Multiscale Characterization of Automotive Surface Coating Formation for Sustainable Manufacturing

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Abstract  Automotive surface coating manufacturing is one of the most sophisticated and expensive steps in automotive assembly. This step involves generating multiple thin layers of polymeric coatings on the vehicle surface through paint spray and curing in a multistage, dynamically changing environment. Traditionally, the quality control is solely post-process inspection based, and process operational adjustment is only experience based, thus the manufacturing may not be (highly) sustainable. In this article, a multiscale system modeling and analysis methodology is introduced for achieving a sustainable application of polymeric materials through paint spray and film curing in automotive surface coating manufacturing. By this methodology, the correlations among paint material, application processes and coating performance can be identified. The model-based analysis allows a comprehensive and deep study of the dynamic behaviors of the material, process, and product in a wide spectrum of length and time. Case studies illustrate the efficacy of the methodology for sustainable manufacturing.

Keywords  sustainable manufacturing, multiscale modeling and analysis, automotive surface coating

1 INTRODUCTION

In automotive coating manufacturing, paints of different types are applied on a vehicle’s surface to generate a basecoat and a clearcoat (together called topcoat, 10-60 μm). Each layer is commonly developed in two consecutive operational steps: paint spray and film curing. In operation, vehicle bodies are moved steadily one by one by a conveyor through a spray booth and then an oven. In paint spray, the emulsified paint particles (1-10 μm in size) fly at a high speed (initial speed at 70-80 m·s⁻¹) from the spray devices to the target vehicle panels [1]. The particles missing the panels will be swept away by the air to the drain through the grids on the floor. In production, material transfer efficiency, wet film topology, and volatile organic compound (VOC) emissions are the main economic, quality, and environmental concerns. The oven for film curing is usually divided into a number of zones to allow for the use of different heating mechanisms (i.e., radiation from the oven walls and hot air convection) under different conditions [2]. In the end, the cured coating with the desired properties is developed on the vehicle surface; hopefully, it is defect free (at any length scales). Besides, energy consumption and VOC emission are expected to be at a minimum [3].

Paint spray and coating curing experience various technical challenges. First, high productivity requires vehicle bodies to continuously move on a conveyor while being sprayed and baked. This makes it extremely difficult to ensure coating thickness uniformity and a defect free finish [4]. Second, almost all process variables are not measurable during manufacturing. This has forced the current quality control practice to rely only on post-process sampling, which causes various quality problems, leads to inefficient energy and material utilization, and generates excessive amounts of waste and pollutants [5, 6]. Third, which is probably the most challenging issue, is the knowledge disconnection between macroscopic bulk production, finer-scale material properties, and product behavior. In production, operational settings (at the macroscopic level) are always adjusted based on experience; hence the true manufacturing optimality cannot be realized in reality.

The challenges listed above have attracted various efforts to two types of modeling: process and facility modeling and product modeling. In studying paint spray, booth air condition, ventilation and electric field are usually simulated using computational fluid dynamics (CFD) codes [7-9]. The modeling of detailed particle behaviors (e.g., particle collision and breakup) during paint spray is also attempted [10-12]. While the known studies can provide valuable insights into paint spray, the models are functionally limited, as they are incapable of predicting detailed film behavior in specific locations on panels and they do not take real operating conditions into account. Efforts have also been made to model oven baking operations [13-15], most of which are at the lab level, studying the curing of small coated substrates. Lou and Huang [16] were among the earliest to introduce a first-principles-based, integrated dynamic modeling approach for characterizing the dynamics of oven curing. Based on that model, Xiao et al. [5, 17-19] solved two classes of curing optimization problems and proposed a proactive quality control approach. However, all the efforts focus only on macroscopic characterizations of general coating behavior and optimization of macroscopic operational conditions.

The existing mono-scale modeling studies disallow the resulting models to provide the information necessary for addressing the whole spectrum of coating quality (macro to microscale), material efficiency...
(macro to mesoscale), and energy efficiency (macro-scale) simultaneously. Since sustainable manufacturing in automotive coating requires the understanding of material, product, and process behavior in a wide range of length scale \((10^{-6}-10^m)\) and time scale \((10^{-6}-10^3)\), multiscale modeling is necessary.

Multiscale modeling and simulation has become increasingly attractive over the past decade. Many investigations have shown successful applications in different fields, such as crystallization, plasma and thermal spray, hard material design, and reactor design [20–24], which have generated various new understandings of the target products and/or process systems. Needless to say, however, the realm of multiscale modeling and simulation methodologies and techniques needs further exploration. How to describe multiscale phenomena mathematically, and how to utilize multiscale information properly in a holistic framework remain as a mountaintop area.

