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Integrated multiscale product and process control of polymeric coating curing

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ABSTRACT

In automotive coating manufacturing, control of curing of thin films of wet paint on vehicle panels is always a very challenging operational task. This is especially true when both process efficiency and product quality need to be controlled simultaneously. The challenges in this task are multiple. First, coating quality is not measurable online and its characterization is multiscale in length and time. Second, coating curing is a multistage process where heat and mass transfer and polymerization take place also in multiscale of length and time, most of which are not measurable online either. In this paper, we introduce an integrated multiscale product and process control (IMPPC) scheme that can be used to control effectively the reactive drying process. By resorting to this scheme, a set of advanced methodologies for multiscale modeling, model simplification, and multiscale controller synthesis can be seamlessly integrated to construct a high-performance control system. It is demonstrated that this control system has extraordinary performance on set-point tracking and disturbance rejection. Most importantly, it offers unique opportunities to achieve all-time on-aim control of both coating quality and process performance covering a wide range of time and length scales.

1. Introduction

Coated products are pervasive in our lives. One of important coating demands comes from automobile, which needs coatings for ‘body’ protection, such as anti-corrosion and stone-chip resistance, as well as a durable and appealing finish. The automotive coating consists of several thin layers, i.e., phosphate, electro-coat, basecoat, and clearcoat, and each layer performs distinctive functions. The associated manufacturing system includes a series of highly automated processes, such as pretreatment, priming, paint spray, and oven curing [1].

In the past decades, automotive OEMs and paint manufactures have devoted tremendous efforts to the process efficiency and product quality improvement in coating manufacturing. Nevertheless, the development of energy-efficient and environmental-benign processes that can ensure a full demonstration of the anticipated coating performance still remains as a very challenging task. High productivity requires vehicle bodies to continuously move on the conveyors, while being sprayed on and being baked. This makes it extremely difficult to ensure the uniform quality of the coating. Moreover, almost all product performance variables and a number of key process variables are not measurable *during* manufacturing. This makes current quality control rely only on post-process sampling, causes various quality problems, leads to inefficient energy and material utilization, and generates excessive amounts of waste and pollutants [2,3]. Furthermore, there exists a clear knowledge disconnection between the macroscale bulk production and finer-scale material properties and product behavior [4,5]. In production, operational settings are always being adjusted based on experience in the macroscale; hence the true optimality could almost never be realized.

A reliable prediction of the process and product performance during coating manufacturing is critical for deriving a better understanding of the system behavior and hence fulfilling system-level tasks such as control and optimization. A set of macroscopic models have been developed for the solvent-borne based coating drying and curing [6–10]. Those models can generate very valuable quantitative information about how (i) the coating topology (from wet to dry) could be dynamically changed, (ii) the solvent could be smoothly removed, (iii) the crosslinking reaction could take place, and (iv) common defects could be successfully detected, analyzed, and prevented. More sophisticated modeling and simulation techniques for characterizing the paint spray operations were developed, where neural networks, fuzzy logic, and CFD techniques were used in different components of the modeling and simulation systems [11–16]. However, the existing models are usually monoscale based. They cannot provide the comprehensive information necessary for addressing the whole spectrum of coating quality (macro- to microscale), material and energy efficiency

