g}{\eta_g}\frac{\partial P}{\partial r} \tag{24}$$

where, by applying the ideal gas law:

$$\rho_v' = \frac{P_w M_w}{RT} = \frac{a_w P_w^o M_w}{RT} \tag{25}$$

Because paper drying occurs at rather high temperatures it is assumed here that local thermodynamic equilibrium exists and therefore a_w in Equation (25) is taken

from the water vapour sorption isotherm at the local moisture concentration. Especially at low moisture concentrations and low temperatures this assumption might be no longer valid.

The diffusive vapour flux can be worked out further by transforming the concentrations into vapour pressures and activities by means of the ideal gas law:

$$j_{v,diff}^{s} = -D_{eff}\frac{M_a}{\overline{M}}\frac{P_w M_w}{RT}\left[\frac{\partial ln a_w}{\partial u}\frac{\partial u}{\partial r}+\left(\frac{\partial ln a_w}{\partial T}+\frac{\partial ln P_w^o}{\partial T}\right)\frac{\partial T}{\partial r}-\frac{1}{P}\frac{\partial P}{\partial r}\right] \quad (26)$$

The total vapour flux reads now:

$$j_v^s = -\left[D_{eff}\frac{M_a}{\overline{M}}\frac{P_w M_w}{RT}\frac{\partial ln a_w}{\partial u}\right]\frac{\partial u}{\partial r}$$

$$-\left[D_{eff}\frac{M_a}{\overline{M}}\frac{P_w M_w}{RT}\left(\frac{\partial ln a_w}{\partial T}+\frac{\partial ln P_w^o}{\partial T}\right)\right]\frac{\partial T}{\partial r} \quad (27)$$

$$-\frac{P_w M_w}{RT}\left[\frac{K_g}{\eta_g}-D_{eff}\frac{M_a}{\overline{M}}\frac{1}{P}\right]\frac{\partial P}{\partial r}$$

Transport of Bound Water

Within the solid phase the mass transfer of water can be seen as a diffusion process:

$$j_b^s = -D_b\frac{\partial \rho_b}{\partial r} \quad (28)$$

This equation, which in fact gives the definition of the diffusion coeffcient D_b can also be written as:

$$j_b^s = -D_b\left(\frac{\partial \rho_b}{\partial u}\frac{\partial u}{\partial r}+\frac{\partial \rho_b}{\partial T}\frac{\partial T}{\partial r}\right) \quad (29)$$

Total transport of water

By combining the above equations (20), (27) and (29) the total mass flux of water can be found.

LUMP MODEL

In this model the paper sheet is considered as a pseudo binary system with the components water (w) and solid fibers (s). The effect of air and bound water both on mass and heat transfer are assumed to be of minor importance. For the sake of convenience only those situations are considered here, where pressure gradients are very low and do not need to be taken into account. Thus mass and heat fluxes are expected to be dependent on gradients of moisture concentration and temperature only.

Mass and heat transfer

Similar to Bird et.al. (8) the basic equation for mass transfer in a pseudo binary system is given by

$$n_w = (n_w + n_s)\omega_w - D_u\rho\frac{\partial\omega_w}{\partial r} - D_T\frac{\partial T}{\partial r} \tag{30}$$

In fact the transport parameters D_u and D_T are defined by this equation, which expresses the mass flux with respect to a fixed coordinate system (Euler). By eliminating the solids flux n_s by using Equation (17) and transforming $\omega_w \to u$ and $n_w \to j_w^s$ and $r \to z$ gives:

$$j_w^s = -D_u\rho_s^2\frac{\partial u}{\partial z} - D_T\rho_s(1+u)\frac{\partial T}{\partial z} \tag{31}$$

For an adequate approach of the heat transfer it still remains necessary to split up the moisture flux in a liquid flux and a vapour flux:

$$j_w^s \approx j_\ell^s + j_v^s \tag{32}$$

and by defining a new set of transport parameters L and V:

$$j_\ell^s = -L_u\frac{\partial u}{\partial z} - L_T\frac{\partial T}{\partial z} \tag{33}$$

and

$$j_v^s = -V_u \frac{\partial u}{\partial z} - V_T \frac{\partial T}{\partial z} \tag{34}$$

According to equation (10) the heat flux is given by:

$$q^s \approx j_\ell^s h_\ell + j_v^s h_v - \lambda \rho_s \frac{\partial T}{\partial z} \tag{35}$$

or by defining the transport parameters Q:

$$q^s = -Q_u \frac{\partial u}{\partial z} - Q_T \frac{\partial T}{\partial z} \tag{36}$$

The transport parameters are interrelated by:

$$D_u \rho_s^2 = L_u + V_u \qquad\qquad D_T \rho_s(1+u) = L_T + V_T$$

$$\tag{37}$$

$$Q_u = L_u h_\ell + V_u h_v \qquad\qquad Q_T = L_T h_\ell + V_T h_v + \lambda \rho_s$$

