KEY CONCEPTS IN BLEND MORPHOLOGY DEVELOPMENT BY CHAOTIC ADVECTION: EXPERIMENTS AND MODELING

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Abstract – The application of chaotic advection to polymer blends and composites originated in the corresponding author's laboratory in 1991. Research has resulted in smart blending devices now being adopted by industry. In the accompanying talk, key concepts and recent results are described where polymer melt components are more controllably formed in situ into a wide variety of blend morphologies and where solid additives are more deliberately organized into functional arrangements. A desired blend morphology or arrangement can be specified to smart blending devices via a computer interface and extruded to give improved and new plastic products. Chaotic advection is an enabling recent sub-field of fluid mechanics for smart blending. Recent advances in fluid mechanics have thereby been implemented to reconsider how blending is done and render in situ structure development more controllable and predictable. By organizing melts and progressively refining them, methods are also amenable to predictive modeling.

Introduction

Due to polymer immiscibility, the physical properties of many polymer blends derive from the fine-scale structural arrangements, or blend morphologies. obtained during processing in addition to the proportion of each polymer type present. Interestingly, most immiscible polymer blends are produced by mixing in sharp contrast to many other types of composite materials where methods are designed to deliberately form material components into functional shapes and give arrangements associated with property enhancements. Because mixing constrains the variety of morphologies producible, many immiscible polymer blends and composites are not necessarily optimized with regard to structure, composition, and properties. Technologies such as co-extrusion have been developed to obtain structured plastic materials. However, methods to create directly functional structures in immiscible polymer blends in compounding steps are less developed.

In this paper, a recent advance in fluid mechanics is a basis for a new blending approach that allows specification via a computer interface such as a keyboard of desired blend morphologies or structured distributions among solid additives¹. As will be shown, a single continuous chaotic advection blender (CCAB) can produce a large variety of fine-scale structures in plastics that are pursued currently with very different compounding equipment or post-processing steps. CCABs can also be comparatively simpler in construction. The effective operation of a CCAB depends on an ability to stretch and reorient melt domains. This requisite characteristic of blending is accomplished with a recent advance in fluid mechanics. H. Aref did some independent thinking and articulated in a seminal paper² the potential importance

of what had been regarded only as rather strange fluid motion. With a Lagrangian perspective and in consideration of dynamical systems theory, he noted that the equations of motion for passive markers in a fluid can produce nonintegrable (i.e., chaotic) dynamics even in simple flow fields. This type of fluid motion was appropriately dubbed by Aref as chaotic advection, where the term advection denotes movement. The derivative term, chaotic mixing, is often used^{e.g.,3}, but the parent term is deemed more appropriate here where in situ structuring is the focus. Because in situ structuring can be done controllably, CCABs are also referred to as smart blenders. Smart blending has been characterized as a new area of chaotic advection research that may hold particular promise⁴. Morphology development and morphology characteristics are consistently repeatable.

General Description of a CCAB (Smart Blender)

A CCAB prototype is shown schematically in Figure 1. This device has been described in detail⁵ and a summary description is given here. (Other related devices are also in operation or have been designed in the LAPM&T.) The CCAB consists of a barrel with an oval cross-section over the barrel mid-span. Separate melt flows of polymer A and polymer B are supplied by metering pumps to give extrusions with a prescribed overall composition. In some cases, melt flow B can be a pre-compounded masterbatch that consists of polymer A and a solids additive. Chaotic advection is induced in response to the rotations of stir rods driven by variable speed motors. Because melt structuring occurs predominantly upstream of the die, attached dies shape the structured melt into a desired form such as film, rod or tubing. Blend morphology changes that occur in a die can be countered if desired by altering in situ structuring in the CCAB. Processing conditions

and melt properties that are needed to produce a particular blend morphology are compiled in a morphology map. Such maps are currently the products of prior experiments but are aided by computer models.



Figure 1. Schematic representation of a continuous chaotic advection blender (CCAB) and its control system. Blend morphology is selectable.

Examples of Polymer Blends and Composites

Unlike conventional mixing where the aim is to achieve compositional uniformity and small domain sizes, a CCAB converts initially large injected melt streams into physically expansive multi-layers of small thicknesses even at viscosity ratios much larger than unity. Melt components are organized into a multilayer arrangement where average layer thicknesses decrease controllably in response to chaotic advection. The multilayer arrangement is a parent morphology to derivative morphologies, which arise volumetrically at a distance along the stir rods of the CCAB of Figure 1. This *progressive morphology development* is a key to process controllability and the wide variety of morphologies producible. Two examples are given.

In Figure 2, the formation of an interpenetrating blend from the multilayer melt can be seen. Injected melt streams are converted to thick layers which stretch and fold to give thinner layers. Ruptures (or holes) arise as the layer thicknesses continue to reduce in response to chaotic advection. Previously separated layers become connected via the ruptures to give an interpenetrating blend. In Figure 3, clay nano-platelets are volumetrically aligned and placed within platelet-rich layers in nylon. Platelet alignment is a direct outcome of chaotic advection. Interestingly, by continuing chaotic advection further, virgin nylon layers become vanishingly thin so the resulting composites have aligned platelets that are also very well dispersed.



Figure 2. Conversion of a multilayer melt arrangement to an interpenetrating blend for a PP-LDPE blend with 30% LDPE.



Figure 3. TEM micrograph of PA nanocomposite with platelets organized within discrete layers and oriented. A virgin PA layer and multiple nano-scales are evident.

Closing Remarks

The novel ability to control blend morphology in CCABs is derived from processing conditions which evolve structure in the melt (progressive morphology development). By organizing melts in lieu of mixing them, predictive modeling may also be done more readily. Modeling results and modeling opportunities will be described in the accompanying talk.

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