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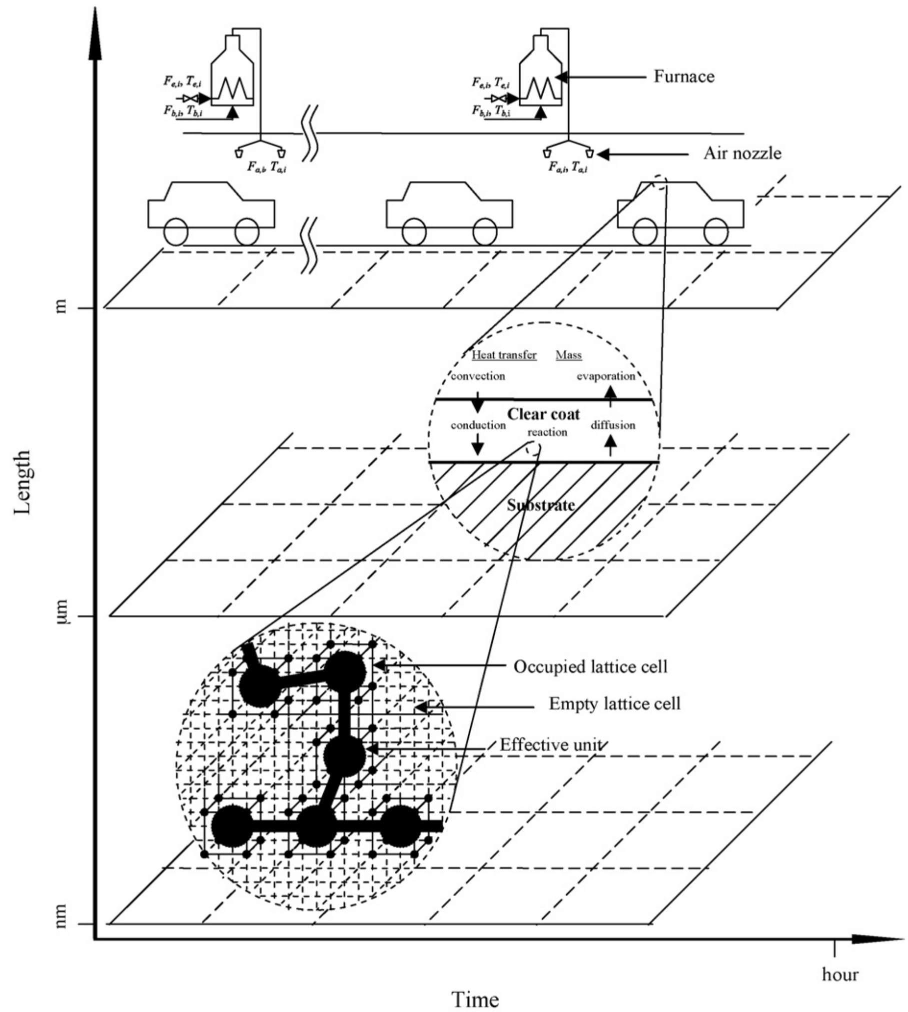

Fig. 1. Multiscale illustration of automotive coating curing system.

(macro- to mesoscale), and environmental cleanness (macro- to mesoscale).

It is anticipated that superior product and process performance have to be assured throughout the course of coating manufacturing. This requirement disqualifies various reactive quality control (QC) approaches [17] that rely mostly on post-process quality inspection. A proactive QC approach must be predictive and preventive, aiming at performance assurance starting from the earliest stage of product manufacturing. This kind of QC approach can be realized by resorting to integrated product and process (IPP) control [18]. Theoretically, IPP control can ensure all-time on-aim control of both process and product performance, if complete and reliable predictions of system behavior are available and an effective control system can be synthesized. Although the IPP control concept is generic and powerful, the control scheme and controller synthesis methodologies introduced in Xiao et al. [18] are only applicable to the over-simplified linear SISO systems characterized by monoscale (i.e., macroscopic) models. There is an urgent need to extend the original methods to the characterization and proactive control of integrated process and product systems covering a wide range of time and length scales, which becomes the focus of this paper.

In the remaining part of this paper, the automotive coating manufacturing system as well as the need for a multiscale model based control are discussed at the outset. After that, a high-performance control system is constructed by seamlessly integrating methodologies for multiscale modeling and simulation, multiscale information coupling, model simplification, control scheme and strategy development, and controller synthesis. Finally, methodological effectiveness will be fully demonstrated by a detailed case study.

2. Automotive coating manufacturing

In automotive coating, paint of different types is used to develop a basecoat (with color) and a clearcoat. Each of the two layers (together called topcoat) is commonly developed in two consecutive operational steps: spray and curing. Besides the composition of the paint material and its properties, the design and operating conditions of the spray and curing facilities are the key factors affecting coating quality and process performance.