Expressing the lump parameters L and V in terms of the mechanistic parameters gives:

$$L_u = -\rho_s d_w \frac{K_\ell}{\eta_\ell} \frac{\partial P_{cap}}{\partial u} \tag{38}$$

$$L_T = -\rho_s d_w \frac{K_\ell}{\eta_\ell} \frac{\partial P_{cap}}{\partial T} \tag{39}$$

and

$$V_u = \rho_s D_{eff} \frac{M_a}{\overline{M}} \frac{P_w M_w}{RT} \frac{\partial ln a_w}{\partial u} \tag{40}$$

$$V_T = \rho_s D_{eff} \frac{M_a}{\overline{M}} \frac{P_w M_w}{RT} \left(\frac{\partial ln a_w}{\partial T} + \frac{\partial ln P_w^o}{\partial T} \right) \tag{41}$$
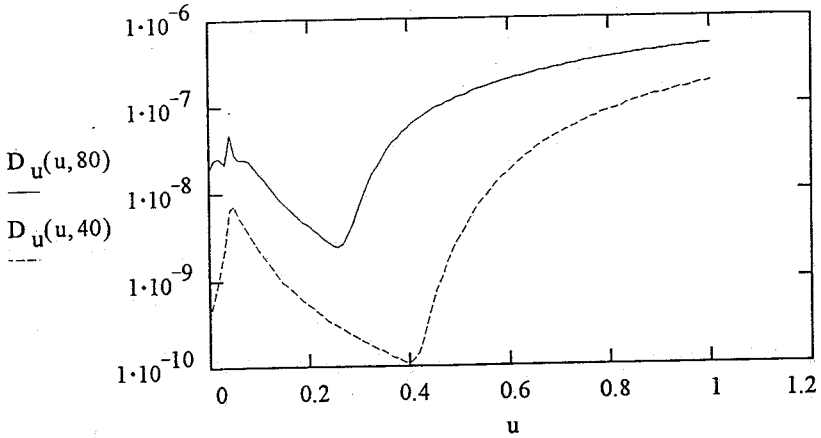
$D_u(u,80)$
——
$D_u(u,40)$
- - -

FIGURE 2. Moisture diffusivity D_u calculated from transport parameters L_u and V_u at 40 °C respectively 80 °C.

SIMULATION OF DIFFUSION COEFFICIENT

In order to calculate the transport parameters the following properties of the paper sheet (2, 9) are required:

   Densities d_s and $d_{s,ap}$.
   Water vapour sorption isotherm $a_w = a_w(u,T)$.
   Capillary pressure $P_{cap} = P_{cap}(u,T)$.
   Liquid permeability $K_\ell = K_\ell(u,T)$.
   Gas permeability $K_g = K_g(u,T)$.
   Effective vapour/air diffusivity $D_{eff} = D_{eff}(P,T)$.
   Shrinkage coefficient $\sigma = \sigma(u,T)$.
   Moisture concentration at fiber saturation $u_{fs} = u_{fs}(T)$.
   Heat conductivity $\lambda = \lambda(u,T)$

More details about these properties will be published in future. As an example in Figure 2 a simulation of the diffusion coefficient D_u, according to equations (37), (38) and (40) in Mathcad®4.0 is given.

In Figure 2 the effects of the transport mechanisms can clearly be distinguished. At high moisture contents liquid flow due to capillary forces is dominating. At

decreasing moisture content the amount of liquid in the pores also decreases and a gas phase is built up, causing a decrease of the liquid permeability. In the porous structure with an increasing vapour permeability the mass transfer is taken over gradually by vapour diffusion. These effects cause a minimum in the diffusivity. At the fiber saturation point (u_{fs}= 0.37 kg w/kg solid at 40 °C and u_{fs}=0.23 kg w/kg solid at 80 °C) there is no longer liquid available in the pores and the mass transport is taken over completely by vapour diffusion. The maximum in the diffusivity at low moisture concentrations is due to a maximum in the slope of the sorption isotherm. A similar behaviour of the diffusivity has also been found by Ketelaars (10) for clay materials, where the diffusivity has been calculated from moisture profiles, determined accurately by neutron absorption in isothermal and isobaric drying experiments.

CONCLUSIONS

In modelling the drying behaviour of paper sheets the effects of shrinkage can be accounted for adequately by introducing the solids based parameters u, H, z, j_ℓ^s, j_v^s, q^s and a shrinkage coefficient σ. The transport parameters for mass and heat can be expressed in terms of mechanistic parameters. As an example the classical isothermal moisture diffusion coefficient is calculated as function of the moisture content; this relationship shows a maximum and a minimum. More research will be needed to establish the experimental data and to verify the mechanistic approach.

ACKNOWLEDGEMENTS

NOTATION

			Subscripts	
ε	volume fraction gas phase	[m³/m³]	a	air
η	viscosity	[Pa.s]		

λ	heat conductivity	[W/m K]
ρ	concentration	[kg/m^3 total]
σ	shrinkage factor	[m^3/m^3]
ω	weight fraction	[kg/kg total]
D	diffusivity for mass	[m^2/s]
D	diffusivity for enthalpy	[kg/(m s K)]
d	density	[kg/m^3]
H	humid enthalpy	[J/kg solid]
h	enthalpy	[J/kg]
j	diffusive mass flux	[kg/m^2 s]
K	permeability	[m^2]
L	transport parameter	[see Eq. (38), (39)]
M	molecular mass	[kg/mol]
n	mass flux in fixed coordinate system	[kg/m^2 s]
P	pressure	[Pa]
Q	transport parameter	[see Eq. (36)]
q	heat flux	[J/m^2 s]
R	gas constant	[J/mol K]
r	fixed space coordinate	[m]
T	temperature	[K]
t	time	[s]
u	moisture concentration	[kg w/kg solid]
V	transport parameter	[see Eq. (40), (41)]
v	velocity	[m/s]
z	solids based space coordinate	[kg solid/m^2]

ap	apparent
b	bound
cap	capillary
eff	effective
fs	fiber saturation
g	gas
ℓ	liquid
max	maximum
s	solid
v	vapour
w	water

Superscripts

o	saturated
s	solid
/	gas phase

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