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MODELING OF INFRARED DRYING OF POLYMER SOLUTIONS

by

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B.Sc. in Chemical Engineering, Bangladesh University of Engineering and Technology,

Bangladesh, 2001

A thesis

presented to Ryerson University

in partial fulfillment of the

requirements for the degree of

Master of Applied Science

in the program of

Chemical Engineering

Toronto, Ontario, Canada, 2008

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MODELING OF INFRARED DRYING OF POLYMER SOLUTIONS

Md Zia-ul Islam

Master of Applied Science, 2008 Department of Chemical Engineering

Ryerson University

Abstract

This thesis presents the development of dynamic models for drying a coating polymer layer placed on fixed and moving substrate in a dryer using infrared (IR) heat source. The IR drying model is a set of coupled nonlinear partial differential equations (PDEs) arising from simultaneous mass and heat balances and they describe variations of the solvent concentration and the polymer system temperature during the drying process. The model was numerically solved in MATLAB environment and then validated using data from literature. Using polyvinyl acetate (in toluene) as a coating material on a polyester substrate, the simulation revealed that the model agrees with data and describes adequately well the drying kinetics. The modeling approach was also extended to simulate the drying of a polymer solution in a container. Since solvent and polymer molecular sizes are quite different, the diffusion coefficient was better described with free volume theory.

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Dedication

I would like to dedicate this thesis to those who work hard and sacrifice for the betterment of others.

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Nomenclature

A, B, C	Antoine constant
C ₀ -C ₃	Coefficients
Ср	Specific heat, J/g. K
с	concentration, g/cc
D _h	Hydraulic diameter, cm
Da	Diffusivity of solvent in air, cm ² /s
d	Distance, cm
ŴFH	Available free volume
h	Convective heat transfer coefficient, W/cm ² .K
h _{des}	Heat of desorption of toluene, J/g
Н	Solvent content, g solvent/100 g dry solid
Ha	Air solvent content, g solvent vapor/100 g dry air
H _{sat}	Saturated solvent content
k _a	Thermal conductivity of air, W/cm. K
k _m	Mass transfer coefficient, g/cm ² .s
1	Thickness, cm
L	Length, cm
m	Mass, g
М	Mass flow rate, g/s

т _{еvар}	Rate of evaporation, g/s.cm ²	
Р	Atmospheric pressure, mm Hg	
Pr	Prandtl number, $Cp_a\mu_a/k_a$	
P _{sat}	Saturated vapor pressure, mm Hg	
q	Heat flux, W/cm ²	
Re	Reynolds number, $\rho_a V_a D_h / \mu_a$	
Sc	Schmidt number	
Т	Temperature, K	
t	Time, s	
V	Velocity, cm/s	
\widehat{V}^*	Critical hole free volume	
Ŷ	Specific volume (cc/g)	
W	Width, cm	
z	Distance along the length of the dryer	

Greek Letters

Δh_{v}	Latent heat of vaporization, J/g
Δz	Space interval, cm
8	Emissivity
μ	Viscosity, g/cm.s

ρ	Density, g/cc	
σ	Stefan-Boltzmann constant, W	$V/cm^2 K^4$
3	Shape factor	
ω	Mass fraction	
x	Flory _ Huggin parameter	
φ	Volume fraction	
α	correcting factor	

Subscripts

а	Air	
des	Desorption	
exp	Experimental	
р	Polymer/ product	
ра	Polymer solution to air	
r	Radiant	
ra	Radiant to air	
sat	Saturated	
sim	Simulated	
sol	Solvent	
sub	Substrate	
v	Vapor	

CHAPTER 1

1. Introduction

Since drying process is one of the oldest and most commonly encountered unit operation in chemical engineering, it has been extensively studied, as it depends upon the nature of the processing mode, physical state of the feed, mode of heat and mass transport, operating temperature and pressure, and other factors. A detailed drying transport phenomenon is not quite well understood. Drying requires massive amounts of energy to heat the drying gas and thus has high operating costs. Drying equipment also represents one of the greatest capital expenditures for the production of coated webs. Recent data show that 10-15% of the total industrial energy consumption is due to drying (Kerkhof et al., 2002) which is substantially high. Many products and processes require a range of quality aspects, e.g. moisture content, bulk density, particle size distribution, flowability, wettability, dust formation and more specific aspects such as color, flavor, brittleness, cracks, enzymes, volatile flavor compounds, removal of solvents. Hence, the drying process is much more than just the removal of water or solvent; it is rather the creation of a number of product properties (Mujumdar, 2002). Besides, the awareness about environmental regulations compels industry to focus on reducing energy consumption and associated CO₂ production, and on minimizing hazardous product emissions (Kerkhof et al., 2002).

Conventional convective drying systems, in which heated air serves as both the source of energy and moisture removal medium, is inherently slow and may not be suitable to dry out some delicate products. As a result, large drying equipments, even though expensive to operate, are inevitably utilized. Hot air flowing over or going through a wet solid surface does not often supply enough thermal energy to extract the moisture out of the solid. Besides, the presence of oxygen in air may not be tolerated in some special applications such as in the drying of minerals, food, and polymer products. Alternatively, thermal energy supplied by electromagnetic waves is able to penetrate deep in moist products and heat up trapped water or solvent. In particular, IR (Infrared) radiation is an electromagnetic spectrum and possesses features that make it attractive for the drying of special materials.

Compared to hot air, steam or other contact drying means, IR drying in particular, presents some advantageous features, for example, it allows a faster rate of evaporation of water without distortion of the material internal structure. IR drying can be beneficial to food industrial products, polymer products, and also to mineral and biological materials. One major advantage of IR drying is that the power density can be six to ten times higher than that in convective drying with hot air, thereby reducing the drying time. Other advantages of IR drying include: possibilities to selective heating; no presence of gas phase as in convective drying; no direct contact as in contact drying, so contamination by dust is avoided, and fast response times are possible.

Many industrial products based on polymer solutions (varnishes, gels, patches) must be dried before being put into final usable form. Most of these products are thin coating layers prepared by spreading polymer-solvent solutions onto moving substrates; for example, adhesive tapes, magnetic media, paints, protective coatings, and imaging coatings are often produced this way. However, improper drying conditions may create a variety of dryinginduced defects such as blister, warping, cracks, etc.

In a simultaneous coating and drying process, a layer of polymer solution is deposited onto a substrate. The solidification of the deposited liquid layer may be achieved in various ways: on the polymerizing a reactive liquid monomer or, the cooling of melt polymer, the drying and crosslinking of a polymer solution, or simply the drying of a solution. The layer can be dried by convective heat with forced air flowing inside an oven, by using IR heating source and or using both of them. The drying of a coating layer is an interesting problem to study as it involves simultaneous mass, momentum and heat transfer.

The drying of coated films involves evaporation of the liquid content by heat, which is supplied by hot gas or radiant elements. The solvent vapor is then carried away by the air flowing over the coated substrate. Thus, the liquid layer recedes as solvent is gradually removed. First, the drying rate is determined by the transport of solvent from the surface of the liquid film to the gas phase (i.e., external conditions such as heat and mass transfer coefficients, gas phase temperature and velocity) and by the partial pressure and activity of the solvent. After that, the drying rate is controlled by the diffusion of the solvent inside the liquid film. The diffusion coefficient of solvents in a polymer matrix is a strong function of temperature and concentration.

Since it is not straightforward to measure the process drying rate, the temperature and concentration of the product to be dried, and in addition pilot plant experiments cost, the overall model is an alternative to study the behavior of a drying process.

An appropriate model for this process must take into account the following phenomena: flow of polymer film, convective heating of coating and evaporation of the solvent from the coating surface, mass transfer resistances in the vapor and polymer phases, etc. The most critical parameter in the drying process is the diffusion coefficient for the polymer –solvent system, which is a strong function of concentration and temperature. The rate of solvent removal from the polymeric coating is controlled by diffusion in the polymer phase during the falling rate period. The heat of desorption also characterizes the falling rate period for drying thin layer of polymer coating.

The objective of this study is to develop mathematical models that can predict the solvent content profile, the temperature profile of the polymer and the air during the batch and continuous drying of a thin (0.01 cm) polymer solution (coating) in an Infrared dryer. Another objective is to develop a model for drying thick (1 cm) polymer solution in an IR dryer.

This thesis is organized into seven chapters. A brief introduction in chapter 1 is followed by the literature review in chapter 2 that highlights the significant past works on IR drying. Chapter 3 discusses the fundamentals associated with drying processes while chapter 4 provides the details of the models developed for IR drying. The simulation procedure is included in chapter 5. Chapter 6 incorporates model validation as well as the effect of important parameters on drying behavior. Finally, some concluding remarks and recommendations for further research are mentioned at the end in chapter 7.

CHAPTER 2

2. Literature Review

Over the last two decades or so, IR drying has attracted much attention and several researchers have worked with different aspects of it. Studies are found on the IR radiation drying in pulp and paper industries, textile industries, food industries, of minerals and polymer solutions. The majority of the studies on drying so far dealt with convective drying only while a few dealt with a combined IR and convective drying. Open literature provides studies that include experimental works, modeling, optimization of batch drying of polymer solution (coating).

Convective Drying of Polymer Solutions

Researchers have proposed quite a few models for convective drying of thin polymer solution consisting of polymer and solvent on a substrate and experimentally validated them. An early study was conducted by Okazaki et al. (1974) who investigated drying of aqueous polyvinyl alcohol (PVA) solution at low airflows using gravimetric measurements. They measured mutual diffusion coefficients for the whole range of solvent concentration and compared the experimental drying rates, weight and temperature of the polymer film with theoretical predictions. Later, Blandin et al. (1987) investigated the convective drying process of coatings with various layers. The calculated results were in good agreement with experimental finding. Duda et al. (1987) introduced a revised version of free-volume theory proposed earlier of polymer solvent diffusion. Upon comparing the predictions of the proposed free-volume theory with experimental data collected over wide temperature and concentration ranges, they found that the theory can accurately describe the diffusional behavior of polymer-solvent systems in convective drying. Also for coating studies, Powers et al. (1990) used a thermogravimetric set-up with controlled flow of gas of known solvent composition across the coating to study the effect of drying gas temperature and composition on drying behavior of poly (methyl methacrylate)/ toluene system. They showed a slight increase in residual solvent at higher drying gas temperature and claim that the increase may be due to skinning.

Vrentas et al. (1994) developed a model in detail for the description of heat and mass transfer in the drying of polymer films. By the utilization of mass and energy balances, they determined the conditions under which the steady-state equations can be converted to an unsteady-state format. Later, Alsoy et al. (1998) studied the convective drying of solvent coated polymer films. They used the model developed by Vrentas et al. (1994) to predict the concentration, the thickness and the temperature profile of a polymer film as a function of time. They demonstrated that temperature gradients in the substrate and polymer film can be neglected. In parallel, Ion et al. (1995) studied the process of convective drying polymer paint in solvent at various constant temperatures. They observed that the diffusivity largely depends on the concentration. It was measured at the beginning and at the end of the drying operation. Being interested in industrial process, Guerrier et al. (1998) described the convective drying pilot plant of a coating of varnish on a moving aluminum substrate, pertaining to packaging industry, where a film of few microns is dried in a few seconds. They showed that the presence of a small amount of solvent in the drying air does not significantly affect the drying kinetics.

