

Modeling the Drying Process of Thin Coatings

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Abstract

There are few computer programs available on the market today for predicting dryer performance and calculating the kinetics of the drying of thin coatings. Additional problems include controversy about which empirical parameters should be used, how much experimental data are required for input, and the fact that the calculations are often complicated. Because of the complexity of the calculations, clarity and insight are lost regarding the drying process and how accurately the models can be applied for dryer design or process optimization. A new drying model was developed which, in the first stage, provides a simulation of the drying process through water/solvent evaporation, and in the second stage, simulates water/solvent transfer through the coating, which is controlled by diffusion transient conditions. Diffusivity, in turn, is dependent upon concentration, temperature and nature of the coating. With these assumptions, two problems arose and were solved: one concerned with the elaboration of a method for determination of the diffusivity and evaporation rate, the other with the construction of a model capable of calculating the weight loss and coating temperature at any time.

This new comprehensive drying process simulator calculates the entire drying process under transient conditions. This model supports multiple coating layers, unlimited amount of drying zones, permits many different conditions to be simulated, and was demonstrated to provide good predictions based on comparison with a large number of experimental data.

Introduction

The removal of volatile solvents from a coated film of polymeric solute that ultimately remains as permanent coating is an important step in forming thin polymer coatings from polymer/solvent solutions. Examples of such coatings include adhesive tapes, photographic films, and gravure inks. Drying ovens can have a variety of configurations, from parallel air flow to air impingement. Dryers may also contain other energy sources including infrared and radio frequency heaters. Infrared heaters are frequently added to the normal convection drying systems to increase the capacity of dryers.

A variety of drying models have appeared in the literature [1-5]. To be adequately modeled, the following facts were considered: the composition dries by solvent/water evaporation without chemical reactions and the solvent plays

the role of diluent. A new three stage drying model was developed which, in the first stage, predicts the rate of temperature change of the film under unsteady state conditions. In the second stage the model provides a simulation of the drying process through water/solvent evaporation in steady turbulent flow over a wetted surface. In the third stage the model simulates water/solvent transfer through the coating, which is controlled by diffusion transient conditions. The accuracy of the diffusion theory for drying depends on the fact that the diffusivity is not constant but varies with moisture content. In practice, an average value of diffusivity established experimentally on the material to be dried is used.

Accurate drying predictions for polymer/solvent/water coatings require a satisfactory description of the polymer/solvent mutual diffusion coefficients. Diffusion coefficients can be determined from sorption/desorption experiments, NMR or infrared spectroscopic techniques, inverse gas chromatography, etc. If experimental data are not available, predictive theories can be used⁶, although they may not lead to quantitative drying calculations. In this paper, we examine the inverse problem of establishing a satisfactory description of the diffusion coefficients from drying experiments. We determine "effective" parameters for the diffusion coefficients from the drying data. We apply the method to water and solvent based solutions and show that the effective parameters can accurately describe the diffusional behavior of polymer/solvent systems, that agree with published diffusion data and lead to quantitative drying predictions in a pilot and production dryers. The model accounts for the very large variations of the diffusivity with temperature and concentration and removes the necessity of having to perform a large number of difficult and expensive experiments and in some cases, the value of the diffusivity is so low that experimental determination is practically impossible. Furthermore, evaluation of the parameters of the model requires information that is usually available (density, viscosity, specific gravity, etc.) plus a small amount of measured parameters (air temperature, relative humidity, total pressure, air velocity, etc.).

Modeling the Drying Process

We assumed that the temperature gradient in the film is negligibly small because of the film being very thin and that there is no convective flow in the film because of the high viscosity of the solution. In a system of convection drying

(Figure 1) when the temperature of the heated air, its humidity, and velocity are maintained constant, the drying process can be divided into three periods of drying. The first period is calculated based on equation for unsteady state conduction ($\partial t/\partial \tau > 0$). The second period is represented by a constant body temperature ($\partial t/\partial \tau = \text{const.}$) and by a constant rate of evaporation ($\partial W/\partial \tau = \text{const.}$). In the third period of drying the rate of moisture content ($\partial W/\partial \tau < 0$) decreases continuously but the temperature of the body increases continuously ($\partial t/\partial \tau > 0$). The transition from one to another is represented by a certain critical moisture content on the surface of the material. The three periods of the drying process are quite clearly separated under mild conditions and high initial moisture content of the body. Under severe conditions the drying process goes on intensively, the moisture content and temperature of the body vary continuously and it becomes impossible to distinguish the periods referred to.

