Twin Screw Extrusion Processing of Graded Composite Materials

Frederick M. Gallant [1] and Hugh A. Bruck[1]

[1] *Department of Mechanical Engineering, University of Maryland, College Park, MD 20742, emails: gallantfm@ih.navy.mil and bruck@eng.umd.edu*

SUMMARY: A new method for fabricating graded composite materials with continuous gradient architectures has been developed using the technology of continuous processing with a Twin-Screw Extruder (TSE). While TSE processing has been investigated for controlling the fabrication of homogeneous composites in steady-state operating conditions, there is a lack of knowledge concerning the processing of gradient architectures using transient operating conditions. Therefore, there is a need to characterize and model the relationship between the extruder screw geometry, transient operating conditions, and the gradient architecture that evolves in the extruder. In this investigation, recent interpretations of the Residence Time Distributions (RTDs) and Residence Volume Distributions (RVDs) for polymer composites in the TSE are used to develop a process model for predicting compositional gradients in the direction of extrusion. In situ optical measurements are used to verify the gradient architectures. The process model that has been developed in this research effort will serve as the basis for determining the operating conditions and screw configurations that produce a desired gradient architecture.

KEYWORDS: Functionally Graded Materials, Residence Time Distribution, Residence Volume Distributions, Gradient Architecture, Twin Screw Extrusion

INTRODUCTION

There is a great deal of interest in tailoring structures so the functional requirements can vary with location. In most cases, this will involve varying the materials that are used at specific locations within the structure resulting in discrete interfaces throughout. These discrete interfaces often limit structural performance by introducing weaknesses or impeding transport process. Attempts at mitigating these problems have led to the concept of Functionally Graded Materials (FGMs). FGMs are structures that possess gradual variations in material behavior that enhance material and/or structural performance [1]. For example, at one point the material may be hard and at another point it may be soft. The description of this functional variation is known as the gradient architecture (*Figure 1*) [2]. Currently, there is a challenge to manufacture FGMs using scalable processes that can easily control the evolution of the gradient architecture in a continuous manner. Manufacturing technologies for processing FGMs are categorized as either transport-based or constructive processes [1]. Constructive manufacturing processes primarily produce discretely layered gradient architectures, and include: powder densification, deposition, and lamination techniques. Transport-based processes primarily produce continuous gradient architectures, and include: mass transport, thermal diffusion, inertial separation, and melt infiltration.

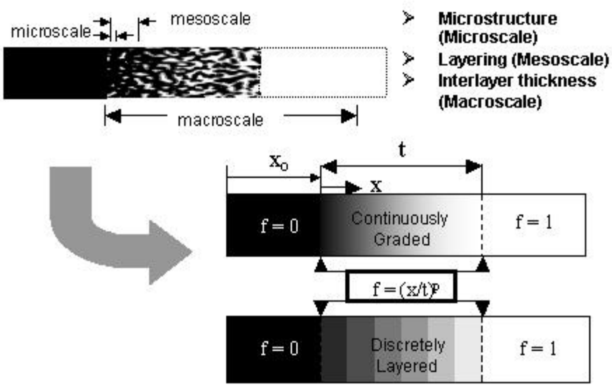


Figure 1. Description of gradient architectures for graded composites [2]

A transport-based manufacturing technology that has yet to be used for manufacturing FGMs is the Twin Screw Extrusion (TSE) process. This paper elucidates on the fabrication of graded polymer composites with continuous gradient architectures using TSE processing technology. Steady-state Residence Volume Distribution (RVD) models are used to describe the TSE process. Convolution of these RVD models with feed input conditions are then used to predict the 1-D composition gradients that evolve during the Twin Screw Extrusion process. Optical measurements are used to verify the composition gradients predicted by the RVD models.

CONTINUOUS PROCESSING OF POLYMER COMPOSITES USING TWIN SCREW EXTRUSION

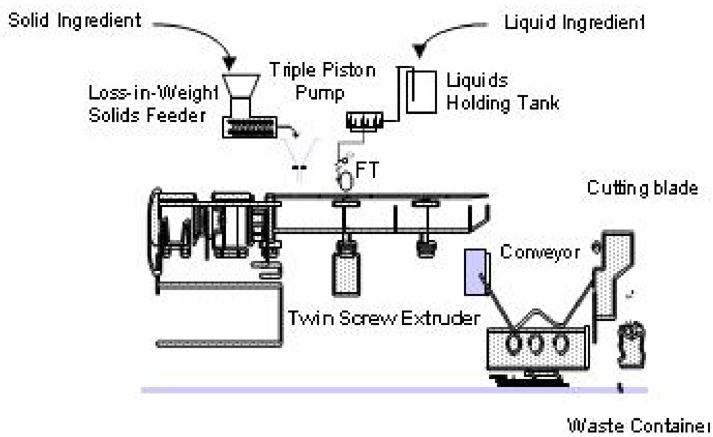


Figure 2. Schematic of Twin Screw Extrusion process

TSE processes are utilized to manufacture a number of consumer and industrial goods from snack foods and medical tubing to plastic pellets and military propellants. The continuous nature of this process has many advantages over batch types, so it has found widespread utility across diverse industries that process polymers and polymer composites. The advantages tend to be universal: economy, quality, and flexibility. Thus, TSE processing is a promising technology for producing graded composite materials.