A theoretical study of convective drying of thin films on a continuously moving flat plate, which occurs in ink and coating solvent has been done by Atakan et al. (2000). By comparing the theoretical results with some experimental data they found that the results were satisfactory particularly for the total drying time. However, their drying model did not consider the velocity of the substrate nor did they present the effect of substrate velocity on drying. Dryer efficiency is of great importance for industrial process. For instance, Peter et al. (2000) discussed an application of automated constrained optimization with a detailed mathematical model of heat and mass transfer to convective drying of polymeric coatings to find the optimal drying conditions for a prototypical coating in a single-zone oven. According to their results, the optimal coating side heat-transfer coefficient is always equal to or greater than the optimal substrate side heat-transfer coefficient. Besides, a study carried out by Alsoy (2001) demonstrated the benefits of using multi-zone ovens for convective drying of coating to obtain better product quality. The validity of the model was limited to drying two components (polymer and solvent) in the coating. Lately, Perez (2007) developed a model and simulation software in order to solve the transient mass and heat transfer equations that describe the convective drying of a polymer solution containing two different solvents. He

used the model as a tool in the optimization of the drying operating conditions of the manufacturing of adhesive tapes at 3M Brazil. The gain in productivity achieved by the analysis was greater than 40%. Further, Cairncross et al. (2001) conducted experimental work to study the drying behavior of polymer solvent coating (PVAc-Toluene). Their model for convective drying accurately predicted the residual toluene in the final stages of drying. However, they attributed the anomalous behavior of residual solvent content to the formation of trapping skinning at higher gas velocities, which cannot be explained with Fick's law of diffusion. Etemad et al. (2002) also carried out an experimental study to investigate the influence of various operating conditions on a convective drying of thin films of Poly vinyl acetate (PVAc) in a drying tunnel where the air velocity and temperature were controlled. Their results demonstrated that the drying rate in the constant drying rate period was influenced by the temperature and the velocity of the air. Increasing the temperature and velocity led to a higher drying rate.

IR Drying

The IR drying process models and experimental work reported in the literature vary in kind, complexity, and application. Earlier, Cote et al. (1991) investigated the important parameters affecting the drying of a cotton web by IR radiation. They concluded that with this dryer, heat transfer by convection is much less important than by radiation. Continuing their work, Dhib et al. (1994) developed a dynamic model to describe the drying of thin sheets in a continuous IR dryer. The model presented the temperature and moisture distribution of air, and the moist sheet, as a function of time and distance (between the material being dried and IR heating source) in the dryer. They have also studied the influence of the sheet velocity and that of the radiant energy on the dryer performance as well as the effect of the moisture content of the entering sheet. In their study, they, however, neglected the diffusion equations but considered desorption phase since the material being dried was very thin.

In a study, Navarri et al. (1997) found that the heat and mass transfer coefficients in IR convective drying verify the analogy's classical result, which expresses the ratio of the coefficients in terms of the Schmidt to Prandtl number.

Blanc et al. (1997) have also made the choice of mixed convective and radiant heating to dry a waterborne epoxy coating. He observed that the response time of the IR heater was very short as 95% of the maximal power was reached in approximately 25 seconds. They developed a model and compared it with the experimental results using PVA coating with different supports. Their work involved the polymerization reaction while drying the polymer film. Similarly, Person et al. (1998) studied the near IR drying of pharmaceutical thin film containing multiple solvents and an active substance. using Fourier transform IR (FT-IR) spectroscopy, Saure et al. (1999) studied the influence of parameters such as air temperature, coating thickness and air velocity on drying of poly (vinyl acetate)-methanol-benzene system. They showed that the total solvent content (methanol and benzene) after drying coating for sufficiently long periods of time is independent of air velocity and decreases with increasing temperature of air. Also an interesting study was carried out by Chen et al. (2000). They analyzed two dimensional heat and mass transfer characteristics arising from a non uniform radiant incidence in polymer solutions whose motion was governed by combined thermo capillary/ bouncy laminar flow. They considered evaporation of solvent at the polymer solution surface and also examined the influence of thermo capillary effect on drying features.

Lamaison et al. (2001) carried out experimental study of transfer phenomena during drying of aqueous paint film under IR heating. They presented the evolution of temperature and evaporated water mass fraction for different heat fluxes during the curing of the film. Similarly but using different mode of heating, Geipel and Stephan (2005) presented experimental results of convective drying of automotive base paints containing near 60% of water mass fraction. Dufour et al. (2004) also studied the experimental control of an IR drying process of a water based epoxy-amine painting.

Combining IR and microwave heat source, Salagnac et al. (2004) presented the modeling of the hygrothermal behavior of a porous medium. Their aim was to study the potential advantages resulting from the introduction of radiating sources in a convective drying process. Afterwards, Allanic et al. (2006) studied the drying of a polymer aqueous solution with some strict constraints (no deformation of Petri dish, limited proliferation of bacteria in the dried polymer solution). The principal objective of their study was to minimize the drying time of the polymer aqueous solution by combining convective and IR radiation. After performing several experiments, they also found that the model predictions were in good agreement with mass and temperature experimental data. Recently, Daniel et al. (2007) presented a mathematical model to describe convective and IR radiant heating of a web and solvent evaporation from a web in an oven during the production of prepregs (composite material made of resin with fiber reinforcement for the electronics industry). The results predicted by computer simulations under different conditions yielded good agreement with a similar study in the literature.

In some studies the source IR heating is clearly mentioned. Using gas-fired IR, Jamal et al. (2001) studied drying of paper. Their experimental study provides basic drying and temperature data for moist paper exposed to gas-fired IR radiation energy.

Most of the studies have so far worked on convective drying. Although few of them worked on IR drying of coating, their works were limited to fixed or batch IR drying. Till date, no study has been done on continuous IR drying of coating as we can hardly find any published article on it, although it has already found its way to industrial application. In the present work, the drying behavior of polymer solutions (consist of one solvent and solute) over an impermeable substrate in an IR-convective oven was simulated using drying models. Two models were developed for drying of thin (0.01 cm) polymer solutions on a fixed (batch drying) and on a continuously moving substrate (continuous drying) inside the drying oven. One more model was developed for drying of thick (1 cm) polymer solution on a fixed substrate. This study also investigated the influence of various physical parameters including radiant temperature, air velocity, substrate velocity, film thickness on the drying of polymer solutions.

CHAPTER 3

3. Drying Processes

The basic principles of drying, drying method and types of dryers are briefly discussed in this chapter.

3.1 Drying Principles

The process of drying is fundamentally a simultaneous heat and mass transfer operation in which the energy to evaporate a liquid (water or solvent) from a solid is provided by drying hot air (for convective) or with an additional means of IR heating source.

For each and every product, there is a representative curve that describes the drying characteristics for that product at specific temperature, velocity and pressure conditions. This curve is referred to as the drying curve for a specific product. Variations in the curve will occur principally in rate relative to carrier velocity and temperature.

Figure 3.1 represents a typical drying curve for virtually any product. Drying occurs in three different periods, or phases, which can be clearly defined. The first phase, or initial period (A-B in Figure 3.1), is where sensible heat is transferred to the product and the contained moisture. This is the heating up of the product from the inlet condition to the process condition, which enables the subsequent processes to take place. In some instances, pre-processing can reduce or eliminate this phase. For example, if the feed material is coming from a reactor or if the feed is preheated by a source of waste energy, the inlet condition of the material is already at a raised temperature. The rate of evaporation increases dramatically during this period with mostly free moisture being removed.



Figure 3.1: A typical drying curve

During the second phase or constant rate period (B-C in Figure 3.1), the free moisture persists on the surfaces and the rate of evaporation alters very little as the moisture content reduces. During this period, drying rates are high and higher inlet air temperatures than in subsequent drying stages can be used without detrimental effects to the product. There is a gradual and relatively small increase in the product temperature during this period. Interestingly, a common occurrence is that the time scale of the constant rate period may determine and affect the rate of drying in the next phase.

The third phase, or falling rate period (C-D in Figure 3.1), is the phase during which migration of moisture from the inner interstices of each particle to the outer surface becomes the limiting factor that reduces the drying rate.

3.2 Heating Methods

In practice, all three heating modes are present in almost every dryer, although one or two modes usually are predominant.

3.2.1 Convection

Convection is possibly the most common mode of drying particulates or sheet-form or pasty solids. Heat is supplied by heated air or gas flowing over the surface of the wet solid. Heat for evaporation is supplied by convection to the exposed surface of the material and the evaporated moisture carried away by the drying medium. Air (most common), inert gas (such as N_2 for drying solids wet with organic solvent), direct combustion gases, or superheated steam (or solvent vapor) can be used in convective drying systems. The convective heat flux from a surface to the process environment can be calculated using Newton's law of cooling which is expressed as:

$$q = h_c (T - T_p) \tag{3.1}$$

Where, h_c is the heat transfer coefficient, T is the drying gas temperature and T_p is the temperature of the product being dried.

3.2.2 Conduction

Conduction dryers are more appropriate for thin products or for very wet solids. Heat for evaporation is supplied through heated surfaces (stationary or moving) placed within the dryer to support, convey, or confine the solids. The evaporated moisture is carried away by vacuum operation or by a stream of gas that is mainly a carrier of moisture. Conduction is well described by Fourier's law:

$$q_x = -k_c \frac{dT}{dx} \tag{3.2}$$

Where, k_c is the thermal conductivity, $\frac{dT}{dx}$ is temperature gradient across the thickness x. The minus sign ensures that heat flows down the temperature gradient.

3.2.3 Radiation

Radiation heat transfer is proportional to the difference in temperatures raised to the fourth power, which follows Stefan-Boltzmann law:

$$q = \sigma \Im \left(T_r^4 - T_p^4 \right) \tag{3.3}$$

Where, σ is Stefan-Boltzmann constant, \Im is shape factor, T_r is radiant temperature, T_p is the temperature of the product being dried.

3.3 Dryer Classification

Neither a certain dryer can dry all kinds of product nor can a single product be dried in all types of dryers. The suitability of dryer depends on various factors such as mode of heat transfer, residence time, dryer efficiency, product quality etc. Depending on the way heat is supplied, dryers are classified into two categories; direct and indirect dryers.

3.3.1 Direct Dryers

In direct dryers or adiabatic, convective heat transfer is done through direct contact of the product with hot gases. The gas transfers sensible heat to provide the heat of vaporization of the liquid present in the moist solid.

Rotary warm air, fluidized bed, flash, spray, tunnel are examples of direct dryers. All these suffer from common disadvantages, viz., the amount of air or hot gas required is fairly large,

which causes the auxiliary equipment needed to be sized accordingly; the thermal efficiency is also lower than that for indirect dryers.

Often a combination of direct and indirect drying results in an optimum and efficient solution to some drying settings.

3.3.2 Indirect Dryers

Indirect dryers, also called non-adiabatic units, separate the heat transfer medium from the product to be dried by a metal wall. These dryers are subdivided on the basis of heat applied by radiation or through heat transfer surface and also by the methods in which volatile vapors are removed.

Indirect dryers have several distinctive operating features: (a) the risk of cross-contamination is avoided since the product does not contact the heating medium, (b) since a limited amount of gas is encountered, solvent recovery is easier than with an adiabatic dryer, (c) dusting is minimized because of the small volume of vapors involved in indirect drying, (d) dryers allow operation under vacuum or in closely controlled atmospheres that can avoid product degradation and (e) explosion hazards are easier to control.