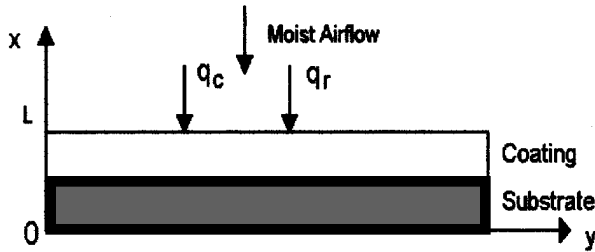


Figure 1. Thin coating in flowing airstream.

Modeling is divided into three steps: the transient period, the constant rate period, and the falling-rate period. The heat transfer coefficient at a drying conditions must be known.

Transient Period of Drying

Before steady-state evaporation will take place, the temperature of the coating increases until the rate of the sensible heat transfer to the surface equals the rate of heat removed by evaporation. We can calculate parameters of this process from the solution of one-dimensional heat transfer equation with assumption that heat of evaporation is negligible.

To predict the temperature change of a film the following equation can be written:

$$\rho * c_p \partial t / \partial \tau = q$$

Solution of this equation is:

$$t = t_0 + \vartheta * \tau / L * \rho * c_p$$

$$\tau^* = L * \rho * c_p * (t - t_0) / \vartheta$$

$$q = \vartheta / L, \text{ heat source per unit volume and time,}$$

$c_p = f_1 * c_{p1} + f_2 * c_{p2}$, specific heat of the mixture, and

$$f_1' = f_1 / (f_1 + f_2)$$

$$f_2' = f_2 / (f_1 + f_2)$$

If ϑ represents the total heat arriving at the surface, then:

$$\vartheta = \vartheta_C + \vartheta_R = \vartheta(t^*)$$

The heat received at the surface by convection is controlled by the appropriate convection heat - transfer coefficient:

$$\vartheta_C = h * (t_A - t^*)$$

The heat received by radiation may be estimated by:

$$\vartheta_R = \epsilon (1730) (10^{-12}) (T_R^4 - T_{WEB}^4)$$

Constant Rate Period

Heat and mass transfer between the air and moving sheet or web are effected by boundary air layer. Boundary air layer is divided into laminar and turbulent zones. The heat is transferred through the boundary layer by conduction and convection, and released vapors are removed by diffusion and convection. Consider a steady turbulent flow over a wetted surface we can assume the liquid-vapor interface to be at zero velocity, which results in a slow moving layer of air in laminar flow next to the evaporation surface. Within the laminar sublayer, only molecular diffusion can occur. In the turbulent region, eddy diffusion is the main mechanism of mass transfer. Reliable mass transfer coefficients were established experimentally for a number of flow geometries⁷⁻¹². Because of the analogy between these transfer processes, heat transfer data have been used to predict mass transfer coefficients.

At the conditions of dynamic equilibrium between the heat transfer and the vapor removal from the surface, when other sources of heat are usually negligible, the drying rate is expressed by the following equation:

$$\partial \omega / \partial \tau = A * h * (t_A - t_s) / \lambda = K_m * A * (p_s - p)$$

At constant rate period the drying proceeds by diffusion of vapor from the saturated surface into the drying chamber. Moisture movement is rapid enough to maintain saturated conditions at the surface, and the rate of drying is controlled by the rate of heat transfer to the evaporating surface. The rate of mass transfer balances the rate of heat transfer, and the temperature of the saturated surface remains constant. The mechanism of moisture removal is equivalent to evaporation from water and is essentially independent of the nature of the polymer in the film. In this case, dynamic equilibrium is established between the rate of heat transfer and the rate of vapor removal from the surface:

$$R = - (L/A) * (\partial W / \partial \tau) = (h/\lambda) * (t_A - t_s)$$

If the drying takes place entirely within the constant rate period, so that W_1 and $W_2 \geq W_C$, and $R = R_C$, equation becomes:

$$\tau_c = [L*(W_1 - W_2)]/(R_C * A)$$

For calculating constant drying rate for this case we can use:

$$R_c = [h_C*(t - t'_w) + h_R*(t_R - t'_w)]/\lambda$$

And if no radiation occurs:

$$R_c = [h_C*(t - t'_w)]/\lambda$$

The heat and mass transfer coefficients are satisfactory related at the same Reynolds number by the Chilton-Colburn relationship:

$$h_C/R_C * C_S = Le^{2/3}$$

At low diffusion rates, where the heat-transfer analogy is valid, the ratio of the heat transfer coefficient to the mass transfer coefficient is equal to the specific heat per unit volume at constant pressure of the mixture:

$$R_c = h_C/C_S$$

In estimating drying rates, the use of heat transfer coefficient is preferred because they are usually more reliable than mass transfer coefficients. Small errors in temperature, have negligible effect on the heat transfer coefficient, but a relatively large error in the partial pressure and so in the mass transfer coefficient.