This paper investigates the clearcoat curing process, which is the most energy-intensive step in an automotive assembly and plays a key role in determining final coating quality. Fig. 1 illustrates an automotive coating curing system in a multiscale fashion. In the process, the vehicle bodies covered by layers of wet films travel one by one on a conveyer at a constant speed through a curing oven. The oven is usually divided into a number of zones so that different heating mechanisms (i.e., radiation from oven walls and hot air convection) can be applied under different operating conditions [10]. The oven wall temperature and the convection air temperature are controlled by adjusting the flow rate of fuel fed into the furnace. During curing, the solvent contained in the wet film is removed by heat, the film thickness and thus its topology change, and crosslink-

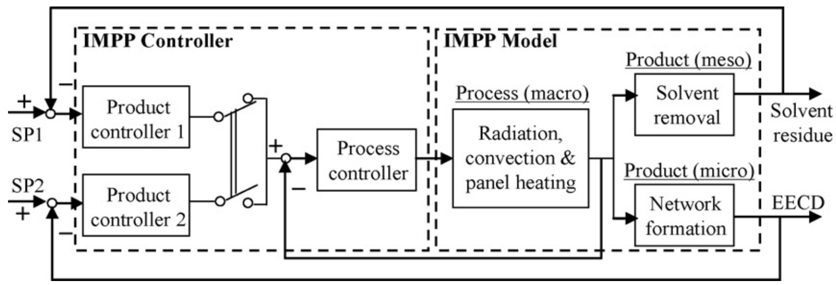

Fig. 2. IMPP control of automotive coating curing.

ing reactions take place within the film. Finally, the cured coating with desired properties is developed on the vehicle surface as the final product.

A curing oven is usually about 120–250 m long and coating curing usually takes ~30 min. Thus, macroscopic heat transfer models are needed to characterize the curing environment in an oven. The solvent removal occurred within the thin wet film of ~110 μm (at mesoscale) determines the thickness and topology of the dry film and thus coating appearance and durability. Consequently, mesoscale solvent diffusion and evaporation models are needed. Note that coating quality in terms of solvent resistance, inter-coat adhesion and scratch resistance is determined by coating microstructure, which is a polymer network formed through crosslinking reactions. Hence, a microscopic polymer network formation model is needed as well. As a result, any monoscale modeling and simulation method is not capable of describing coating curing system precisely and comprehensively. Superior system performance can be realized only if multiscale process and product behavior can be effectively characterized and controlled.

3. IMPPC system design

As stated, the essential merit of an IPP control is the all-time systematic control of both process performance and product quality. The control performance is largely affected by control synthesis. A selected synthesis method should provide answers to the following challenging questions: (i) which control scheme is most appropriate for an IPP system? (ii) how to develop models that can precisely capture dominant process and product behavior and at the same time can be used for real-time control? and (iii) how to design an IPP controller in a systematic way?

An IPP control synthesis methodology has been successfully developed for linear single-input–single-output (SISO) and multiple-input–multiple-output (MIMO) systems, where both process and product are described by monoscale (i.e., macroscale) models [18–20] However, those methods should be extended in order to be applicable to an integrated multiscale product and process (IMPP) system. A key challenging issue to be addressed is the simplification of computationally expensive multiscale models for online control. In this section, a comprehensive IMPP control (IMPPC) synthesis method is introduced.

4. IMPPC scheme

A cascade-control-based IPP control scheme was rigorously derived by Xiao et al. [18], and it has demonstrated attractiveness in controlling both linear SISO and MIMO monoscale systems [18–20]. This scheme is adopted for IMPP control as well. An IMPP control system for automotive coating curing is given in Fig. 2. The inner loop is for the control of macroscale curing process, while the outer loop is for the control of meso- to microscale coating quality. The IMPP controller consists of one process controller and two product controllers, with product controller 1 for solvent content control and product controller 2 for coating microstructure control. A switch strategy is introduced between the product controllers to smooth the transition of control between the mesoscale and microscale product quality targets.