Typically, indirect dryers are used for small-or medium-size production. The product from such a unit has a higher bulk density than the same material processed in direct dryers. The common indirect heated dryers are tubular dryers (with or without vacuum), drum dryers (atmospheric, vacuum, horizontal or rotary vacuum, and others), hollow disk dryers, paddle dryers, mechanically fluidized bed dryers, pneumatically conveyed dryers, cone of twin-shell dryers, and others. IR dryer is one kind of indirect dryer.

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3.3.3 IR Dryers

An IR dryer can be either electric or gas fired. Basically, the IR dryers differ in their construction and in how they transfer heat to the product to be dried.

a) Gas-Fired IR Dryer

The radiation heat produced by a gas-fired IR dryer must be in medium-wave length. The emission spectrum wavelength (radiation) corresponds well to the absorption spectrum of fibers and water. However, in practice, this means that the radiation heat does not penetrate through the web, but remains within the surface fibers of the material to be dried.

A circulating air system can be used to increase drying efficiency, and the energy utilization can be further improved by using a separate air foil unit (Hiden et al., 1998).

b) Electric IR Dryer

In an electric IR dryer, heat is transferred solely as radiation. Convection is negligible. Typically, a row of electric IR units are placed in the direction of the product being dried.

In a previous study, Socha et al. (2001) concluded that the radiation efficiency of electric heater varies between 76-83.5% whereas for Gas-IR burners it varies between 36 and 46% (under ideal burner conditions).

For instance, Hinosawa (1999) mentioned two different factors in choosing between the two types of IR dryers. These factors were the objective of the applications and the cost and availability of energy. While gas IR is almost exclusively used in drying products, electric IR has more flexibility. It can be used strictly for coating drying usually immediately following the coater head to quickly set the coating-or for base sheet moisture profiling prior to coating, or for final moisture profiling before reel. The reason electric IR system have this flexibility over gas is largely due to the modulated control ability inherent to electricity. It is relatively easy to segment an electric IR system and with 0% to 100% power control over each zone.

In this study, electric IR dryer was used for drying the polymer solutions. The IR drying mechanism, the drying systems considered and the mathematical models for drying the polymer solutions are discussed in the next chapter.

CHAPTER 4

4. IR Drying Process and Modeling

This chapter focuses on details of Infrared radiation, the mechanism of IR drying, the drying systems considered, the derivation of mathematical model, the physical properties of polymer solution being dried and the parameter estimation for the drying processes.

4.1 IR Radiation

IR drying is the most widely used type of heating by radiation. Here, electromagnetic energy in the form of IR waves is emitted from radiant and directed to the coated substrate. This radiated energy, when absorbed, causes frictional (vibrational) heating of the coating molecules, which initiates solvent evaporation.

Wavelength of the radiation emitted by an IR heating source is a function of the surface temperature of the emitter. In an industrial environment, the two preferred wavelengths are medium wave and short wave. The choice of a particular IR system very much depends on the particular application. For example, medium wave IR is readily absorbed by water and is often ideal for drying and curing water-based paints. It is also very tolerant of paint formulation and the curing of most single and two-pack coatings can be greatly increased without the risk of causing surface defects such as solvent boil and gassing. Short wave IR emitters have a virtually instantaneous on/off response and provide rapid cure from radiation penetration, with the lowest temperature increase of the coating or substrate. However, the higher intensity of the emitted energy of short wave IR can cause problems with solvent boil on incorrectly formulated coating systems, so that control of solvent type, both in manufacture and in use, is more critical.

A recent development in IR technology includes the introduction of medium wave systems with short wave response characteristics. These are particularly useful for rapid drying and curing of water-based coatings. Nowadays, IR emitters are available in a wide variety of shapes and configurations and include ceramic emitters, metal sheathed emitters and carbon fiber emitters, although the most popular emitters still tend to be quartz units. However, the most important advances in IR technology have probably been in the manner in which the various usable wavelengths of IR radiation have been exploited to offer maximum application advantage.

4.2 The Mechanism of IR Drying

IR radiation, radio, visible light, ultraviolet, x-rays waves and microwaves, as shown in Figure 4.1, are all electromagnetic waves that travel through space at the speed of light. The difference between them is the wavelength of the electromagnetic wave. IR energy travels without heating air as it goes through, since the amount of IR radiation absorbed by the main composition of air is CO_2 , water vapor and other particles in the air is negligible. Any object with a surface temperature above absolute zero will emit IR radiation. Thus, temperature of an object as well as its physical properties dictates the radiant efficiency and wavelengths emitted.

Gamma- rays	X-rays	Ultra- violet	Visible	IR (1- 200 µm)	Microwave	Radio, TV
Nuclear transitions	Inner shell transitions	Val elec trans	ence etron itions	Molecular vibrations	Molecular rotations	Spin in magnetic field

Energy increases

Wavelength increases

Figure 4.1: Energy scale of IR

Like the sun, its IR rays heat the earth and other objects directly. The energy emitted is safely absorbed by cool surfaces that warm up, which in turn, release heat into the atmosphere by convection to raise ambient temperature. IR heating is more efficient for two reasons: it can be directed to heat only occupied space and it does not heat the air in a space.

IR heating is the transfer of thermal energy in the form of electromagnetic waves. IR radiation occupies that part of the electromagnetic spectrum immediately adjacent to visible light, extending from 0.78 μ m to 200 μ m. The technically suitable part of this spectrum extends from 0.8 μ m to 100 μ m and is then further subdivided into short, medium and long wave radiation. In practice, the peak wavelength of the emitted radiation is governed by the operating temperature of the emitter filament, with long wave emitters having a filament temperature of between 500°C and 750°C, medium wave emitters having a filament temperature of between 850°C and 1200°C, while short wave emitters have a filament temperature of between 2000°C.

IR heating works best where convective heaters are not practical. Reliable IR heat should have one common characteristic: that the transfer of heat is emitted or radiated from the heated object or substance. The source emits radiation at a peak wavelength towards an object. The object can absorb the radiation at some wavelength, reflect radiation at other wavelengths and re-radiate wavelengths. It is the absorbed radiation that creates the heat within the object.

Figure 4.2 shows that the penetration of IR energy is a function of its wavelength. The higher is the temperature the shorter the wavelength and the greater its penetrating power. For example, a tungsten filament quartz lamp operating at 3725°C has a greater ability to penetrate into a product than a nickel chrome filament quartz tube operating at 1575°C.

For optimum performance, it is important that the wavelength of the emitted radiation be matched to the absorption characteristics of the liquid to be removed. For example, long wave radiation is less sensitive to color difference and is widely used for plastics applications. Medium wave radiation is readily absorbed by water, making it suitable for moisture removal. It is easily absorbed by many plastics and paints, is highly energy efficient and is ideal for

paint and powder curing operations. Short wave is more penetrating than long wave and can provide extremely rapid cure of paint.



Figure 4.2: Penetration of different IR wavelength for drying a coating layer

A polymer solution is basically comprised of solute (polymer) and solvent. The solute may contain other solids (such as binder, resin, pigment, etc) along with the polymer while the solvent may contain more than one liquid. A homogenous polymer solution is comprised of a polymer and a solvent (liquid). We apply this solution onto a substrate which is most commonly referred to as coating and put this coated substrate (web) to dry inside an oven.

4.3 IR Drying Systems

Depending on the application, a drying process can be either batch or continuous. The polymer solution can be dried on a stationary (fixed) substrate placed inside an oven, which is commonly known as batch process of drying. Alternatively, the polymer solution can be dried on a moving substrate that continuously passes through the oven, which is known as continuous drying process. The thickness of the polymer solution is usually in the order of micrometer. Both types of arrangements are discussed in this thesis.

4.3.1 Fixed System (Batch Drying)

First, we analyze the problem of drying a polymer solution on a fixed substrate (web) placed in an IR oven. The polymer solution can be applied onto different types of substrate. Based on the substrate materials, coated substrate may exist in three categories: coated paper and paperboard, coated plastic films (e.g., photographic films) or tapes (e.g., adhesive tapes, magnetic tapes, pressure sensitive tapes, and photo sensitive tapes) and coated metallic sheets. Physical properties of substrates also contribute a little in affecting the drying kinetics.



Figure 4.3: IR drying of polymer solution on a fixed substrate

Figure 4.3 shows that the substrate containing polymer solution to be dried is placed into an IR oven. Initially, the polymer solution is a mixture made up of two phases: a liquid phase containing solvent (e.g., Toluene), and a solid phase containing the polymer (e.g., Polyvinyl acetate (PVAc)). We consider the size of the IR dryer of a laboratory dryer in order to simulate the drying phenomena in a laboratory scale. The oven is 65 cm wide and 140 cm long. The IR lamp is consist of electric IR emitters of standard industrial type are placed above the substrate containing the coating. The radiant emitters are equipped with reflectors so as to reduce the heat losses into the surroundings and reflect the radiation. The radiant

heater is placed above the coated substrate. The distance between the emitter and the substrate is 5 cm. Air is passed through only above the substrate through the area between the substrate and the emitters to essentially carry away the solvent or water from the coated material being dried. Thus, it favors mass transfer of solvent vapor into the air and lowers the solvent content in the coated material. Figure 4.4 shows a typical phenomenon of drying a polymer solution.



Figure 4.4: Typical drying phenomenon

4.3.1.1 Assumptions and Model Derivation

Usually in any modeling, assumptions are made to keep the system as simple as possible. The models for the drying processes presented are based on the following assumptions.

- The partial specific volumes of the solvent and polymer are independent of composition at each temperature so that there is no volume change on mixing for the solution;
- 2. End effects of the substrate and air flow are negligible;
- 3. There is a single, uniform temperature of the polymer film;
- 4. Heat and mass transfers in x-direction (vertically upward) only;
- 5. No chemical reaction in the polymer;
- 6. The polymer film is considered opaque; as a consequence, the radiation energy which penetrates into the body of the material is completely absorbed;

Drying involves simultaneous mass and energy transport. In many practical cases, the transport equations reduce to one-dimensional mass and energy transport. Referring to the IR set up shown in Figure 4.3, heat is transferred from the surroundings into the wet material (coating), which causes the water (or solvent) to vaporize, and moving air carries this vapor away from the web. Technically speaking, the process of drying consists of supplying energy into the coating and removing the water or solvent as it vaporizes. The drying process involves the vaporization of a liquid and the diffusion the vapor into the flowing air. The governing equations of IR drying of the polymer coating are discussed next.

Simultaneous heat and mass transfer take place for all the components involved in the drying process i.e. the polymer, solvent and the substrate.





a) Polymer, solvent and substrate

From the control volume in Figure 4.5, a mass balance of the polymer solution is expressed as:

$$\begin{bmatrix} Rate \ of \ change \\ of \ solvent \ cotent \\ of \ polymer \ solution \end{bmatrix} + \begin{bmatrix} Rate \ of \ mass \\ of \ solvent \\ content \ out \end{bmatrix} - \begin{bmatrix} Rate \ of \ mass \\ of \ solvent \\ content \ in \end{bmatrix} = - \begin{bmatrix} Rate \ of \\ evaporation \\ into \ air \end{bmatrix}$$
$$\frac{dH_p}{dt} = -\frac{L_p W_p}{m_s} \dot{m}_{evap}$$
(4.1)

Where, \dot{m}_{evap} is the rate of evaporation, and H_p is the solvent content (%) of the polymer, L_p, W_p are the length and width of polymer and m_s is the mass of solvent.