At the heart of the TSE process is the extruder, which is highly configurable and flexible allowing for the optimization of processing for many different types of materials (*Figure 2*). Unlike discrete batch processes that require a number of process steps and facilities, the continuous nature of the TSE process allows for the combination of process steps to reduce facility requirements. By continuously processing materials, it is possible to produce larger quantities with greater consistency (i.e., no batch to batch variation). The process also lends itself to on-line analysis allowing for the quick detection of anomalous conditions or quality that can be used to automatically remove material into a waste container.

RESIDENCE DISTRIBUTION MODELING OF TSE PROCESS

To control gradient architectures manufactured with the TSE process, it is necessary to develop a model of the process. Material transport through a fully intermeshing twin screw extruder is accomplished by screw geometry and screw motion [3]. Because of the complex dependence of material transport on evolving material properties, screw configuration, and operating conditions, the quantitative residence time of material in the system, characterized by the residence time distribution (RTD), has become a convenient way to express the cumulative effect of all processing and material parameters. The RTD is typically normalized in order to describe the probability, *e(t)*, that a given quantity of material will reside in the extruder for a time, *t*, as follows:

$$\mathrm{e(t)} = \frac{\mathrm{c(t)}}{\int_0^\infty \left|\mathrm{c(t')}\right| \mathrm{dt'}} \tag{1}$$

where *c(t)* is a filtered probe response obtained from the extruder [4]. The RTD can be used to quantify various characteristics of the TSE process, such as the dampening that occurs as a result of backmixing in the extruder [5]. A model has been developed to predict the RTD based on a series of ideal mixers [6]. The general form of the RTD model, *f(t)*, for a series of n ideal mixers is as follows:

$$f(t) = \frac{a^n}{(n-1)!}\left(t - t_d\right)^{n-1} e^{-a\left(t-t_d\right)} \tag{2}$$

It consists of two parameters: (a) the delay time, t_d, predicted from operating conditions and screw configuration, and (b) a shape factor, *a*, determined experimentally. The RTD can be converted to the volume domain, equation (3), to obtain a Residence Volume Distribution (RVD) that has been shown to be independent of operating conditions and only dependent upon screw geometry [7]. Thus, the RVD can be used to uniquely identify (i.e., fingerprint) a screw design. The RVD and its associated general mixing model are given as follows:

$$g(v) = \frac{c\left(\frac{v}{Q}\right)}{\int_0^\infty \left|c\left(\frac{v}{Q}\right)\right| dv} = \frac{e\left(\frac{v}{Q}\right)}{Q} = \frac{a_v^n}{(n-1)!}\left(v - v_d\right)^{n-1} e^{-a_v\left(v-v_d\right)} \tag{3}$$

Figure 3. Graded polymer composites manufactured using the TSE process

By converting residence distribution model from the time to the volume domain, it is possible to directly predict the spatial distributions of material in a gradient architecture independent of operating conditions.

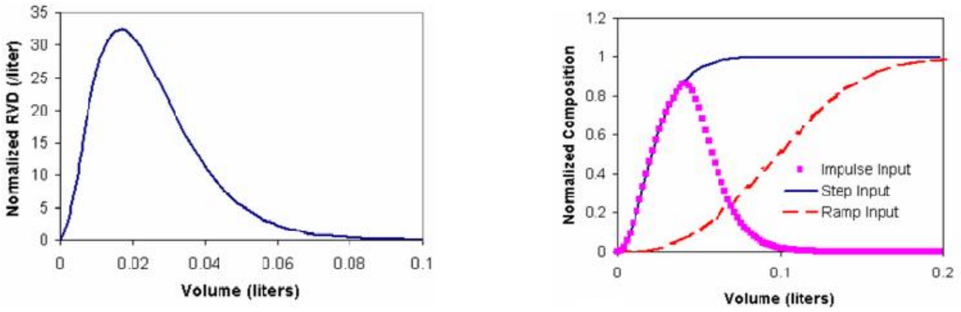
PREDICTION AND MEASUREMENT OF COMPOSITION GRADIENTS

The TSE process is naturally suited to producing continuous composition gradients. These composition gradients can be achieved either by dynamically changing the relative feed rate of ingredients, or by varying the operating conditions. Examples of graded polymer composite fabricated by changing the ingredients in the TSE process can be seen in *Figure 3*.