5. Multiscale model development

The process and product models developed for describing coating curing are briefly presented below.

5.1. Macroscopic curing model

A set of first-principles-based models is developed to characterize the multistage curing environment. Burning natural gas in the furnace provides energy to heat up the oven wall and the convection air. It is reasonable to assume that the fuel and combustion air are well mixed and the heat loss to the surrounding environment is negligible. Thus, the energy balance of the burning process in the furnace can be described as:

$$F_a C_{p,a}^{T_a} T_a - F_e C_{p,e}^{T_e} T_e - F_b C_{p,b}^{T_b} T_b = F_e \Delta H_e, \tag{1}$$

where F, T, and C_p are, respectively, flow rate, temperature, and heat capacity; the subscripts a, e, and b represent, respectively, convection air, fuel, and combustion air. ΔH_e is the energy density of the fuel.

In the work, a convection-only oven is investigated, where the panel temperature dynamics can be expressed as:

$$\rho_m C_{p,m} Z_m \frac{dT}{dt} = h_v (T_a - T), \tag{2}$$

where ρ_m, $C_{p,m}$ and Z_m, T are the density, heat capacity, thickness and temperature of the metal substrate, respectively; h_v is the heat transfer coefficient, that is a function of convection air velocity, the distance between the panel and the convection air nozzles, and others. It is assumed that the thin film has the same temperature as the related vehicle panel.

5.2. Mesoscopic solvent removal model

The following models can reveal the solvent removal process occurred within the thin film and on the coating surface:

$$\frac{\partial X}{\partial t} = \frac{\partial (D(X,T)(\partial X/\partial Z))}{\partial Z}, \tag{3}$$

$$\rho_s Z_s \frac{\partial X}{\partial t} = K \frac{(P_a - \alpha P_{sa})}{P} + \rho_s D(X,T) \frac{\partial X}{\partial Z}, \tag{4}$$

$$D(X,T) = \eta e^{-((\gamma/X)+(E_d/RT))}, \tag{5}$$

where X is the solvent content; D is the diffusivity; ρ_s and Z_s are the density and thickness of unreducible components in the film, respectively; K is the mass transfer coefficient; P_a is the partial pressure of the solvent in the convection air; P_{sa} is the solvent saturation pressure; P is the system pressure; η is a pre-exponential constant for diffusion; γ is a constant; E_d is the activation energy for diffusion.

5.3. Microscopic polymer network formation model

A lattice Monte Carlo (LMC) model based on a bond fluctuation (BF) method is developed to characterize coating microstructure evolution [21]. In the lattice, each cell can be occupied by no more than one effective unit (EU), either an effective monomer or a crosslinker (see Fig. 1). The EUs can move around continuously in the lattice, which mimics the random motion of polymer chains during coating curing in real application. Note that a move is feasible only if it follows the excluded volume restriction and the resulting new bond vectors belong to a set of permissible bond vectors.

The formation of a polymer network can be simulated by following the steps below: (i) to set up a simulation system, (ii) to generate an initial configuration, (iii) to establish an equilibrium state, and (iv) to implement crosslinking reaction for polymer network formation [22,23]. In this paper, only the most important step (i.e., step iv) is detailed below. The crosslinkng reaction proceeds along LMC steps until a preset curing operation is finished. In each LMC step, an EU move is attempted first; the EU is randomly selected. Then, crosslinking reactions are performed between the selected EU and other EUs. A new bond between them is then created only if the following three conditions are all met: (i) a neighbouring EU is located in two lattice cell distance from the selected EU, (ii) the neighbouring EU has a different type of functional groups, and (iii) the neighbouring EU has at least one remaining functional group for reaction. The method for counting the effect of macroscopic curing condition on microstructure evolution will be described later.