On the hypothesis that air-polymer coating interface is saturated with solvent, the drying rate is expressed by:

$$\dot{m}_{evap} = k_m (H_{sat} - H_a) (H_p / H_c)^p \tag{4.2}$$

Where $\beta=0$ for the constant rate of drying and $\beta=1$ for the falling rate of drying. k_m is mass transfer coefficient. H_{sat} is the saturated solvent content at the coating/air interface. H_a is the solvent vapor content of in air and H_c is the critical solvent content. Both these parameters H_{sat} and H_a are calculated using the vapor pressure at polymer temperature which changes with time. The pressure at the upper side of the coating is considered equal to the atmospheric pressure as no external pressure was applied to the system. As we used solventfree air in drying, the solvent partial pressure in the air is zero. The mass transfer coefficient (k_m) is calculated by analogy with a heat-transfer coefficient.

Using the principle of energy conservation, an energy balance gives us:

 $\begin{bmatrix} Rate \ of \ change \\ of \ energy \ of \\ polymer \ solution \end{bmatrix} + \begin{bmatrix} Rate \ of \\ energy \\ out \end{bmatrix} - \begin{bmatrix} Rate \ of \\ energy \\ in \end{bmatrix} = \begin{bmatrix} Rate \ of \ heat \ added \ or \\ removed \ by \ conduction, \\ convection, \ radiation \\ and \ evaporation \end{bmatrix}$

$$(\rho_p C p_p l_p + \rho_{sol} C p_{sol} l_{sol} + \rho_{sub} C p_{sub} l_{sub}) \frac{dT_p}{dt} =$$

$$q_{sub} - h_{pa} (T_p - T_a) + \Im \varepsilon_p \sigma (T_r^4 - T_p^4) - q_{evap}$$
(4.3)

Where *l* represents the thickness, h_{pa} is the convective heat transfer coefficient between polymer and air, q_{evap} is the heat flux of vaporization and is expressed by $q_{evap} = \dot{m}_{evap}(\Delta h_v + h_{des})$ and q_{sub} corresponds to conductive heat transfer between the substrate and the polymer solution. Δh_v is the heat of vaporization of solvent, and h_{des} is the heat of desorption of solvent. ε_p is the emissivity of polymer, \Im is the shape factor; it is also called as form factor, view factor, configuration factor. The heat of desorption of the solvent was found from the similar kind of correlation used by Dhib et al. (1994).

$$h_{des} = 420.72 - 65.02H_p + 9.08H_p^2 - 0.21H_p^3 \tag{4.4}$$

The shape factor depends on the geometry of the emitter, coated substrate and their relative position. We assumed that the reflector emitter arrangement could be considered as a rectangular plane. The shape factor is expressed by the following equation (Cote et al., 1991).

$$\Im = -1.86 \times 10^{-6} W_p^2 + 2.36 \times 10^{-5} W_p + 1.33 \times 10^{-4} d^2 - 7.01 \times 10^{-3} d + 0.113$$
(4.5)

Where, d is the distance between the emitter and the coating in cm.

The IR heating source causes the evaporation of solvent from the polymer solution, and air stream carries away that vapor from the system. In general, since the thickness of the coated substance is thin enough, the temperature of the whole system (solution and substance) can be assumed to be uniform. With this assumption, the temperature of the polymer solution and substance as the same.

b) Air and vapor mixture

Air flows over the solution surface in z-direction only and carries away the solvent vapor. A mass balance for air -vapor mixture gives the following equation:

$$\begin{bmatrix} Rate \ of \ change \\ of \ solvent \ vapor \\ in \ the \ air \end{bmatrix} + \begin{bmatrix} Rate \ of \ mass \\ of \ solvent \\ vapor \ out \ from \ air \end{bmatrix} - \begin{bmatrix} Rate \ of \ mass \\ of \ solvent \\ vapor \ in \ the \ air \end{bmatrix} = \begin{bmatrix} Rate \ of \\ evapor \ atom \\ of \ solvent \end{bmatrix}$$
$$\frac{\partial H_a}{\partial t} + V_a \frac{\partial H_a}{\partial z} = \frac{V_a W_p}{M_a} \ \dot{m}_{evap}$$
(4.6)

Where Ha is solvent content in air, Va is velocity of air, Ma is the mass flow rate of air

And an energy balance for the air- vapor mixture gives us

$$\begin{bmatrix} Rate \ of \ change \\ of \ energy \\ of \ air \end{bmatrix} + \begin{bmatrix} Rate \ of \\ energy \\ out \ of \ air \end{bmatrix} - \begin{bmatrix} Rate \ of \\ energy \\ in \ the \ air \end{bmatrix} = \begin{bmatrix} Rate \ of \ heat \ added \ or \\ removed \ by \ convection \\ and \ evaporration \end{bmatrix}$$
$$\frac{\partial}{\partial t} (M_a C p_a T_a + M_v C p_v T_a) + V_a \frac{\partial}{\partial z} (M_a C p_a T_a + M_v C p_v T_a)$$
$$= V_a \{ W_r q_{ra} + W_p q_{pa} + m_{evap} C p_v W_p (T_p - T_a) \}$$
(4.7)

Where, W_r is the width of radiant (emitter) q_{ra} and q_{pa} are the convective heat fluxes exchanged by the moving air with the IR emitters and the polymer. They are defined as:

$$q_{ra} = h_{ra}(T_r - T_a)$$
(4.8)

$$q_{pa} = h_{pa} \left(T_p - T_a \right) \tag{4.9}$$

After dividing equation (4.5) by Cp_v and M_a we get

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{Cp_a}{Cp_v} T_a + \frac{Cp_a}{Cp_v} H_a T_a \right) + V_a \frac{\partial}{\partial z} \left(\frac{Cp_a}{Cp_v} T_a + \frac{Cp_a}{Cp_v} H_a T_a \right) \\ &= \frac{V_a}{Cp_v M_a} \{ W_r q_{ra} + W_p q_{pa} + m_{evap} Cp_v W_p (T_p - T_a) \} \end{aligned}$$

The above equation then reduces to

$$\frac{\partial T_a}{\partial t} \left(\frac{Cp_a}{Cp_v} + \frac{Cp_a}{Cp_v} H_a \right) + V_a \frac{\partial T_a}{\partial z} \left(\frac{Cp_a}{Cp_v} + \frac{Cp_a}{Cp_v} H_a \right)$$
$$= \frac{V_a}{Cp_v M_a} \{ W_r q_{ra} + W_p q_{pa} + m_{evap} Cp_v W_p (T_p - T_a) \}$$

Now, dividing the above equation by $\frac{cp_a}{cp_v} + H_a$ we get,

$$\frac{\partial T_a}{\partial t} + V_a \frac{\partial T_a}{\partial z} = \frac{V_a}{Cp_v M_a} \frac{\left\{ W_r q_{ra} + W_p q_{pa} + m_{evap} C p_v W_p (T_p - T_a) \right\}}{Cp_a / Cp_v + H_a}$$
(4.10)

Initial conditions along with the boundary conditions are required in order to solve the above mass and energy balance equations. The initial conditions refer to the conditions existing in the dryer when starting the operation. In general, the variables appearing in the mass and energy balance equations are constant values along the length of the dryer for a start-up operation. Boundary conditions refer to the solvent content and temperature of the air and coating material at the starting of the process.

Initial conditions

Boundary conditions

$H_p(z,0) = H_{p0}$	$H_p(0,t) = H_{pe}$
$H_a(z,0) = H_{a0}$	$H_a(0,t) = H_{ae}$
$T_p(z,0) = T_{p0}$	$T_p(0,t) = T_{pe}$
$T_a(z,0) = T_{a0}$	$T_a(0,t) = T_{ae}$
for $0 < z < L_p$	for $t > 0$

4.3.2 Moving System (Continuous Drying)

Here we consider a moving system where the coated substrate passes through the IR oven at a certain speed. In this case, the oven dimension, flow arrangements and other parameters are the same as mentioned earlier in batch drying process.



Figure 4.6: Simplified view of continuous IR drying

4.3.2.1 Assumptions and Model Derivation

In addition to the assumptions previously stated, here we add:

- 1. The movement of the coated web is smooth and continuous.
- 2. Heat loss at the bottom of the web is negligible.

The governing equations of IR drying of polymer traveling through the dryer are developed in this section. The velocity of the coated web has been incorporated in the model.

Mass balance of the coating and air-vapor mixture give the following two equations, respectively.

$$\frac{\partial H_p}{\partial t} + V_p \frac{\partial H_p}{\partial z} = -\frac{W_p V_p}{M_p} \dot{m}_{evap}$$
(4.11)

$$\frac{\partial H_a}{\partial t} + V_a \frac{\partial H_a}{\partial z} = \frac{W_p V_a}{M_a} \dot{m}_{evap}$$
(4.12)

From energy balance we get,

$$\frac{\partial T_p}{\partial t} + V_p \frac{\partial T_p}{\partial z} = \frac{W_p V_p}{C p_{sol} M_{sub} M_p} \frac{q_{pr} - q_{pa} - q_{evap}}{\frac{C p_p}{C p_{sol} M_{sub}} + \frac{C p_{sub}}{C p_{sol} M_p} + \left(H_a/H_p\right)}$$
(4.13)

$$\frac{\partial T_a}{\partial t} + V_a \frac{\partial T_a}{\partial z} = \frac{V_a}{Cp_v M_a} \frac{W_r q_{ra} + W_p q_{pa} + \dot{m}_{evap} Cp_v W_p (T_p - T_a)}{Cp_a / Cp_v + H_a}$$
(4.14)

Where,

$$q_{pr} = \Im \sigma \epsilon_p \alpha_r (T_r^4 - T_s^4) \tag{4.15}$$

 α_r is a correcting factor that corrects the shape factor globally for the moving substrate and its value lies between 1 and 0.

4.4 Modeling of Thick Layer Drying of Polymer Solution (batch process)

In the previous section 4.3, we developed model for thin layer (0.01 cm) of polymer solution (coating). In this section we will talk about a model for thick layer (1 cm) of polymer solution. This is mainly important for the polymer manufacturing industries as the final product of polymer solution is dried in the end to remove the solvent from the polymers.