Coefficient of heat transfer is constant only during the constant rate period of drying; in falling rate period it decreases continuously, gradually approaching the value of the coefficient of heat transfer for dry material.

Most air calculations are based on an atmospheric pressure of 760mmHg. If the total pressure is different from 760mmHg, the humidity at a given wet-bulb and dry-bulb temperature must be corrected. Also corrections should be made for specific volume, the saturation-humidity curve, and the relative humidity curves.

Temperature of Evaporating Surface

When radiation and conduction are negligible the temperature of the evaporating surface approaches the wet-bulb temperature and is readily obtained from the humidity [13] and dry-bulb temperature:

$$t_w = t_A - \lambda / [(0.24 + 0.446 w) * Le^{2/3}]$$

If in addition to convection heating we assume that an amount q_R of infra-red energy per unit area is added to the drying film, then a rate balance between evaporation and heat transfer may be written as follows:

$$\lambda*(w_s - w)/C_S = (t - t'_{WEB}) + h_{CW}*(t - t'_{WEB})/h_C + h_R*(t_R - t'_{WEB})/h_C$$

It is assumed that heating with air on both sides of the web. This equation may be solved to estimate value of the wet-bulb temperature t'_s . For the air-water vapor mixture:

$$C_S = C_A + C_{sv}*w$$

For the solvent containing air:

$$C_S = C_A + (C_{solv} - C_A)*w_{sv}$$

And humidity ratio and saturation humidity are:

$$w_{sv} = [p_A/(p - p_A)] (M_{sv}/M_A)$$

$$w_s = [p_{ws}/(p - p_{ws})] (M_{sv}/M_A)$$

Water vapor saturation pressure over liquid water for the dry-bulb temperature is calculated according:

$$p_{ws} = e^{-A/T} * e^{-B} * e^{-C*T} * e^{-D*T^2} * e^{-E*T^3} * e^{H*\ln(T)}$$

Where temperature is expressed in degrees Rankine by the relation:

$$T^{\circ}R = t^{\circ}F + 459.67$$

Partial pressure of water vapor can be calculated from:

$$p_w = p_{ws} * \phi$$

Radiation heat transfer coefficient h_R can be estimated by the following equation if the web temperature t'_s is known¹⁴:

$$h_R = \epsilon (1730)^*(10^{-12})*(T_R^4 - T_{WEB}^4)/(t_R - t'_{WEB})$$

The Falling Rate Period

As soon as liquid concentration on the surface decreases below saturation, the drying enters into falling rate period. The rate of water removal decreases with drying time during this period. The drying rate during the falling rate period becomes more dependent upon the transport of the liquid through the film to the surface, rather than on the rate of heat transfer, and the solvent evaporates as soon as it reaches the surface. Solvent transport to the surface may take place by liquid diffusion and the temperature of the film should not be raised above the boiling point.

The following assumptions were made: thin films were considered to have a one-dimensional diffusion; at the beginning of the evaporation process the concentration of solvent/water throughout the coating was constant; solvent/water transfer through the coating was controlled by diffusion under transient conditions, with concentration-dependent diffusivity; the rate of evaporation from the surface was either constant or proportional to the surface

concentration; despite the shrinkage of the coating during the process, the thickness of the coating was assumed to remain constant for calculations. The solvent/water transfer through the coating follows the one-dimensional diffusion equation:

$$\partial\rho/\partial\tau = \partial/\partial x (D*\partial\rho/\partial x)$$

The falling rate period begins when the moisture content is below the critical moisture content point (W_c). The plane of evaporation moves into the film. The drying is now governed by the rate of internal moisture movement. In drying to low moisture contents, this period is mainly determining the over-all drying time. The diffusion rate within the film is dependent upon the form of water/solvent binding and process parameters. The relative diffusion resistance indicates the reduction factor for the diffusion rate in the film to the rate of evaporation from the surface to the air stream at the same pressure and temperature. The relative diffusion resistance can be estimated¹⁵. Since the outer layers lose moisture before the interior, the moisture gradient near the surface increases and also increases the resistance to diffusion in the outer layers.