5.4. Process and product performance model

The process performance is evaluated in the context of energy efficiency. The fuel consumption (i.e., a direct indicator of energy efficiency) can be easily calculated by integrating the fuel flow rate along the curing time. The coating quality is assessed by quantifying the solvent residue in the film and the elastically effective crosslink density (EECD) of the 3D polymer network in a coating. In the dry film, the solvent content must be lower than a certain value [10]. For a specific polymeric material, there exists a preferred EECD region. A very low EECD indicates that the coating is underbaked and thus tends to be sensitive to humidity and solvent. On the other hand, a very high EECD is a sign of overly baked coating, which means a typical inter-coat adhesion failure in the coating [24–26].

6. Multiscale information coupling

The models listed above can provide the process–product information at different time/length scales. Hence, how to fully utilize the information is critical. For the coating curing system, there exists a clear time-scale gap between the macroscopic curing simulation and the microscopic polymer network evolution simulation. A complete curing process takes ~30 min, while the characteristic time for a local diffusive motion of a coarse-grained polymer chain is only 10^{-4}–10^{-8} s.

A special bi-directional coupling approach is developed to bridge the existing time-scale gap. The curing temperature at a specific time instant obtained from the curing model is sent to the LMC model for evolving the polymer network microstructure. On the other hand, the crosslinking conversion derived from the microstructure is transmitted back to the curing model. By utilizing the reaction rate information, the succeeding time instant for transmitting a temperature to the LMC model can be determined [22]. In this way, the microstructural evolution throughout a curing process under known curing conditions can be derived.

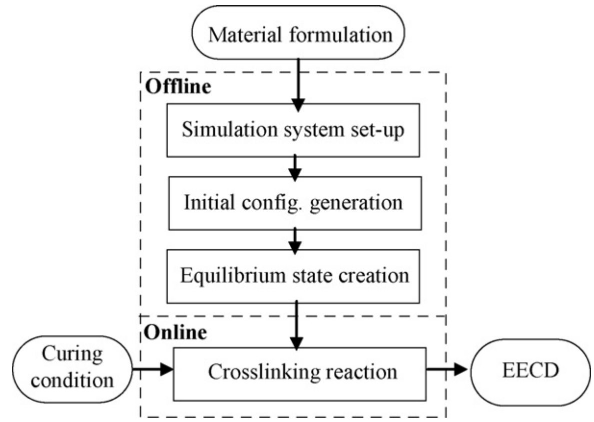

Fig. 3. LMC model simplification by task division.

7. Model simplification

Multiscale models can provide a comprehensive description of the system behavior, but at the same time they are computationally expensive and thus cannot be directly used for real-time control. A superior model simplification method has to be developed that is capable of achieving a desirable balance between the precision and computational efficiency.

7.1. Microscale LMC model simplification

It is found that for a system consisting of $\sim 10^4$ polymer beads, the LMC-based polymer network formation simulation will take ~32 min, ~94% of which will be for creating an equilibrated structure, and only ~6% of time for crosslinking reaction simulation. Based on this finding, a special task division strategy is utilized.

As shown in Fig. 3, a complete simulation task is divided into two parts: an offline part for preparing a well equilibrated system and an online part for implementing crosslinking reaction for polymer network formation. The online part is used as the microscale product model in the IMPP control system shown in Fig. 2. A unique feature of this special strategy is that the precision of the model keeps unchanged. It should be more attractive than some conventional MC simulation simplification methods, e.g., reducing the total number of entities in the simulation system at the expense of sacrificing prediction precision.

8. Controller design and operational strategy development

Dynamic system simulation shows that most of the solvent is removed in the initial stage of curing, while during that time period, EECD value remains at zero. The EECD starts to rise from zero only after the gel point, when the polymer network of infinite size begins to form [22]. It is also noticed that, after the gel point, the solvent residue decreases very slowly and its dynamics are not sensitive to the curing history. These interesting phenomena suggest application of a two-stage control strategy shown in Fig. 2. In the first stage, the solvent is removed under the control of product controller 1. The outer loop is then switched to the closed-loop control of polymer network formation at the gel point, when product controller 2 begins to function. In order to ensure a smooth transition from product controller 1 to 2, the switch point is determined as the earliest time instant when either the EECD set-point or the EECD real curve begins to rise from zero.