Here we consider a system where a polymer solution (PVAc-toluene) of thick layer on an inert impermeable container (polyester) is being dried in an IR oven. The oven dimensions are the same as described earlier in section 4.2. For this thick solution we consider diffusion of

solvent taking place inside the solution. The value of the diffusion coefficient characterizes how quickly a solvent can transport to the surface. The solvent mass balance in polymer solution phase can be written as

$$\frac{\partial c_{sol}}{\partial t} = \frac{\partial}{\partial x} \left(D \, \frac{\partial c_{sol}}{\partial x} \right) \tag{4.16}$$

 C_{sol} is the solvent concentration in the solution in g/cc, x is the vertical position in the coating, D is the solvent-polymer mutual diffusion coefficient. We used free volume theory to describe the concentration and temperature dependence of the mutual diffusion coefficient and that can be expressed as (Duda et al, 1982):

$$D = D_0 D_1 exp\left(-\frac{E}{RT}\right) exp\left(-\frac{\left(\gamma \omega_{sol} \widehat{V_{sol}^*} + \omega_p \xi \widehat{V_p^*}\right)}{\widehat{V_{FH}}}\right)$$
(4.17)

 D_0 is a preexponential factor, E is activation energy, ω is mass fraction and D_1 is a thermodynamic parameter that converts the self –diffusion coefficient of solvent into the mutual diffusion coefficient:

$$D_1 = (1 - \phi_{sol})^2 (1 - 2\chi\phi_{sol})$$
(4.18)

Where, χ is Flory Huggins parameter, ϕ is volume fraction

 $\widehat{V_{FH}}$ is the free volume available for diffusion inside the polymer solution:

$$\frac{\hat{V}_{FH}}{\gamma} = \frac{K_{11}}{\gamma} \omega_{sol} \left(K_{21} + T - T_{g1} \right) + \frac{K_{12}}{\gamma} \omega_{sol} \left(K_{22} + T - T_{g2} \right)$$
(4.19)

The initial solvent concentration is assumed uniform:

$$c_{sol}(x,0) = c_{sol}^0 \tag{4.20}$$

Since the substrate (web) is impermeable, the concentration gradient of solvent must be zero at the coating/ substrate interface:

$$\frac{\partial c_{sol}}{\partial x} = 0 \quad at \ x = 0 \tag{4.21}$$

Another boundary condition on the top of the coating surface can be obtained from an interfacial mass balance.

$$-D\frac{\partial c_{sol}}{\partial x} = k_m (P_1 - P_a) \left(1 - c_{sol} \widehat{V_{sol}}\right)$$
(4.22)

 P_a is solvent vapor pressure in the air, the solvent partial pressure P_1 at the surface is given by:

$$P_1 = P_s \phi_{sol} exp(\phi_p + \chi \phi_p^2) \tag{4.23}$$

We can get P_s from Antoine equation:

$$\log P_S = A - \frac{B}{T+C} \tag{4.24}$$

Where, A, B and C are Antoine constants and T in °C

From energy balance we can get for the coating

$$\rho_p C p_p \frac{\partial T}{\partial t} = k_c \frac{\partial^2 T}{\partial^2 x} + q_{rp}$$
(4.25)

Where, kc is the thermal conductivity of the coating, q_{rp} is the radiative heat transfer between the radiant and the coating. The initial temperature in the polymer is uniform

$$T(x,0) = T_0 (4.26)$$

We assume that at the solution / container interface, the energy flux is zero to avoid heating of the container.

$$\frac{\partial T}{\partial x} = 0 \quad at \ x = 0 \tag{4.27}$$

The energy flux to the upper surface of the coating is the result of an interfacial energy balance.

$$-k_c \frac{\partial T}{\partial x} = -h_{pa}(T - T_a) + \Delta h_v k_m (P_1 - P_a)$$
(4.28)

The heat and mass transfer coefficients are related to heat transfer coefficients by the Chilton-Colburn analogy as mentioned in equation (4.34).

We used the free volume parameters for this PVAc-toluene system as reported by Funda et al. (2000). The authors used these parameters to find the mutual diffusivity of toluene in PVAc.

Parameters	Values for PVAc-Toluene
$\widehat{V}_1^*(cc/g)$	0.917
$\hat{V}_2^*(cc/g)$	0.728
$K_{11}/\gamma \left(cc/gK\right)$	2.21×10^{-3}
$K_{12}/\gamma \left(cc/gK\right)$	6.145×10^{-4}
$K_{21} - T_{g1}(K)$	-86.32
$K_{22} - T_{g2}(K)$	-258.2
ξ	0.709
X	0.7
$D_0(cm^2/s)$	0.0975
E (cal/mol)	3923

Table 4.1: Free volume parameters (Funda et al., 2000)

This system of equations (equation 4.16 and 4.25) is highly nonlinear and hence requires to be solved numerically.

4.5 The Physical Properties

The polymer solution properties used in this study are documented here. Physical properties of the oven, air, polymer, solvent, and solvent vapor were collected from the open literature. The presence of a small amount of solvent in the drying air does not significantly affect the drying kinetics. Therefore, the physical properties of solvent vapor/ air mixture can be taken as those of pure air. The heat and mass transfer coefficients are related to heat transfer coefficients by the Chilton-Colburn analogy. The density, specific heat, thermal conductivity, viscosity, diffusivity of the solvent in air, etc. are evaluated at the average temperature of air and radiant.

Dependence of specific heat (Cp) on Temperature can be expressed approximately by the following equation.

$$Cp = C_0 + C_1 T + C_2 T^2 + C_3 T^3 ag{4.29}$$

Where C_0 , C_1 , C_2 , C_3 are coefficients, T is in K, and Cp is in J/g/K

Water (liquid)	Toluene (liquid)
2.822232	-6.1169E-01
1.1182771E-2	1.9192E-02
-0.350477E-4	-5.6354E-05
3.601070E-8	5.9661E-08
	2.822232 1.1182771E-2 -0.350477E-4 3.601070E-8

Table 4.2: Coefficients of approximating equations for Cp of liquids (Majumdar, 2006)

Table 4.3: Coefficients of approximating equations for Cp of vapors (Majumdar, 2006)

Coefficients	Water (vapor)	Toluene (vapor)
C ₀	1.88300	-4.2440E-01
C_1	-0.16737E-3	6.2933E-03
C ₂	0.84386E-6	-3.9623E-06
C_3	-0.26966E-9	9.3604E-10

Ср	Co	C1	C ₂	C ₃
Air	1.02287	-0.5512E-3	0.181871E-6	-0.05122E-9

Table 4.4: Coefficients of approximating equations for Cp of air (Majumdar, 2006)

Density of air was found by the following expression (Majumdar, 2006):

$$\rho_a = 0.34145/T \tag{4.30}$$

Following equation was used to find the thermal conductivity (W/cmK) of air (Majumdar, 2006):

$$k_a = -3.933E - 4 + 1.10184E - 4 \times T - 4.8574E - 8 \times T^2 + 1.5207E - 11 \times T^3$$
(4.31)

Viscosity of air in g/cm.s is given by (Majumdar, 2006):

$$\mu_a = 4.569E - 7 \times T + 4.73E - 5 \tag{4.32}$$

Density of Toluene (g/cc) was approximated by the following equation (Majumdar, 2006):

$$\rho_{toluene} = \frac{M_w}{1000} \frac{C_1}{C_2^{1+(1-T/C_3)^{C_4}}}$$
(4.33)

Where, M_w is the molecular weight

Table 4.5: Coefficients of approximating equations for density of toluene (Majumdar, 2006)

ρ	C1	C ₂	C3	C_4
Toluene	0.8488	0.26655	591.8	0.2878

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4.5.1 Parameters Estimation

Air velocity, temperature of air and geometry of oven determine heat transfer coefficient (h_{pa},h_{ra}) in dryer.

For a flowing gas confined between two parallel planes the convective heat transfer coefficient is expressed by the following equation (Treybal, 1980)

$$h_{ia} = \alpha_{ia} \rho_a V_a C p_a R e^{-0.29} P r^{-0.67} , \qquad i = r \text{ or } p$$
(4.34)

Where, r stands for radiant and p stands for polymer and α_{ia} corrects the convective heat transfer coefficients. The value of α_{ia} are determined using a nonlinear regression.

From the Chilton –Colburn analogy, the mass transfer coefficient of vapor between the polymer and air may be expressed as

$$k_m = \frac{h_{pa}}{Cp_a} S_c^{-0.67} P r^{0.67} \tag{4.35}$$

Air in direct contact with the polymer sample is assumed to be saturated with solvent all along the dryer length and therefore its relative humidity H_{sat} may be computed from the relation in equation (4.34) at a given total pressure P_t (Mujumdar, 2006)

$$H_{sat} = \frac{M_{\nu}}{M_g} \frac{P_{sat}}{P_t - P_{sat}}$$
(4.36)

Where, M_v and M_g are the molecular weight of vapor and drying gas, respectively. In the case of toluene vapor and air this ratio of molecular weights is 92/29 = 3.17And P_{sat} may be calculated using Antoine Equation (Mujumdar, 2006)

$$log_{10}(P_{sat}) = A - \frac{B}{T_p + C}$$
(4.37)

Where, A, B and C are Antoine constants and T in °C

Antoine parameters	А	В	С
Water	8.107	1750.28	-38.15
Toluene	6.954	1344.80	-53.67

Table 4.6: Parameters for Antoine equation (Mujumdar, 2006)

Equation (4.37) assumes that the coating is pure solvent. But in reality the coating also contains dissolved materials, which will lower the vapor pressure of the solvent. In aqueous coatings this vapor pressure reduction generally can be neglected with negligible error; in solvent coating where many of the solids are dissolved rather that dispersed, the vapor pressure reduction is appreciable. The vapor pressure is reduced by an adjustable vapor pressure factor, which varies between zero and one, to allow for the reduction in vapor pressure due to dissolved species. Theoretically one should calculate activity coefficients, but in most cases, the data is not available. The activity coefficient is adjusted between and 1 and 0.25 so as to have the predicted coating temperature, and the final solvent level match the experimental runs. In aqueous system it is usually one; in solvent systems it often is on the order of 0.25.

Diffusivity of solvent (toluene) in air is expressed by the following equation (Bird et al., 2002)

$$D_a = 1.886 \times 10^{-7} T^{2.334} \tag{4.38}$$

The next chapter discusses in detail about the numerical method used to solve the system of equations.

CHAPTER 5

5. Numerical Method Used

All the mathematical models developed in chapter 4 include Partial Differential Equations (PDE) that are highly nonlinear and therefore, they need to be solved numerically. There are several methods available for solving a system of Partial Differential Equations (PDE). In the present work, method of lines (MOL) has been applied to find the solution of the system of partial differential equations. The method of lines (MOL) is a general technique for solving PDEs by typically using finite difference relationships for the spatial derivatives and ordinary differential equations for the time derivative. This is based on the concept of converting the PDE into a set of ODE by discretizing only the spatial derivatives using finite differences and leaving the time derivatives unchanged. The method requires the construction of a mesh defining local coordinate surfaces. For each node of this mesh, the unknown function values are found, thus replacing the PDEs with a set of ODEs. An ODE integrator is then used to integrate the system of ODEs to obtain the solution of the original PDE. Employing Taylor series expansion, we can derive the finite difference approximations of derivatives. Second order (three-point) forward, backward and centered difference approximations for the first derivative $\frac{\partial f(x_i)}{\partial x}$ are three main approximations derived from Taylor series expansions. Finite difference approximations for different nodes (Chapra and Canale, 1988) can be written as:

a) Forward finite-divided-difference formula (for the first node):

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2\Delta x}$$

b) Backward finite-divided-difference formula (for the last node):

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2\Delta x}$$

c) Centered finite-divided-difference formula (for all other node):

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}$$

For the second derivative a central difference formula can be used (Chapra and Canale, 1988):

$$\frac{\partial^2 f(x_i)}{\partial x^2} = f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x^2}$$

The success of the MOL originates in the availability of efficient time integrators for solving a wide range of problems, including ordinary differential equations (ODEs) and mixed systems of algebraic equations (AEs) and ODEs (AEs and ODEs forming a system of differential-algebraic equations, DAEs). Since our system of equations for both batch and moving drying is highly nonlinear, we used MATLAB integrator ode15s for integrating the set of ODEs.



Figure 5.1: Discretization along the length of the dryer using N number of nodes

Direction of Integration



Figure 5.2: Formation of ODE at each node

Equations (4.1) to (4.10) describe the model developed for IR drying of polymer solution on a fixed substrate (batch process) whereas Equations (4.11) to (4.14) describe the modeling of IR coating drying on a moving substrate (continuous process). The modeling of IR drying of thick layer involves two PDEs; Equations (4.16) and (4.25).

