Temperature influence on drying regime maps for the prediction of particle distribution in particle-filled polyvinyl alcohol films

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Incorporation of nanoparticles into a polymer matrix is a way to modify material properties such as tensile strength, biocompatibility or optical properties. The functionality of these composites depends on the material selection as well as on the component distribution. The latter is strongly affected by the dispersion stability as well as the process conditions during drying.

In this work drying regime maps for particle dispersions with dissolved polymer were calculated with a 1D simulation of the early drying phase, based on predictive models of Cardinal and Jung [1] and Buss [2]. In the model sedimentation of particles, diffusion of particles and polymer and evaporation with consideration of the mass transport in the gaseous phase was implemented. The ternary diffusion in the system was modelled with quasi-binary approach. The simulation shows that three different regimes exist: An evaporation regime with particle accumulation at the top of the coating, a sedimentation regime with particle accumulation at the bottom of the coating and a diffusion regime where the particles are distributed equally over the film thickness. The borders of the regimes can be described as function of sedimentation N_S and Peclet Number Pe_c:

$$N_s = \frac{U_0}{E_0} \qquad Pe_c = \frac{E_0 h_0}{D_0} \tag{1}$$

To account for evaporative cooling that occurs during industrial drying an energy conservation equation was implemented in the model. The non-isothermal boundary condition which is schematically shown in Fig. 1 causes a temperature shift during drying which induces a shift of the drying regime borders.

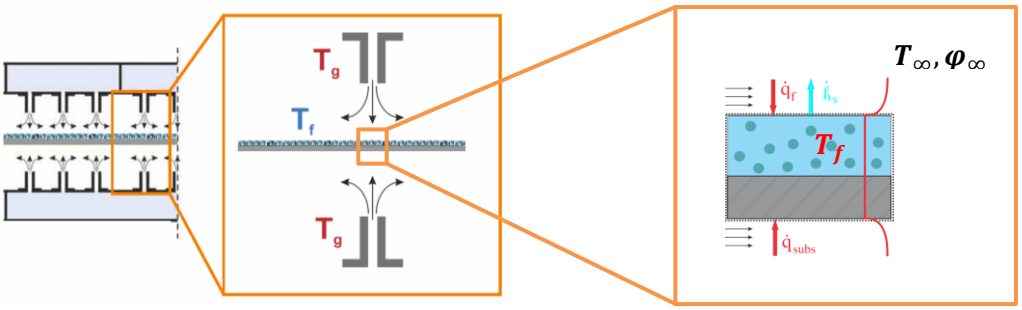

Fig. 1. Schematic drawing of the boundary conditions for the energy conservation equation

For the validation of the model two different experimental methods were used: Cryogenic scanning electron microscopy and 3D Micro Raman Spectroscopy. In Cryo-SEM experiments, PVA-films with silica particles were dried for a certain time. The drying process was stopped by vitrifying the films. The vitrified films were subsequently fractured to expose their cross-sections and imaged on a liquid nitrogen cooled stage. The fracture exposes particles along the cross-sections. All three regimes predicted by the simulation could be qualitatively shown with this technique. Additionally, PVA films with incorporated PS particles were prepared under similar conditions. The lateral 3D component distribution in the dry films was measured by imaging cross sections with confocal 3D Raman Spectroscopy. The experimental results match the predictions of the drying regime maps very well.

References

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2. F. S. Buss, K. Crawford, C. C. Roberts, K. Peters, and L. F. Francis, *J. Colloid and Interface Sci*., **359**, 112-120 (2011).