8.1. Process controller design

The nonlinear heat transfer ODE model is first linearized using a piecewise linearization method. For any specific linearization zone, a control law and a set of controller parameters can then be derived using a target-oriented method [27].

8.2. Product controller design

The two product controllers adopt usual PID control laws. The complete control horizon is first divided into a number of zones. The standard Ziegler–Nichols tuning method is applied in each zone to derive a set of PID controller parameters.

9. Case study

An automotive coating curing system is thoroughly investigated in this section. It is to show how the introduced methodology can offer quantitative predictions and high-performance control of process and product behavior over multiple time and length scales.

9.1. System specification

9.1.1. Material

The coating material contains a resin that is composed of hydroxyl-functional acrylic copolymer and hexamethoxymethylmelamine (HMMM) crosslinker. The resin has a number average molecular weight of 3000 g/mol and the hydroxyl equivalent weight of the resin is 650 g/mol. The molecular weight of an effective monomer is 360 g/mol, and the crosslinker has a molecular weight of 390 g/mol and a functionality of 6. The number ratio of the methoxy group of HMMM to the hydroxyl group of the precursor polymer chains is set as 1.5.

9.1.2. Process

The oven is 125 m long and consists of seven zones. Each vehicle body, initially at 300 K for each panel, moves through the oven at the line speed of 0.069 m/s. Other normal operating conditions (e.g., the flow rate and temperature of fuel for each furnace, the flow rate of the convection air in each zone, and the temperature of the fresh air fed into the furnace, etc.) are specified using industrial data.

9.1.3. Product

The wet clearcoat on the vehicle surface has a solvent content of 0.18 and an initial thickness of 70 μm. For the coating product after curing, the solvent content in the dry film should be less than 0.03 and the coating microstructure should have an EECD value between 0.8×10^{-3} mol/g and 1.25×10^{-3} mol/g. Furthermore, in order to prevent defects caused by improper heating, the temperature increment of the film cannot exceed 7 K/s and the temperature of the convection air must be below 470 K.

9.2. Multiscale system characterization

The modeling and simulation method developed in this work offers unique opportunities to monitor process performance and product quality at multiple scales throughout coating manufacturing. Fig. 4 displays the dynamics for the film temperature, the solvent content and the EECD. As shown in the inset of Fig. 4(c), a coating microstructure is a crosslinked polymer network. The green and blue beads represent monomers, while the crosslinkers are plotted as red and pink beads. This 3D structure is used for EECD calculation. The shaded areas indicate the permissible regions of coating quality. It is clear that the final coating quality is fully acceptable in this case.

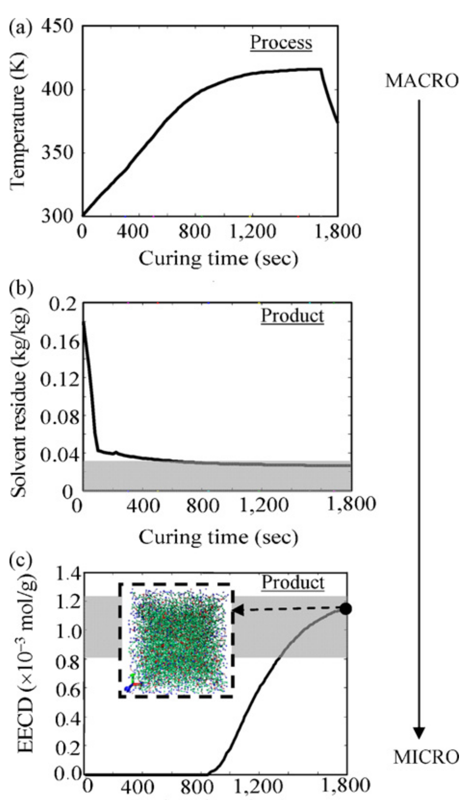

Fig. 4. Process and product dynamics: (a) film temperature, (b) solvent content, and (c) EECD (the inset shows the coating microstructure at the end of the curing).