99 equally spaced nodes were used to discretize each Partial Differential Equation (PDE) in the models. Consequently each PDE was converted into 99 ODEs. For instance, the discretization of equation (4.11) is discussed here. Equation (5.1) represents the same equation (4.11).

$$\frac{\partial H_p}{\partial t} + V_p \frac{\partial H_p}{\partial z} = -\frac{W_p V_p}{M_p} \dot{m}_{evap}$$
(5.1)

The total number of nodes taken for discretizing the spatial derivative $\frac{\partial H_p}{\partial z}$ is 99.

For the first node, i=1, the forward finite difference approximation may be used for discretization.

For i=1;

$$\frac{dH_p}{dt} = -V_p \frac{-3H_{p_{i+2}} + 4H_{p_{i+1}} - 3H_{p_i}}{2\Delta z} - \frac{W_p V_p}{M_p} \dot{m}_{evap}$$
(5.2)

The value of H_{p_1} could be found from the given boundary condition.

For all the nodes between the last and first node, i.e. $I \le i \le N$, the centered finite difference approximation may be used to discretize the equation. After discretization it will generate 99-2= 97 ODEs.

For $1 \le i \le N$;

$$\frac{dH_p}{dt} = -V_p \frac{H_{p_{i+1}} - H_{p_{i-1}}}{2\Delta z} - \frac{W_p V_p}{M_p} \dot{m}_{evap}$$
(5.3)

For the last node (i=N), the backward finite difference approximation may be used for discretization.

For *i*=N;

$$\frac{dH_p}{dt} = -V_p \frac{3H_{p_i} - 4H_{p_{i-1}} + H_{p_{i-2}}}{2\Delta z} - \frac{W_p V_p}{M_p} \dot{m}_{evap}$$
(5.4)

As these ODEs thus found after discretization were highly nonlinear and stiff, ode15s solver in MATLAB was used to integrate them.

ode15s is a variable order solver based on the numerical differentiation formulas (NDFs). Optionally, it uses the backward differentiation formulas (BDFs, also known as Gear's method) that are usually less efficient. Like ode113, ode15s is a multistep solver. ode15s is used when ode45 fails, or is very inefficient, and if the problem is stiff, or when solving a differential-algebraic problem.

All the results of numerical solution of the system of equations are discussed in the next chapter.

CHAPTER 6

6. Results and Discussion

In this chapter, model validation is reported for both convective and IR drying. The following section illustrates the effect of several parameters on the IR drying of a coating process as obtained from simulation results for both conditions of drying (i.e., fixed and moving substrate) of thin layer.

6.1 Convective Model Validation

We obtained a model of convective drying of coating in batch process by simply removing the radiation term from the model (equations 4.1 to 4.10) developed earlier in section 4.3.1.1. After that we confirmed the validity of the model by comparing the predicted results of this model with the available data from the literature.

We considered the drying of a polymer solution of polystyrene in toluene on an inert substrate (polyester). For the purpose of model validation, the model was integrated using the same operating conditions as reported by Alsoy et al. (1998). They dried the coating by passing hot air both on top and bottom side of the substrate. Therefore, heat transfer for both the surfaces with hot air was incorporated in our model.

The model was validated by adjusting the parameters to minimize the deviation between the actual data and the model predictions at the same time. In this study, the convective heat transfer coefficients (h_{pa} , h_{ra}), activity coefficient (ac) were adjusted to compensate for model imperfections. The parameters were constrained to physically reasonable values. To find that minimum deviation requires extensive trial and error calculation or automated optimization.

Operating conditions:	
Air flow velocity, V _a	1 m/s
Air supply temperature, T _a	834°C
Initial conditions:	
Polymer Temperature, T _p	24°C
Polymer thickness, l_p	0.01033 cm
Initial solvent content, H _{pi}	70 %
Substrate physical properties:	- Les a men alla pag
Heat capacity, C _p	1.25 J/g/K
Density, ρ_{sub}	1.37 g/cc
Base thickness, <i>l_{sub}</i>	0.0036 cm
Coating physical properties:	an Tanad Middle Constant or re-
Heat capacity, Cpp	1.93 J/g/K
Density of polymer, ρ_p	1.08 g/cc
Heat of vaporization of solvent, Δh_v	360 J/g

Table 6.1: Parameters used for polystyrene - toluene system

Optimization techniques are used to find a set of design parameters, $x = \{x_1, x_2, ..., x_n\}$, that can in some way be defined as optimal. In a simple case this might be the minimization or maximization of some system characteristic that is dependent on x. In a more advanced formulation, the objective function, f(x), to be minimized or maximized, might be subject to constraints in the form of

Equality constraints, $G_i(x) = 0$ ($i = 1... n_e$);

Inequality constraints, $G_i(x) \le 0$ (i = n_e + 1... n);

And/or parameter bounds, x1, xu

A General Problem description is stated as:

$$\min_{x} f(x) \tag{6.1}$$

Subject to:

$$G_i(x) = 0$$
 $i = 1, \dots, n_e,$ (6.2)

$$G_i(x) \le 0$$
 $i = n_e + 1, \dots, n,$ (6.3)

where x is the vector of length n design parameters, f(x) is the objective function, which returns a scalar value, and the vector function G(x) returns a vector of length m containing the values of the equality and inequality constraints evaluated at x.

An efficient and accurate solution to this problem depends not only on the size of the problem in terms of the number of constraints and design variables but also on characteristics of the objective function and constraints. When both the objective function and the constraints are linear functions of the design variable, the problem is known as a Linear Programming (LP) problem. Quadratic Programming (QP) concerns the minimization or maximization of a quadratic objective function that is linearly constrained. For both the LP and QP problems, reliable solution procedures are readily available. The more difficult of the two to solve is the Nonlinear Programming (NP) problem in which the objective function and constraints can be nonlinear functions of the design variables. A solution of the NP problem generally requires an iterative procedure to establish a direction of search at each major iteration. This is usually achieved by the solution of an LP, a QP, or an unconstrained sub problem.

Solver "fmincon" in MATLAB is a very good choice to find a minimum of a constrained nonlinear multivariable function, keeping in mind that our models are highly nonlinear. We used that optimization scheme to locate the optimum heat transfer coefficients and activity coefficient which results in the lowest discrepancy.

The solver "fmincon" uses the methods of Sequential Quadratic Programming (SQP). SQP methods represent the state of the art in nonlinear programming methods. The method allows us to closely mimic Newton's method for constrained optimization just as is done for unconstrained optimization. At each major iteration, an approximation is made of the Hessian of the Lagrangian function using a quasi-Newton updating method. This is then used to generate a QP sub problem whose solution is used to form a search direction for a line search procedure.

The optimization routine minimizes the following objective function for a given set of parameters values, as a least square criterion for N data points:

$$J = \sum_{k=1}^{N} (Y_k - X_K)^2$$
(6.4)

Where Y_k represents the data points collected from the literature and X_k the values predicted by the models.

Equation (6.4) can be expanded as:

$$J = \sum_{k=1}^{N} \left(H_{p,exp} - H_{p,sim}(h,ac) \right)^{2} + \sum_{k=1}^{N} \left(T_{p,exp} - T_{p,sim}(h,ac) \right)^{2}$$
(6.5)

As our model involves the critical solvent content, for this system it was observed that the model fits well with the literature data, as shown in Figure 6.1, when the critical solvent content is 10%. Thus it proves the influence of critical solvent content on drying kinetics. As the solvent in the system contains polymer, its vapor pressure needs to be corrected. Vapor pressure correction factor was calculated as a product of volume fraction of solvent at any time and the activity coefficient. The optimum activity coefficient of the solvent (toluene) was found it to be 0.2382. However, no data about the geometry of the oven or coating sample was available in their work; we chose them arbitrarily as well. The air velocity was not mentioned either and so we assumed it to be 1 m/s. The optimum heat transfer correcting coefficient (α_{pa}) was found to be 0.2912, which resulted in a corresponding heat transfer

coefficient of 0.0012 W/cm²/ K. By Chilton-Colburn analogy we found the mass transfer coefficient to be 9.6710e-004 g/cm²/s. The total mass of solvent and polymer used in the simulation was 9.167 gm. This very simulation results also generated the temperature profile for both the polymer and air, although these profile are not available in their work. As Figure 6.2 shows, the polymer temperature approaches the drying air temperature after drying for 80 seconds. Furthermore, the air temperature decreases faster during the early stage of drying and this is pretty obvious in a typical convective drying. For this particular case, model prediction deviates by 13% from the literature data. Detail of error estimation on solvent remaining can be found in the appendix.



<u>Figure 6.1:</u> Comparison of literature data (Alsoy et al., 1998) and simulation results for the solvent remaining (%) in solution as a function of time for PS/Toluene system on polyester substrate. (lp= 0.010 33 cm, T_{pi} = 24°C, Va= 1 m/s, T_a =83.4 °C)



<u>Figure 6.2:</u> Simulated temperature profile for polymer and air for PS/Toluene drying (convective) on polyester Substrate. (lp= 0.010 33 cm, T_{pi} = 24°C, Va= 1 m/s, T_a =83.4 °C)

6.2 IR model Validation

Equations (4.1) to (4.10) describe the model developed for IR drying of polymer solution on a fixed substrate (batch process). This model was validated here with the literature data collected from the work done by Lamaison et al. (2001). They dried a paint film consisting of a water suspension of pigment and polymer particles of polyester on a stainless steel substrate in an IR oven under free convection. The thickness of the film was 100 micrometer, the initial weight of the solution was 0.275 g, and the applied heat flux was 4.2 kW/m². The paint film was applied on a stainless steel substrate of 53 mm diameter and 0.8 mm thickness.

We implemented an automated optimization scheme to find the optimum parameters that could make the curves fit best. The optimum values for the activity coefficient, heat transfer correcting coefficients (α_{pa} , α_{ra}) were found to be 0.3, 0.22 and 0.45, respectively. Figure 6.3 shows the predicted polymer temperature match the literature data with about 2% deviations. Figure 6.4 shows the predicted fraction of water evaporated is in a good agreement with the literature data with approximately 5% deviations. Detail of error calculation can be found in the appendix. The deviation could be attributed to the fact that in our simulation we assumed binary solution of water and polyester only, whereas originally the solution contained a third component (pigment) in a very small quantity. In our calculations we took the dimension of the stainless steel substrate as a square of having sides of 53 mm. But in practical, it was a round substrate with the diameter of 53 mm. This could also contribute to the deviation of prediction from the literature data.

The heat and mass transfer coefficients for this case were calculated from the conditions of natural convection. That is why the drying is a bit slow as it takes 400 seconds for almost all the water to evaporate.



<u>Figure 6.3</u>: Comparison of predicted polymer temperature profile with literature data (Lamaison et al., 2001) for aqueous polyester film drying on stainless steel substrate. (lp= 0.01 cm, T_{pi} = 24°C, E= 4.2 kW/m²)



<u>Figure 6.4</u>: Comparison of fraction of water evaporated from aqueous paint drying on steel with literature data (Lamaison et al., 2001). (lp=0.01 cm, $T_{pi}=24^{\circ}C$ K, E =4.2 kW/m²)

6.3 Simulation

The numerical predictions of the temperature and solvent content profile of thin coating on the substrate (web) are presented here for two cases; when the web is fixed and when it passes through the solvent removal IR oven. Equations (4.11) to (4.14) describe the modeling of IR coating drying on a moving substrate. The coating is supposedly a polymer solution which is composed of one solid polymer (PVAc) dissolved in only one solvent (Toluene) and is being dried on polyester substrate. From the large number of parameters, the web velocity, heater temperature, inlet air velocity and coating thickness were chosen and then varied in successive program simulations in order to compare the results. The first three parameters listed are variables that can normally be controlled during the operation of the oven. The last parameter, coating thickness, is normally set at the very beginning and remains nearly constant for thin coating during the operation. Results obtained are only applicable for the material, air and solvent properties given in section 4.5 and oven dimensions as described in section 4.3. Temperature dependent properties such as air density, viscosity, and thermal conductivity were changed accordingly for each simulation. The simulation time was taken as the residence time for a moving substrate in an IR oven. Therefore for a substrate traveling at a speed of 10 cm/s, the residence time is 140/10= 14 seconds. The parameters that were used for the simulation are presented in the table below.