The falling rate frequently can be expressed with a fair accuracy, over the required range of moisture content, by the following equation:

$$\partial W/\partial\tau = -K_1*(W - W_p)$$

Drying rates are always specified in the quantity of water/solvent that can be evaporated per square foot per hour. K_1 is a function of the constant rate as follows:

$$K_1 = -R_c/(W_c - W_p)$$

Drying coefficient K_1 is found from:

$$K_1 = -[h_c * (t_A - t_w)]/[\rho*s*\lambda*d*(W_c - W_p)]$$

The falling rate for this case:

$$\partial W/\partial\tau = -[h_c*(t_A - t_w)*(W - W_p)]/[\rho*\lambda*d*(W_c - W_p)]$$

Thus:

$$\tau = \{4*d^2 * \ln [(W_c - W_p)/(W - W_p)]\}/(D*\pi^2)$$

Web Temperature in the Falling-Rate Period

The following equation is written for general case, when coating heated by air from both sides and with radiation heat supply added from coated side:

$$\Sigma(C_{pi} m_i)*\partial t_{WEB}/\partial\tau = h_c*(t_A - t_{WEB}) + h_R*(t_A - t_{WEB}) + h_{CW}*(t_A - t_{WEB}) - \lambda*\partial W/\partial\tau$$

This equation can be solved numerically for the web temperature:

$$t_{w_i}(\tau) = [B*t_{w_{i-1}} + t_A*(h_c + h_{CW} + h_R) - \lambda*R_i]/(B + h_c + h_{CW} + h_R)$$

Where B is:

$$B = 1/(\tau_i - \tau_{i-1}) * [C_w * m_w * L + m_c*(C_s + C_{sv} * W_i)/100 - W_i]$$

The Program

We developed the original model of the drying process built on the theoretical base and proven by significant numbers of experimental data. The model has an accurate predictive capabilities and many different conditions can be simulated with this model. Multiple areas of the program windows reflect the structure of design information: Dryer Input Data, Results of Calculations, Ink/Coating Parameters, Database, Graphics and Tables.

It will increase productivity and profitability and reduce drying time by improving dryer efficiency, analyzing and changing dryer conditions and heat transfer. With experimental data model can be customized to a particular drying system, providing an accurate representation of the drying process.

The calculations below were performed for drying of water based inks in impingement drying system with five intercolor dryers. The main screen with the calculations for the first dryer is shown in Figure 2.

Graphs for the water content and drying rate are presented in Figure 3 and 4. Agreement between the model calculations and the experimental data shows the reliability of the proposed drying model as shown in Figure 3.

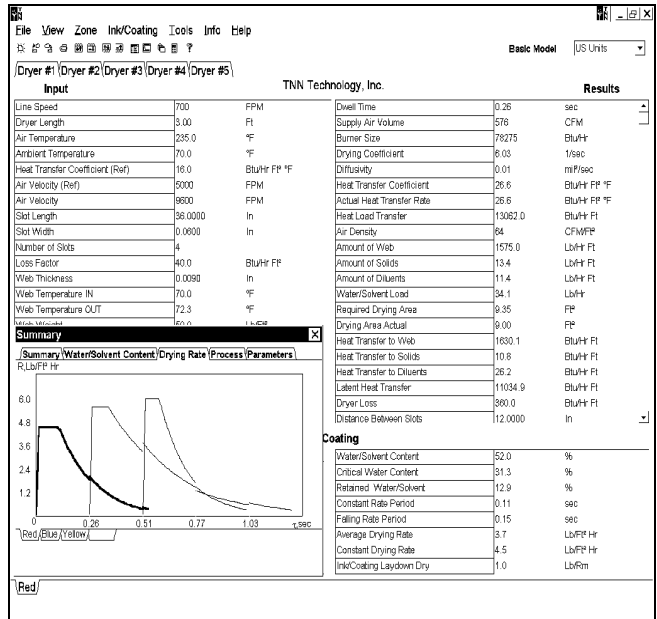


Figure 2. Output main screen of the program.