In this article, a definition of the sustainable manufacturing of paint-based automotive coatings is presented first. An integrated multiscale modeling and simulation methodology is then introduced for characterizing paint spray and film curing. The resulting multiscale system models can describe simultaneously product and process dynamic behaviors at the different spatial and temporal scales, thus enabling comprehensive and deep analyses on the multiple-stage coating manufacturing. Model-based simulation has revealed various usually inconceivable opportunities for sustainable manufacturing.

2 SUSTAINABLE COATING MANUFACTURING

As stated, the multiscale system approach introduced in this article is mainly for helping achieve sustainable coating manufacturing, which is defined as follows.

A paint material application for automotive surface coating manufacturing is sustainable if the resulting products meet quality specifications (on appearance, durability, and styling), and the manufacturing consumes the minimum amount of materials and energy, and has the minimum adverse environmental impact (i.e., minimum VOC emission and paint-containing wastes).

Note that product life cycle analysis is of great importance in a sustainability study, but it is out of the scope of this work. The analysis of economical, environmental, and social impacts (restricted to social satisfaction on product quality) requires the information in a wide spatial and temporal spectrum.

Figure 1 shows a framework of the multiscale analysis of multi-objectives for paint spray and curing, where individual manufacturing objectives are allocated at the appropriate scales of length and time. The paint material properties span from the microscale to macroscale of length and time. In paint spray, energy consumption is reflected mainly by the setting of downdraft (macroscopic). Material efficiency and environmental quality are basically macroscopic, and coating quality has a wider span of length and time scale (macro-meso), as it is reflected by panel-based topology and defect as well as very much localized surface roughness, etc.

For coating curing, no material efficiency needs to be considered, as all the paint materials are already on the vehicle panels. The energy issue is clearly macroscopic, but the environmental concerns are directly related to the mesoscale phenomena as the solvent is removed from the thin film on the panel surface. The quality has wider length and time scales, as the crosslinked network structure within the coating is a main concern.

Figure 1 Multiscale analysis for sustainable manufacturing of polymeric surface coating

- 1—polymer & crosslinker MWD & functionalities;
- 2—water & solvent level;
- 3—viscosity;
- 4—downdraft;
- 5—transfer efficiency;
- 6—paint particle velocity & trajectory;
- 7—film thickness;
- 8—surface roughness;
- 9—coating topology;
- 10—defects;
- 11—coating microstructure;
- 12—oven temperature, air temperature & velocity;
- 13—VOC emission
3 MULTISCALE MODELING FOR PAINT SPRAY AND FILM CURING

Assume the domain $\Omega$ of a product-process system consists of sub-domains $\Omega_1$ and $\Omega_2$, which are for defining the system behaviors at the macroscale and meso/microscale, respectively. A macroscale model set can be generalized as:

$$F(t, Y(t, z), X(t), U, z, t) = 0$$

where $F$ is a nonlinear vector function; $X$ and $Y$ are the system input and output variable vectors, respectively; $U$ includes the time-independent parameters; $z$ is the vector of spatial coordinates; $t$ is the time. The model set is associated with its initial and boundary conditions in the boundary domain $\partial \Omega$.

The micro/meso-scale models can be generalized as:

$$\tilde{Y}(t_i) = \Gamma(\tilde{Y}(t_i); \Delta t; X(t), Y(t, z))$$

where $\tilde{Y}(t_i)$ is the meso- or microscopic system states at the time instant $t_i$; $\Delta t$ (i.e., $t_{i+1} - t_i$) is the time interval. Function $\Gamma$ can be treated as a time-stepper, which uses $\tilde{Y}(t_i)$ and macroscopic states $Y(t, z)$ as the inputs, evolving over the time interval $\Delta t$ and producing $\tilde{Y}(t_{i+1})$ [25, 26]. Note that some mesoscopic models can have a closed form when describing certain finer-scale phenomena (e.g., particle flying during paint spray, and heat transfer and solvent diffusion through the film in coating curing). System design variables $X(t)$ in the model can be material properties related (e.g., polymer molecular weight distribution, paint viscosity and density).