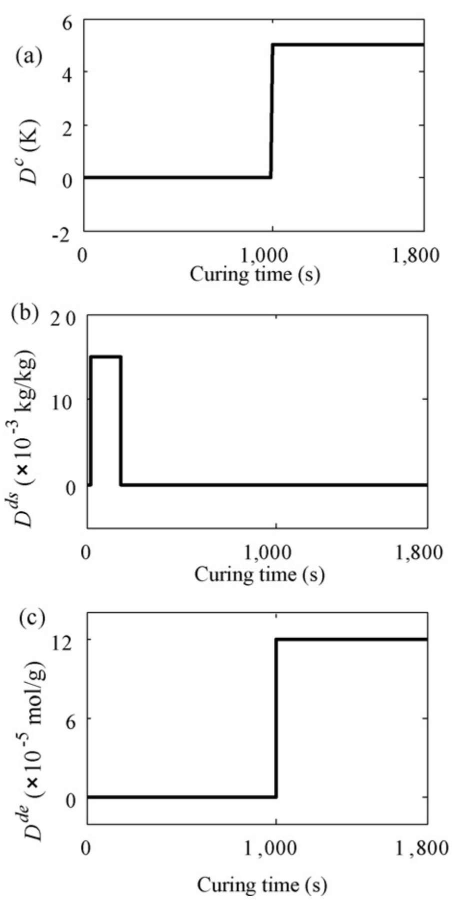

Fig. 5. Introduced process and product disturbances: (a) disturbance on film temperature, (b) disturbance on solvent residue, and (c) disturbance on EECD.

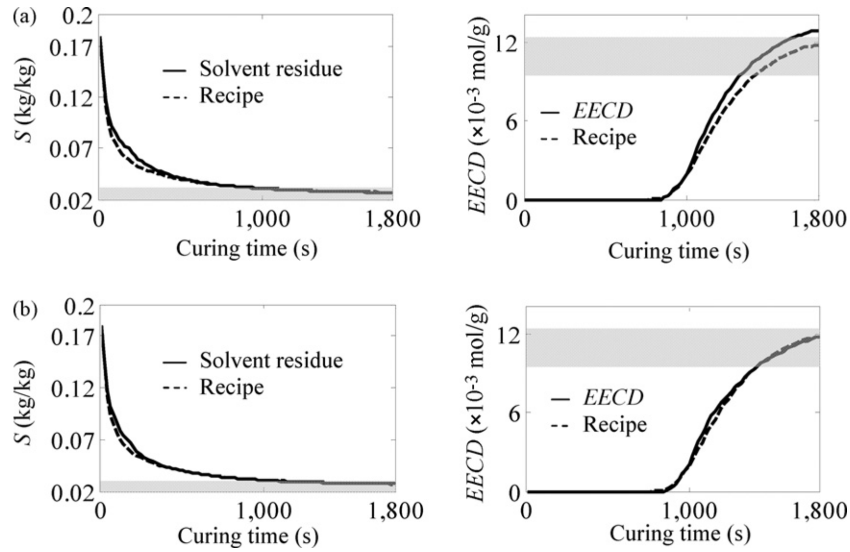

Fig. 6. System performance under: (a) process control and (b) IMPP control.

9.3. System performance analysis

In this section, system performance under IMPPC is compared with performance under conventional process control to demonstrate the attractiveness of IMPPC in all-time on-aim control of both process and product.

9.3.1. Process and product disturbance

The system is studied under three types of disturbances, one on the process (see the film temperature disturbance (D^c) in Fig. 5(a)), and the other two on the product (see the solvent residue and EECD disturbances (D^{ds}, D^{de}) in Fig. 5(b) and (c)).

9.3.2. System performance comparison

The IMPP system is first investigated using only a process controller. Fig. 6(a) shows that although the process controller takes actions immediately after the process disturbance is introduced at the time instant of 1000 s, it is incapable of reacting to the product disturbances. Finally, the coating is over baked (see the final EECD value that is higher than 1.25×10^{-3} mol/g in Fig. 6(a)).