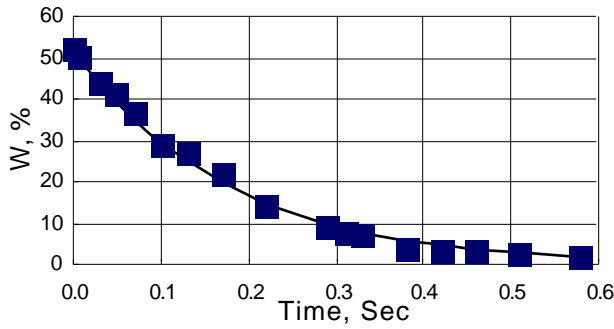


Figure 3. Model calculations vs. experimental data for water based ink.

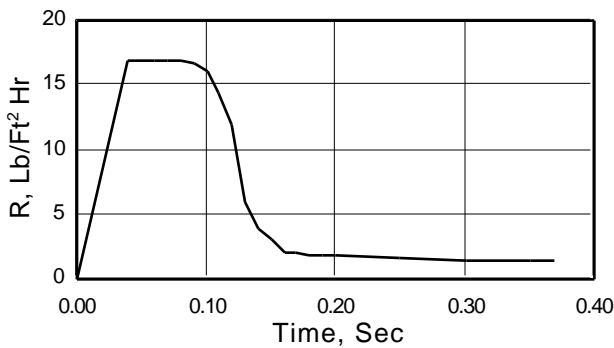


Figure 4. Calculated drying rate for the first ink layer.

The Data Summary dialog is presented in Figure 5.

This new comprehensive drying process simulator calculates the entire drying process under transient conditions. This model supports multiple coating layers, unlimited amount of drying zones, permits many different conditions to be simulated, and was demonstrated to provide good predictions based on comparison with a large number of experimental data. Our model applicable for the coating thickness from 0.0001in to 0.006 in, for air temperature range 50°F -500°F, and air velocity range 2000FPM - 15000FPM. We believe that our approach will have considerable value to practicing engineers who would like to apply mathematical models to their drying problems, process optimization, and design projects.

Summary						
Summary		Water/Solvent Content		Drying Rate		Process Parameters
Total Dwell Time		1.29				sec
Maximum Air Temperature		275.0				°F
Maximum Air Velocity		11000				FPM
Total Water/Solvent Load		140.3				Lb/Hr
Average Drying Rate		2.3				Lb/Ft² Hr
Total Supply Air Volume		4572				CFM
Total Burner Size		699970				Btu/Hr
Air/Solvent Ratio		11742.626				SCF/Gal
25% LEL		2807.563				SCFM
40% LEL		1754.727				SCFM

Summary						
Summary		Water/Solvent Content		Drying Rate		Process Parameters
Name	Units	1	2	3	4	5
Dryer Length	Ft	3.00	3.00	3.00	3.00	3.00
Air Temperature	°F	235.0	275.0	275.0	275.0	275.0
Air Velocity	FPM	9600	9600	11000	9600	11000
Web Temperature IN	°F	70.0	72.3	79.7	84.5	92.1
Web Temperature OUT	°F	72.3	79.7	84.5	92.1	110.1
Heat Transfer Coefficient	Btu/Hr Ft² °F	26.6	26.6	29.6	26.6	29.6

Figure 5. Portion of Summary dialog, showing some of the dryer specification data.

Symbols

- τ - time, sec
- w - humidity ratio
- w_s - saturation humidity ratio
- W - water content, %
- C - heat capacity, Btu/Lb
- D - diffusivity, mil²/sec
- λ - latent heat of evaporation, Btu/Lb
- t - dry-bulb temperature, °F
- t_s - wet bulb temperature, °F
- t_w - web temperature, °F
- t_A - supply air temperature, °F
- T - absolute temperature, °R
- ϕ - relative humidity
- p - pressure, psia
- p_w - partial pressure of water vapor, psia
- p_{ws} - saturation vapor pressure, psia
- h_c - convection heat transfer coefficient, Btu/Hr Ft² °F
- h_r - radiation heat transfer coefficient, Btu/Hr Ft² °F
- h_c - convection heat transfer coefficient from web side, Btu/Hr Ft² °F
- m - amount of material, Lb/Ft²

ρ - mass density or concentration, Lb/Ft³
 M_{sv} - molecular weight of the solvent
 M_A - molecular weight of the air
 Le - Lewis Number
 f_1 - volume fraction of the coating
 f_2 - volume fraction of the web
 L - thickness of the coating, Ft

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