Note that sub-domains $\Omega_1$ and $\Omega_2$ may share certain types of information. For instance, for paint spray, the domain used for describing the macroscopic spray booth condition (i.e., the air flow and the electric field) is also the domain defined for characterizing mesoscale paint particle flying. On the other hand, $\Omega_1$ and $\Omega_2$ may share a narrowed interfacial region. For example, for a topcoat curing description, a macroscopic domain is used for characterizing oven curing conditions (i.e., the convection air flow and the radiation intensity), and a micro/mesoscopic domain is used for describing film dynamic behavior. The two domains share a common interface: the film surface.

3.1 Model need identification

Various product and process models are needed to characterize either paint spray or coating curing operations, which should be sufficient for generating necessary information about coating quality, material and energy consumption, and environmental quality.

3.1.1 Integrated multiscale paint spray model

Figure 2 shows a general model structure where two sets of models exist: (1) the macroscale spray-booth air flow and electric field models, and (2) the mesoscale particle flying and collision models. In addition, three following multiscale integration approaches are needed (see the rectangular box with one corner cut): (1) an approach for developing a (macro) coating topology from a static spray pattern, (2) an approach for coupling continuous (macro) booth condition models with discrete (meso) particle models, and (3) an approach for creating (meso) surface roughness from a static spray pattern [27].

3.1.2 Integrated multiscale coating curing model

The detailed curing model structure is shown in Fig. 3, where there is a macro-scale oven model set, a mesoscale film physical behavior model set, and a micro-scale chemical behavior model (all in rectangular box). In addition, three model integration approaches are needed to generate the multiple information necessary for studying coating behavior and manufacturing performance (see those rectangular boxes with one corner cut).
3.1.3 Performance assessment models

The economic, environmental, and social impacts of the coating manufacturing are assessed based on production cost, productivity, energy and material use efficiencies, waste reduction performance, and product quality (i.e., end users’ satisfaction). Figs. 2 and 3 include the performance assessment models (see the rectangular boxes with rounded edges), each of which takes the information from the macro, meso, and/or microscale models. For example, for oven curing, an energy model needs the information of energy used for maintaining the required oven wall temperature, convection air temperature and velocity. An environmental quality model can be used to calculate VOC emission due to solvent evaporation. The product quality models are for quantifying macro-to-microscale coating physical/chemical properties, appearance, and durability.

3.2 Integrated process and product modeling

The needed models shown in Figs. 2 and 3 have been properly developed. Due to space limitations, only general model descriptions are provided below.

3.2.1 Paint spray model set

The following types of models have been developed.

1) Macroscopic booth condition models The booth-condition model set includes a booth air flow model and an electric field distribution model; both are at the macroscale of time and length. In the booth air flow model, the well-known conservation equations for mass and momentum, together with a standard $k$-$\varepsilon$ turbulence model, are used [8, 9]. The electric field model describes the physics of an electric field between the bells and the grounded surfaces generated by the emitting electrode of the spray bells. The model consists of a Poisson equation and a correlation between the electric field intensity and electrostatic potential [28].

2) Mesoscopic particle models Two mesoscopic particle models are developed to identify the correlation between booth condition and particle dynamics. In the particle flying model, spherical paint particles with the same density are assumed to be delivered from spray nozzles, and the momentum of particles is affected by three dominant forces: the drag force from the surrounding turbulent air flow, the electrical force from the electric field, and gravity. Based on these assumptions, the velocity of each particle is modeled based on Newton’s second law of motion [9]. O’Rourke’s statistics-based collision algorithm is used for characterizing particle collisions [10].

3) Performance assessment models These necessary models are described below.

Energy consumption In the paint spray booth, the high-power fans mounted on the booth ceiling provide air downdraft, and the spray devices generate shaping air and an electric field. Industrial practice shows that the power needed for maintaining downdraft is dominant in energy consumption. According to Perry and Green, the power for the fans is proportional to the downdraft air flow velocity [29].

Material transfer efficiency Material transfer efficiency is defined as the ratio of the amount of paint received by the panels over the total amount of paint delivered by the spray devices [30]. The mass of paint particles landing on the panel surface and that of the particles delivered from the nozzles can be readily obtained through CFD simulation [27].

Environmental quality The spray booth air quality is reflected by the particle concentration in the air. During paint spray, the particles reach their destinations (i.e., a vehicle panel surface, a booth wall, or the floor) at different time instants. It is conceivable that the number of particles in a location at a time instant can be never exactly known. In this work, an alternative way of estimating the particles’ average flying time (AFT) is used. A longer AFT indicates increased particle concentration in the air, and an increase of VOC released from the particles to the booth. In estimation, the particles failed to land on vehicle panels are counted.