Based on the RVD model in equation (3), the 1-D composition gradient, *f[z(v)]*, can be predicted by convolving the feed input conditions, *h(v),* for the extruder with the RVD model as follows:

$$f[z(v)] = \int_{o}^{v} g(v - v')h(v')dv' \tag{4}$$

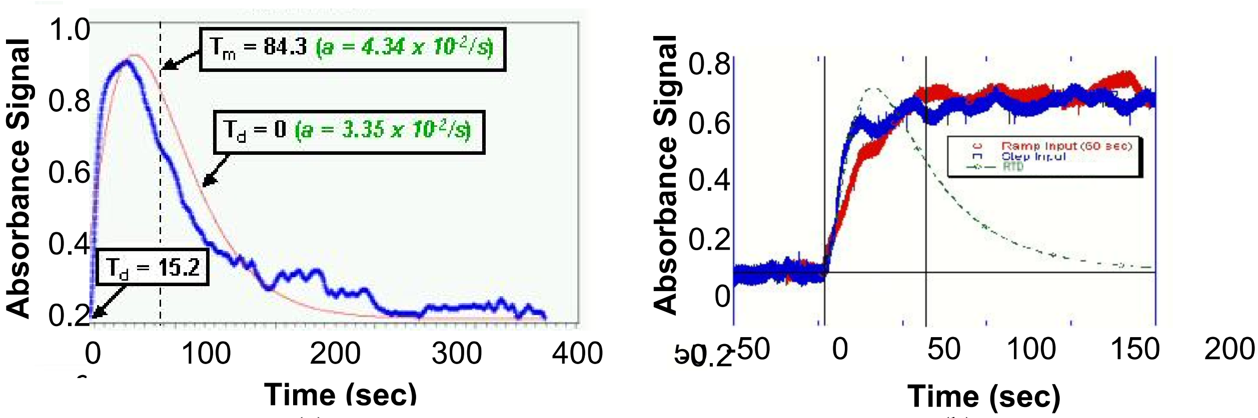
A RVD representative of the TSE process and a prediction of the gradient evolution from convolution of the RVD with impulse, step, and ramp input conditions can be seen in *Figures 4a* and *4b* respectively.



(a) (b)

Figure 4. (a) RVD representative of TSE process, and (b) prediction of gradient architecture from convolution of RVD with impulse, step, and ramp input conditions

The 1-D composition gradient that evolves in the TSE process has been characterized using in situ optical measurements of the composite ingredients. The optical measurement system consisted of a bifurcated fiber optic cable inserted into a probe that screws into a Dynisco-profiled barrel instrumentation port. The twin-screw extruder used in these experiments was a laboratory scale Werner & Pfleiderer model ZDSK-28 with co-rotating fully-intermeshing screws. A model polymer composite system was chosen for this experiment that consisted of 200 μm KCl particles and DuPont Dow Engage 8401, a high melt index polyolefin elastomer (POE). The RTD for this material system and the screw configuration along with an experimental fit to of equation (2) can be seen in *Figure 5a*. The gradient architectures that evolved for step and ramp changes from 40 wt% to 60 wt% particle input can be seen in *Figure 5b*. The general variation in the gradient architecture is qualitatively very similar to the predicted variations seen in Figure 5. Thus, the convolution model exhibits excellent potential for predicting 1-D composition gradients in polymer composites fabricated in the TSE process.



(a) (b)

Figure 5. Experimental optical measurements of (a) RTD and (b) gradient architectures for step and linear changes in input conditions

CONCLUSIONS

TSE processing has been used to fabricate continuously graded polymer composites. Residence distribution models were used to characterize the TSE process. These models were then convolved with feeder input conditions to predict the 1-D composition gradients that evolve in the TSE process. Experimental studies were conducted using a model polymer composite system consisting of an elastomer with KCl particle reinforcement. In-situ optical measurements were used to characterize the RTD and gradient architectures that evolved from step and linear changes in KCl particle reinforcement from 40 wt% to 60 wt%. These measurements were qualitatively similar to the predictions from the convolution model, indicating that the convolution model has excellent potential for predicting gradient architectures in TSE-processed polymer composites.

ACKNOWLEDGEMENTS

This work was supported by Dr. James Short under ONR contract no. N00014-00-1-0472 and Indian Head-Naval Surface Warfare Center under contract no. TI01-9.

REFERENCES

1. Suresh, S. and Mortenson, A., *Fundamentals of Functionally Graded Materials*, Institute of Materials, London, UK (1998).
2. Bruck, H.A., Evans, J.J., and Peterson, M.L., "The Role of Mechanics in Biological and Biologically Inspired Materials," *Experimental Mechanics*, 42, 361-371 (2002)
3. Rauwendaal, C., *Polymer extrusion*, first ed., Hanser Publishers, New York (1986).
4. Gao, J., Walsh, G.C., Bigio, D., Briber, R.M., and Wetzel, M.D., "A Residence Time Distribution Model for Twin Screw Extruders", *AICHE Journal*, 45, 2541-2549 (1999).
5. Danckwerts, P.V., "Continuous Flow Systems: Distribution of Residence Times." *Chemical Engineering Science*, 2, 1-18 (1953)
6. Gao, J., Walsh, G.C., Briber, R.M., and Wetzel, M.D., "Mean Residence Time Analysis for Twin Screw Extruders", *Polymer Engineering and Science*, 40, 227-237 (2000)
7. Gasner, G.E., Bigio, D.I., Marks, C., Magnus, F., and Kiehl, C., "A New Approach to Analyzing Residence Time and Mixing in a Co-Rotating Twin Screw Extruder", *Polymer Engineering and Science,* 39**,** 286-298 (1999)