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Initial air temp (T _i)	25°C
Initial coating temp (Tp _i)	23°C
Initial coating solvent content (Hpi)	70%
Velocity of substrate (V _p)	10, 15, 20 (cm/s)
Velocity of air (V _a)	3.5, 2.5, 1.5 (m/s)
Hc (g/100 gm of dry solid)	30
Air flow area (A _a)	360 cm^2
Shape factor correcting coefficient (α_r)	0.4
Convective heat transfer coefficient (between radiant and air) correcting factor (α_{ra})	0.1
Convective heat transfer coefficient (between polymer and air) correcting factor (α_{pa})	0.3
Total pressure (P)	760 mm Hg
Width of polymer (W _p)	25 (cm)
Width of radiant (W _r)	45 (cm)
Hydraulic diameter (D _h)	13 (cm)
Stefan-Boltzmann constant (σ)	5.67e-12 (W cm ⁻² K ⁻⁴)
Emissivity of polymer (ε_p)	0.9
Radiant Temperature (T _r)	225, 200, 175 (°C)

Table 6.2: Values of different initial conditions and parameters suggested for IR drying simulation

6.3.1 Batch Drying of coating (Fixed Substrate)

a) Effect of Radiant Temperature

From Figure 6.5 and Figure 6.6, the effect of radiant temperature on solvent content and polymer temperature is quite evident. As Figure 6.5 shows, at the end of drying, the solvent content reduces to 1% from 3% when radiant temperatures are 225°C and 175°C respectively. Figure 6.6 demonstrates that final polymer temperature rises to about 130°C and 100°C when radiant temperatures are 225°C and 175°C for the same thin layer (0.01 cm) of coating and air velocity (3.5 m/s). As expected, the solvent content decreases and the coating temperature increases with increasing radiant temperature. The temperature of the radiant (T_r) was chosen to a certain maximum in order to avoid the boiling of the solvent and to make sure that the solvent content reduces to zero at the same time. Boiling of solvent can many times lead to coating defects in the form of blisters or bubbles. The boiling temperature of pure solvent (Toluene) is 110.62°C. However, the bubble point of toluene in a solution is a function of the solvent content and it is higher than that of pure solvent. The PVAc polymer normally degrades under vacuum at an appreciable rate at temperatures above 227°C. PVAc degrades in two stages. In the first stage, 237-307°C, the thermal degradation of PVAc leads to production of a high proportion of acetic acid. In the second stage (322-372°C), aromatic hydrocarbons are produces almost exclusively. More about thermal degradation of PVAc could be found elsewhere (Barry et al., 2002). Figure 6.7 shows that the air temperature rises more rapidly at the very beginning than it does at the later stage of drying. This is because the heat transfer between the solvent vapor and air does not start right at the beginning of drying. At the very beginning of drying air only gains energy by convection heat transfer from the radiant before it actually starts losing heat to the solvent vapor.







<u>Figure 6.6</u>: Effect of radiant temperature on polymer temperature profile (lp = 0.01 cm, Va = 3.5 m/s)





b) Effect of air Velocity

Figure 6.8 shows that high air velocity (air flow) favors the drying process by rapidly reducing the solvent content in the polymer solution. As Figure 6.8 demonstrates, after 14 seconds of drying, the final solvent content is reduced from 3% to 1% by simply increasing the air velocity from 1.5 m/s to 3.5 m/s. The polymer solvent content decreases faster with the increase of air velocity. This is due to the fact that the higher the velocity of air the faster it carries away the solvent vapor evaporating from the polymer solution coated on the substrate and thus the air flow serves the principal purpose behind it. Air velocity, temperature of air and geometry of oven determine heat transfer coefficient in dryer. High air velocity results in high heat transfer coefficient and hence can increase the drying rate.





Figure 6.9 shows that polymer temperature is strongly affected by air velocity as final polymer temperatures are 135°C and 115°C for the air velocity of 3.5 m/s and 1.5 m/s, respectively. Figure 6.10 represents the air temperature profile for various air velocities. It is observed from Figure 6.10 that the air temperature increases with increase in air velocity.



<u>Figure 6.9</u>: Effect of air velocity on polymer temperature profile ($l_p = 0.01$ cm, $T_r = 225^{\circ}C$)



<u>Figure 6.10</u>: Effect of air velocity on air temperature profile ($l_p = 0.01$ cm, $T_r = 225^{\circ}$ C)
c) Effect of Coating Thickness

Figure 6.11demonstrates the effect of coating thickness on solvent content profile in polymer solution. As Figure 6.11 shows, after 14 seconds of drying, the solvent content of thinner coating (0.01 cm) has gone down to 1% while the thicker (0.03 cm) one still contains about 7% of the solvent. Figure 6.12 shows the polymer temperature profiles for various coating thickness. Figure 6.12 reveals that the temperature of 0.01 cm thick coating rises to 135°C after 14 seconds of drying, while that of 0.03 cm thick coating reaches 80°C. How the coating thickness affects the air temperature is shown in Figure 6.12.



<u>Figure 6.11</u>: Effect of coating thickness on the profile of solvent content ($T_r = 225^{\circ}C$, $V_a = 3.5$ m/s)

Figure 6.12 shows, after 14 seconds of drying, for thin coating (0.01 cm) the final air temperature is higher (165° C) than that for thick coating (0.03 cm). Examining these Figures, we observe that drying rates are lower for thicker coatings. Thicker coatings have more total mass and more solvent mass; thus, they heat more slowly.



<u>Figure 6.12</u>: Effect of coating thickness on the profile of polymer temperature ($T_r = 225^{\circ}C$, $V_a = 3.5 \text{ m/s}$)





6.3.2 Continuous Drying of Coating (Moving Substrate)

a) Effect of Radiant Temperature

Figure 6.14 represents the effect of radiant temperature on solvent content profile for drying of coating on moving substrate. Figure 6.14 shows that the final solvent content in the coating goes down to zero when radiant temperature is 225°C. For exactly the same drying condition, the final solvent content is 5% when radiant temperature is 175°C.



<u>Figure 6.14</u>: Effect of radiant temperature on solvent content profile ($l_p = 0.01$ cm, $V_a = 3.5$ m/s, $V_p = 10$ cm/s)

As has been mentioned before in the earlier section of drying of coating on fixed substrate, higher radiant temperature radiate higher heat flux, which is the principal source of heat and mass transfer to take place. Obviously, higher heat flux increases the temperature of the coating and also the vapor pressure of the solvent, thereby increasing mass transfer rate. From Figure 6.15, it is observed that the thinner coating (0.01 cm) temperature reaches 108°C while for the same residence time the thicker coating (0.03 cm) temperature is below 90°C.



<u>Figure 6.15</u>: Effect of radiant temperature on polymer temperature profile ($l_p = 0.01$ cm, $V_a = 3.5$ m/s, $V_p = 10$ cm/s)

Figure 6.16 shows how air temperature gets affected by various radiant temperatures. As the figure shows the air temperatures are 142°C and 132°C when radiant temperatures are 225°C and 175°C, respectively.



<u>Figure 6.16</u>: Effect of radiant temperature on air temperature profile ($l_p = 0.01$ cm, $V_a = 3.5$ m/s, $V_p = 10$ cm/s)

b) Air Velocity

Like drying of coating on fixed substrate, air velocity favors the drying of coating on moving substrate as well. As Figure 6.17 demonstrates, high air velocity enhances drying rate significantly. The coating dries in about 14 seconds when air velocity is 3.5 m/s and it exits with 9% solvent content when air velocity is 1.5 m/s.



<u>Figure 6.17</u>: Effect of air flow (air velocity, Va) on solvent content profile ($T_r = 225^{\circ}C$, $l_p = 0.01$ cm, $V_p = 10$ cm/s)

Figure 6.18 demonstrates how polymer (coating) temperature changes with different air velocity. Air velocity helps determine the convective heat transfer coefficients (h_{pa} , h_{ra}). The higher the air velocity, the higher are the heat transfer coefficients.



<u>Figure 6.18</u>: Effect of air flow (air velocity, Va) on polymer temperature profile ($T_r = 225^{\circ}C$, $l_p = 0.01$ cm, $V_p = 10$ cm/s)

Figure 6.19 shows how air temperature also changes with varying air velocity. The higher the air velocity, the higher is the mass flow of air and as a result the higher are the final air temperatures.



<u>Figure 6.19</u>: Effect of air flow (air velocity, V_a) on air temperature profile ($T_r = 225^{\circ}C$, $l_p = 0.01$ cm, $V_p = 10$ cm/s)

c) Effect of Coating Thickness

Figure 6.20 shows that for the same residence time, thinner coating temperature rises to above 100°C and the thicker coating temperature is somewhere around 70°C. Thinner coatings have less total mass and less solvent mass, which leads to more rapid heating. As shown in Figure 6.21, it takes only 14 seconds for 0.01 cm thick coating to dry whereas 0.03 cm thick coating still contains about 40 % solvent after the same residence time of 14 seconds.



<u>Figure 6.20</u>: Effect of coating thickness on polymer temperature profile ($T_r = 225$ °C, $V_a = 2.5$ m/s, $V_p = 10$ cm/s)



<u>Figure 6.21</u>: Effect of coating thickness on solvent content profile ($T_r = 225^{\circ}C$, $V_a = 2.5$ m/s, $V_p = 10$ cm/s)

Figure 6.22 demonstrate the effect of coating thickness on air temperature profile. The air temperature (142°C) is higher for thinner (0.01 cm) coating.



<u>Figure 6.22</u>: Effect of coating thickness on air temperature profile ($T_r = 225^{\circ}C$, $V_a = 2.5$ m/s, $V_p = 10$ cm/s)

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d) Effect of Substrate (Web) Velocity

Figure 6.23 shows that the substrate traveling at a speed of 20 cm/s and 10 cm/s exit the dryer after 7 seconds with containing 35% and 2% solvent, respectively. Figure 6.24 represents a display of temperature distributions in the coated substrate in the oven as a function of the web velocity. The polymer final temperature is only 45°C when the web speed is 20 cm/s, whereas, it is about 90° when the web speed is 10 cm/s. The polymer temperatures are each seen to decrease with increasing web velocity. The difference in polymer temperatures for different web velocity is greatest towards the end of the oven as the web exits. It is the web velocity that determines the residence time of the web inside the oven as it is equal to the length of the dryer divided by the web velocity. The higher the web velocity, the lesser is the residence time. Consequently, the profile end after the residence time for respective web or substrate velocity. Hence the web that passes with the higher velocity gets actually less time to stay inside the oven than the one that passes with lower velocity. And, the web can absorb more heat when it passes at a lower velocity. Problems can arise when excessively fast web speed (> 20 cm/s) is used or when the web speed is too slow (< 10 cm/s). If the web speed is too fast, the newly coated web will still hold a large percentage of water or solvent as it proceeds on for possible further processing. The presence of any remaining unwanted component can affect the properties of an adhesive or coating, reducing the cohesive strength of the material, and affecting the final bond of an adhesive or the performance of a coating. If the web speed is too slow, the newly coated web, particularly if it is of a thermosetting nature, will be affected by the excessive residence time. It's been mentioned earlier, the simulation time was taken equal to the residence time of the coating inside the oven, the curves (solvent content, temperature, air temperature profile) for different web velocity (10, 15, 20 cm/s) end at their respective residence times (of 14, 9.3, 7 seconds). It is also observed in Figure 6.24 that the temperature profile has a slightly decreasing trend at the end of its residence time. This is because the web is exposed to ambient temperature when it comes to the other end of the dryer. Figure 6.25 shows the air temperature profile for various web speeds. It also shows that the air temperature is higher $(130^{\circ}C)$ for slower web (10 cm/s) than that (100°C) of faster web (20 cm/s).