Coating topology In industry, the film topology is measured by the film thickness in a limited number of locations on each panel of a sampled vehicle. Obviously, a large difference in the thickness at each pair of adjacent locations of a panel indicates a poor coating topology. According to this, a topology quality indicator is created by counting the mean gradient of the thickness of the adjacent measurement locations throughout the panel, which can reflect the severity of thickness change in both magnitude and frequency.

Surface roughness A common approach to quantifying surface roughness is to estimate the standard deviation of film thickness at the mesoscale. In this work, the surface roughness in a variety of small areas ($10^{-6}$ m$^2$ each) on a panel is investigated. In modeling, each target area is divided into numerous grids, and the film thickness at the location of each grid point is evaluated. These estimations are compared with the average thickness of the target area.

3.2.2 Coating curing model set

The following models have been fully developed.

1) Macroscopic oven models The oven model set contains a convection air flow model and an oven-wall radiation model, both at the macroscale. The conservation equations of mass, momentum and energy are used to model the convective heat transfer, and a standard $k$-$\varepsilon$ turbulence model is applied to describe the turbulent air flow. The radiation intensity within the oven is obtained from a radiative transfer equation (RTE) [31].

2) Mesoscopic models Four mesoscopic models are developed to characterize the physical/chemical phenomena occurring in the thin film. The solvent diffusion and evaporation, and film thickness change modeled by Lou and Huang are adopted in this work [16]. By concerning possible defects on the film surface, the crater formation model by Evans et al. [32] for instance, is enhanced to study crater formation in curing by incorporating the correlation of the paint viscosity, the resin molecular weight, the solvent amount, and the film temperature.

3) Microscopic crosslinked network structure model Monte Carlo (MC) simulation is used to derive a network structure. With the given polymer and
crosslinker information, a molecule database is generated, which contains detailed information (including the molecular weight, the functional groups number and the type) for each molecule to be used in simulation. A small part of the overall reaction volume needs to be picked out as a suitable simulation space, where the chemical species are assumed to be mixed homogeneously. In each MC step (corresponding to a certain time instant in the curing operation), one reaction is first selected from a list of possible reactions according to its reaction rate (note that the film temperature at time \( t \) is used in this step), then the molecules involved in this reaction are selected. After this reaction, the molecule database is updated and the time is advanced by \( \Delta t \) (calculated from the kinetic model) for the next step [33]. The simulation proceeds until the curing operation ends, which will give rise to the information of effective crosslink density, gel point, and molecular weight distribution.

(4) Performance assessment models These models are described below.

Energy consumption and environmental quality
The energy consumption of an oven is calculated from the oven operational settings (i.e., the wall temperatures, the air temperatures and velocities) [17]. The VOC emission from each vehicle surface is quantified by calculating the amount of evaporated solvents.

Coating quality The coating topology and surface roughness quantification methods are described above in the paint spray model set. The solvent resistance and inter-coat adhesion are modeled according to the effective crosslink density values [34].

4 MULTISCALE INFORMATION UTILIZATION

The models listed above can describe various types of phenomena occurring in product manufacturing at different time/length scales. In this section, two major integration tasks are described to explain the approaches for handling the information generated from the spray paint and coating curing model sets.

4.1 Coating topology generation

A real paint application process is very complicated, where each vehicle body moves at a certain line speed and the spray devices move in different ways (e.g., the spray bells above the vehicle roof move side by side at a certain frequency and amplitude). For a given spray device, the number of paint particles from each bell is on the order of \( 10^9 \) per second. Thus, for example, to paint a 1.3×1.8 m² roof panel with three bells within 27 s, the total number of particles sprayed can be on the order of \( 10^{11} \), according to Li et al. [27]. In model-based simulation, particle collision and spray bell oscillation must be considered in order to have a better approximation of real spray operations. Due to these complexities, it is impractical to simulate particles on the order of \( 10^{11} \) directly for a multiple-bell operation when studying the generation of a coating layer of about 70 \( \mu \)m on a panel. On the other hand, it should be reasonable to use the paint-spray (mesoscopic) information obtained from a static spray pattern (i.e., the simulation based on the fixed locations of bells and receiving panels) repeatedly in a constructive way to generate a coating layer (macroscopic) on the panel [27]. This allows the use of a superposition approach to add the static spray patterns in the pathway that a bell movement follows.