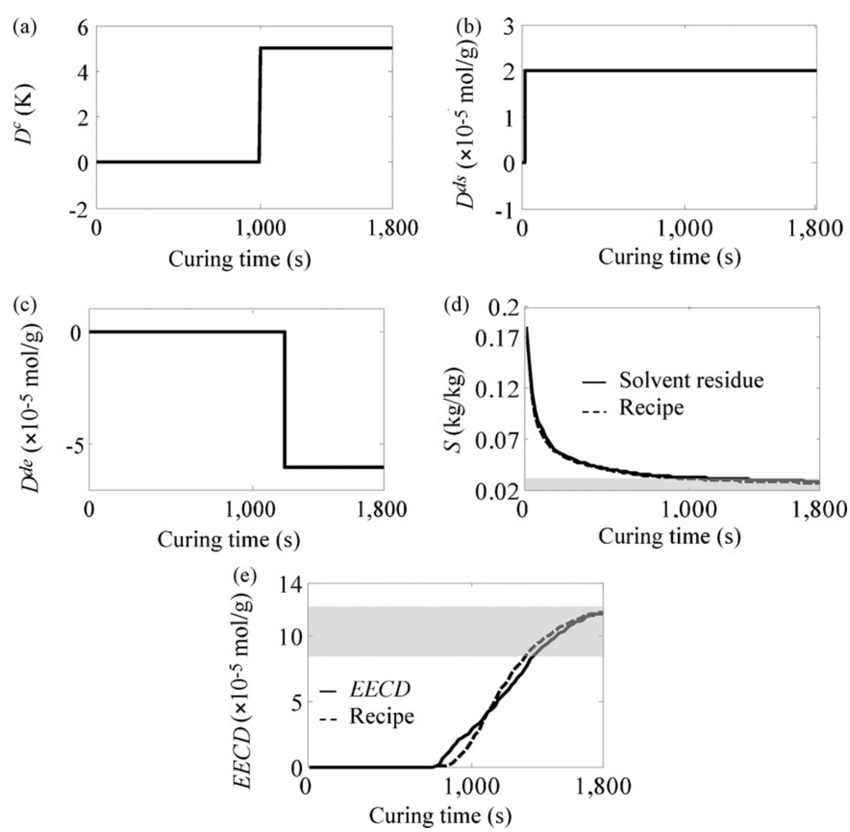

Fig. 7. System performance under IMPP control: (a) disturbance on film temperature, (b) disturbance on solvent residue, (c) disturbance on EECD, (d) solvent residue dynamics, and (e) EECD dynamics.

The product quality problem identified under the conventional process control can be readily prevented by the application of IMPP control. Fig. 6(b) shows that both solvent content and EECD can be all-time ensured under IMPPC. It is also demonstrated that excellent system performance can be achieved regardless of the introduced disturbances (see the control performance under another set of completely different disturbances in Fig. 7). Moreover, IMPPC offers superior process performance over conventional process control. It is demonstrated that a change from process control to IMPPC can give rise to a ∼2% reduction in fuel consumption.

10. Concluding remarks

Automotive surface coating manufacturing faces various technical challenges, which include a multistage dynamic operation under a high production rate, the lack of process and product online measurements, and the knowledge disconnection between macroscale bulk production, finer-scale material property and product behavior. The current manufacturing practice is far from optimality in terms of coating quality, energy and material use efficiency.

In this paper, an integrated multiscale characterization and control approach is introduced to effectively address above listed challenges. The multiscale characterization method can provide a comprehensive and precise description of product and process behavior covering a wide range of length and time scales. It enables a deep understanding of the crucial correlations among material, processing condition, microstructure, product property and quality, and energy efficiency. Thus, it allows identification of improvement opportunities of system performance. Furthermore, the introduced IMPP control methodology ensures all-time on-aim control of both process performance and product quality. The IMPP control synthesis method is generic and thus should be valuable for the control of a wide range of multiscale process–product systems. A case study on an automotive coating curing system has demonstrated that effective control systems can be constructed that have excellent performance on set-point tracking and disturbance rejection.

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