<u>Figure 6.23</u>: Effect of Substrate velocity (V_p) on solvent content profile ($T_r = 225^{\circ}C$, $l_p = 0.01$ cm, $V_a = 3.5$ m/s)



<u>Figure 6.24</u>: Effect of substrate velocity (V_p) on polymer temperature profile (T_r = 225°C, l_p = 0.01 cm, V_a= 3.5 m/s)



<u>Figure 6.25</u>: Effect of substrate velocity (V_p) on air temperature profile ($T_r = 225$ °C, $l_p = 0.01$ cm, $V_a = 3.5$ m/s)

6.4 Comparison of two Different Drying Systems (Fixed versus Moving)

Figure 6.26 demonstrates that drying is faster for fixed sample than moving one for the same drying conditions. For instance, after 4 seconds of drying, the solvent content of the fixed substrate is only 12% whereas that of moving is about 38%. As shown in Figure 6.27, the temperature profile also follows the same kind of trend. As is shown in Figure 6.27, coating temperature on fixed substrate reaches around 80°C after 6 seconds of drying. For the same drying condition the coating temperature on moving substrate reaches just about 70°C after 6 seconds when it travels at 10 cm/s. The faster the substrate passes through the dryer the lower is the rise in coating temperature. The temperature difference of coating between the two cases, fixed and moving substrate, is the greatest near the middle of the oven. The moving web exits with slightly lower temperature (110°C) than the temperature that the fixed substrate reaches (135°C) after the same residence time. The comparisons are all made under a fixed oven residence time of 14 seconds. The oven residence time sets the time scale for which the comparative statements are meaningful.



<u>Figure 6.26</u>: Solvent content profile for coating drying on moving and fixed substrate ($T_r = 225^{\circ}C$, $V_a = 3.5 \text{ m/s}$, $l_p = 0.01 \text{ cm}$)



<u>Figure 6.27</u>: Polymer temperature profile for coating drying on moving and fixed Substrate ($T_r = 225$ °C, $V_a = 3.5$ m/s, $l_p = 0.01$ cm)

6.5 Simulation of Drying Thick Layer on fixed container

Next two figures (Figure 6.28 and Figure 6.29) represent the IR drying kinetics of thick layer of polymer solution applied on inert impermeable container of polyester. Figure 6.28 reveals that at radiant temperature of 225°C, the solvent concentration goes down close to 0.1 g/cc. At low radiant temperature of 175°C, the solvent concentration remains little higher than 0.15 g/cc. In every case of simulation the residence time was taken to be 200 seconds. Since the solution is 100 times thicker than thin solution (0.01 cm) it takes longer time to dry.



<u>Figure 6.28:</u> Solvent concentration profile for IR drying of thick polymer solution at different radiant temperature. ($l_p=1$ cm, $V_a=1.5$ m/s)

Figure 6.29 shows the temperature profile of the polymer for different radiant temperature. The polymer temperatures rise to 118°C and 92°C when radiant temperatures are 225°C and 175°C, respectively.



<u>Figure 6.29</u>: Polymer temperature profile for IR drying of thick polymer solution at different radiant temperature ($l_p=1$ cm, $V_a=1.5$ m/s)

A conclusion has been drawn at the end on the overall work in the next chapter.

CHAPTER 7

7. Concluding Remarks

7.1 Summary

Mathematical models have been developed to describe IR and convective heating of a coated substrate and solvent evaporation from a substrate in an oven for both thin and thick layers. The models were used in this study to predict the temperature and solvent content of the substrate. The models developed are validated with published literature data. Both the convective and IR drying models yielded good agreement with similar study in the literature. From the large number of oven parameters, the substrate velocity, heater temperature, inlet air velocity, and coating thickness were chosen and then varied in successive program simulations in order to compare the results. The effect of substrate speed on drying is well characterized by the model of moving system. Simulated results show that the coating thickness is the most influential parameter for coating drying. Thick layer model of IR drying can be used to predict drying profiles in paint and polymer manufacturing industry. We may conclude that higher radiant temperature and air flow, lower speed of substrate help enhancing drying rate. Depending on the specific application, these parameters may be chosen to customize the design and operation of a coating processing oven. The results presented are dependent upon the accuracy of the numerical formulation, which is limited by the assumptions made. This is not a complete analysis for all coatings, but the qualitative results for this particular system (PVAc-toluene) should extend to many other systems. Careful analysis of the results of computer simulations under different conditions, such as presented in this study, can be expected to lead to better design decisions prior to building an IR oven for coating drying application.

7.2 Future Work

Lack of significant amounts of analytical or experimental research on the continuous IR drying process of coating provides a lot of important future works. The models can be used for the following works.

- To find the optimum drying condition for continuous drying of coating in an IR oven in order to achieve desired goals, for example, to maximize profits, minimize costs, minimize residual solvent in the film for a specified substrate speed, etc.
- To design a controller that can control the drying process for this particular problem by means of controllable variables.
- It would be an interesting idea to carry out experimental works on drying of coating on moving substrate so as to calibrate the models.

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Appendix

A.1 Data for Convective Drying

Here we represent all the data we collected from the literature and also the data predicted by the models. Afterwards, we calculated the percentage of error at which the predicted data deviates from experimental data.

The experimental data were collected from open literature (Alsoy et al, 1998) for the convective drying of polystyrene in toluene on polyester substrate. These data were plotted in Figure 6.1 against the predicted data from simulation for the same system.

% of error was calculated by the following equation

$$Er = \frac{|ed - sr|}{ed} \times 100$$

Where, ed and sr stand for experimental data point and sr for corresponding predicted results from simulation.

And the average % error was calculated by

$$Er_{avg} = \frac{1}{N} \sum_{i=1}^{N} Er_i$$

Where N is the total number of data points.

Table A.1 repsrents the literature data, predicted results of the simulation and error percentage of "% solvent remaining" in coating for convective drying of polystyrene in toluene on polyester substrate.

Time (s)	% Solvent remaining			Average
	Literature data	Predicted	Error %	error %
0.00	100.00	100.00	0.00	and a set of the
5.87	90.35	87.88	2.73	
10.54	82.59	72.32	12.43	
15.55	71.56	56.70	20.76	
20.39	58.71	43.94	25.15	
25.50	45.85	32.89	28.28	
30.60	32.38	24.20	25.26	
35.41	17.91	17.86	0.28	13.45
40.63	10.33	12.82	24.13	
45.55	8.04	9.87	22.64	
50.36	7.60	8.02	5.54	
55.58	6.52	6.64	1.80	
60.39	5.46	5.71	4.57	
65.36	5.82	4.98	14.34	
70.31	4.75	4.42	7.03	
75.54	4.28	3.94	7.96	
79.69	4.89	3.63	25.69	

Table A.1: Data (plotted in Figure 6.1) and error percentage of % solvent remaining in coating for convective drying of polystyrene in toluene on polyester substrate.

A.2 Data for IR drying

IR drying in a fixed frame has been validated, as shown in Figure 6.3 and 6.4, with the experimental data collected from the work done by Lamaison et al. (2001). They dried a paint film consisting of a water suspension of pigment and polymer particles on stainless steel substrate in an IR oven under free convection. The error percentage calculation was done the way as it has been explained earlier. Here we calculated error for both the temperature of polymer and fraction of water evaporated. Table A.2 represents the data of Temperature and error % for each data point as well as average error % at a specific time. Table A.3 represents the data and error percentage of fraction of water evaporated for IR drying of polyester-water paint on stainless steel substrate.

Time	Temperature (°C)		Error	Average
(s)	Literature data	Predicted	%	Error %
0.00	26.04	26.00	0.14	
12.20	39.62	35.54	10.31	
24.39	50.94	49.03	3.75	
35.37	57.74	58.45	1.23	
46.34	62.26	68.22	9.56	
58.54	66.79	77.28	15.70	
70.73	74.72	85.62	14.60	
95.12	90.57	93.49	3.23	
106.1	99.62	100.8	1.22	
119.5	106.4	107.6	1.15	
130.5	114.3	113.9	0.41	
142.7	120.0	119.6	0.37	
154.9	125.7	124.7	0.75	
165.9	130.2	129.4	0.63	
178.0	134.7	133.5	0.87	2.361
190.2	138.1	137.3	0.61	
201.2	142.6	140.3	1.65	
214.6	143.8	143.3	0.34	
225.6	146.0	146.2	0.11	
237.8	149.4	148.5	0.61	
250.0	150.6	150.6	0.01	
262.2	152.8	152.4	0.29	
274.4	154.0	154.0	0.01	
285.4	155.1	155.2	0.09	
297.6	156.2	156.6	0.23	
309.8	157.4	157.7	0.19	
322.0	157.4	158.6	0.79	
345.1	158.5	159.3	0.54	
369.5	159.6	161.3	1.03	
393.9	161.9	162.5	0.40	

Table A.2: Data (plotted in Figure 6.3) and error percentage of temperature for IR drying of polyester-water paint

Time (s)	Fraction of wat	Fraction of water evaporated		Average
	Literature data	Predicted	%	error %
0.000	0.000	0.000	0.000	
9.521	0.026	0.031	17.873	
23.770	0.093	0.112	20.765	
34.384	0.204	0.206	1.142	
46.152	0.348	0.346	0.641	
57.924	0.489	0.512	4.676	
69.718	0.611	0.655	7.120	
81.561	0.693	0.754	8.845	
93.431	0.752	0.822	9.288	
105.322	0.793	0.868	9.536	
117.223	0.826	0.901	9.028	
129.137	0.848	0.923	8.863	
141.046	0.874	0.940	7.509	
152.969	0.889	0.952	7.066	1 000 1
164.887	0.907	0.961	5.865	4.9234
176.809	0.922	0.967	4.897	
187.542	0.933	0.972	4.155	
199.469	0.944	0.976	3.371	
212.595	0.952	0.980	2.944	
224.522	0.963	0.983	2.025	
236.453	0.970	0.985	1.462	
248.389	0.974	0.986	1.254	
260.321	0.982	0.988	0.636	
271.063	0.985	0.989	0.369	
284.192	0.989	0.990	0.108	
296.133	0.989	0.991	0.196	
308.064	0.996	0.992	0.474	
318.806	1.000	0.992	0.784	
354.622	1.004	0.994	0.998	
390.443	1.004	0.995	0.893	

Table A.3: Data (plotted in Figure 6.4) and error % for fraction of water evaporated for IR drying of polyester- water paint

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