4.2 Macro (curing environment)–micro (network structure formation) coupling

It is reasonable to assume that the heat generated/consumed by cross-linking reactions can be neglected in the initial study, which means that a coupling between the curing environment and the network structure formation is only one-way. Note that film temperature dynamics in curing can be derived by a CFD solver. By compromising solution resolution and computational expense, the total vehicle surface area is divided into 20 zones in this work. In each zone, the average temperature is passed for one MC simulation. It is assumed that in each zone, those homogeneously mixed chemical species (i.e., the polymers and crosslinkers in this case) are reacted at the same film temperature. Using periodic boundary conditions, the crosslinked network structure formed in each zone can be predicted by using only a few thousand molecules. In this manner, a total of 20 MC simulations can generate a network structure in the coating that covers the complete vehicle surface.

5 INTEGRATED ANALYSIS OF PROCESS AND PRODUCT PERFORMANCE

The comprehensive analyses on paint spray and coating curing have revealed various opportunities for achieving sustainable coating manufacturing. Part of the results is briefly presented below.

5.1 Paint spray system analysis

A clearcoat spray system in Fig. 4 (a) is studied in this work. The geometries of the spray booth, the
vehicle panel (the roof in this case), the spray bells, the normal operating conditions, and the paint material properties resemble practical industrial data.

Figure 5 shows an air velocity profile, an electric field profile, and a particle flying time distribution that are obtained from CFD simulation. The film topology on the roof and the surface roughness details in a localized small area (i.e., 1 mm × 1 mm) are shown in Fig. 6 [27].

Four cases with different downdraft settings are studied. It is found that downdraft mainly affects both booth air quality and energy consumption. Increasing downdraft will decrease VOC emissions in the spray booth but consume more energy. Also, three cases are investigated to assess the effect of different initial distributions of particle sizes on the performance of product and process. It reveals quantitatively that smaller sized particles can produce a better coating topology, but result in lower material efficiency and worse environmental quality. Thus, the initial particle size distribution should be properly controlled to achieve a better tradeoff between product performance and process performance [27].

5.2 Coating curing system analysis

The clearcoat oven curing system is illustrated in Fig. 4 (b). The clearcoat studied is a type of high-solid acrylic-melamine enamel. The hydroxyl functional acrylic copolymers (the number average molecular weight of 3,000 g·mol⁻¹) are crosslinked with hexamethoxymethylmelamine (HMMM) (the functionality of 6). Note that clearcoat contains no pigment and in this study, the effect of solvent and additives on curing is neglected. The oven geometry and the operational settings resemble practical industrial data.

Figure 7 (a) is a snapshot of the 3-vehicle panel-heating through a 137.16 m (450 ft) long oven [only the first 27.43 m (90 ft) of the oven is shown]. The temperature profile at any specific location of any panel of each vehicle at any specific time instant during curing can be obtained, which is critical for studying solvent removal, topology change, cross-linking conversion and crosslinked network structure formation. Fig. 7 (b) shows the cross-linking conversion of the film throughout the vehicle body at the 1500th sec after the curing starts [35]. It shows that the cross-linking conversion is not uniform at that time.
In a more detailed study on coating curing quality, the curing temperature dynamics for the film in the center of roof panel is obtained [see Fig. 8 (a)]. This information is used in MC simulation to generate a crosslinked network structure, based on which an effective crosslink density dynamics is generated [see Fig. 8 (b)]. Also, the gel point [Fig. 8 (c)] and the molecular weight distribution [Fig. 8 (d), at the hydroxyl groups conversion of 15%] are obtained.

Three paint materials having different initial number average molecular weight (MW) are investigated. The study has revealed that under the same curing condition, a decrease of the initial resin MW can lead to a decrease of the final effective crosslink density. It means that a lower MW resin requires a higher curing temperature or a longer curing time. Consequently, a decrease of the resin MW will consume more energy in curing, although the amount of emissions can be reduced. This information will be valuable for identifying the most desirable material formulation with well acceptable material application conditions.

6 CONCLUSIONS

Polymeric coating manufacturing on vehicle surfaces is one of the most sophisticated and expensive steps in automotive assembly. Most known studies on coating quality through paint spray and coating curing have focused on the product’s macroscopic behavior, and for those lab-based studies, the operation simulated has been limited to the use of many ideal operational settings. Thus, many important issues in production, such as energy consumption, material use efficiency, and work-zone environmental quality, which are key indicators of manufacturing sustainability, can hardly be addressed.

This article has illustrated that all the major process and product issues in paint spray and coating curing can be simultaneously addressed properly by means of a multiscale system modeling and analysis approach. The integrated process and product performance analysis introduced in this article illustrates its potential in generating important product and process information that is critical for achieving sustainable manufacturing in automotive surface coating applications.

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