RHEOLOGY-BASED MODELING TO IDENTIFY THE MOLECULAR WEIGHT DISTRIBUTION OF LINEAR POLYMERS

Technical Field

[0001] The present disclosure relates to rheology-based modeling to identify the molecular weight distribution of linear polymers. Such techniques can be particularly useful to predict the molecular weight distribution in order to tune the molecular weight distribution to manipulate the flow behavior of polymer formulations.

Background

[0002] Polymer rheology is an important aspect of polymer solution design and processing control. Techniques to manipulate the flow behavior of polymer formulations can be exemplified by tuning the molecular weight distribution (MWD), designing branching structures, adding flow modifiers, and/or adjusting processing conditions. The resulting rheology behaviors, such as shear thinning and strain hardening, determine the processability of the formulations and impact the properties of final products.

[0003] Polymer rheology has been used as a characterization method to probe molecular structure. Measuring such rheological properties can require significantly larger sample sizes (e.g., quantity of sample, etc.) than other characterization techniques such as gel permeation chromatography (GPC), light scattering, and/or membrane osmometry for one experiment. The application of rheology to characterize polymer structure holds value for the conditions beyond the capability of other techniques, such as the MWD measurements of ultrahigh molecular weight polyethylene (UHMWPE), which have higher molecular weight chains than the upper limit of the capability of GPC.

[0004] Characterization of the molecular structure of polymeric materials can rely on separation methods. The separation methods can be time consuming, sensitive, and/or incomplete. In instances where separation methods may not be available (e.g., plant laboratories, recycling facilities) the molecular structure characterization of plastics is challenging. Linear rheology measurements on the other hand are robust enough to be implemented in plant environments, and experimental execution along with data analysis and interpretation can be sufficiently automated. A reliable method to study the structure-property-performance

relationships can be utilized to help with an increasing demand to recycle plastics for the manufacture of new products.

Summary of the Disclosure

[0005] The present disclosure is directed to using improvements in machine learning technology to predict properties of a polymer sample. The prediction can be based on a data set that has been categorized based on rheology properties of a plurality of polymer ensembles with a defined range of molecular weights. The data set can be generated and input to an artificial neural network (ANN) trained to predict the molecular weight distribution of an unknown polymer sample based on the rheology of the polymer sample. The trained neural network can be utilized to provide information to reverse engineer polymers with a particular rheological behavior, characterize post-consumer recycled polymers, and/or design new polymers or resins.

[0006] The above summary of the present disclosure is not intended to describe each disclosed embodiment or every implementation of the present disclosure. The description that follows more particularly exemplifies illustrative embodiments. In several places throughout the application, guidance is provided through lists of examples, which examples can be used in various combinations. In each instance, the recited list serves only as a representative group and should not be interpreted as an exclusive list.

Brief Description of the Drawings

[0007] Figure 1 illustrates one example flow diagram of a method to generate a rheology-based model to identify the molecular weight distribution of linear polymers.

[0008] Figure 2 is one example diagram illustrating an approach to generate a rheology curve for a plurality of polymer ensembles.

[0009] Figure 3 is one example diagram illustrating an approach to rescale a modulus value for a plurality of input features associated with rheology curves to generate a plurality of output features.

[0010] Figure 4 illustrates an example of a method for rheology-based modeling.

[0011] Figure 5 illustrates an example of a machine-readable medium for rheology-based modeling.

[0012] Figure 6 illustrates an example of a device for rheology-based modeling.

Detailed Description

[0013] The present disclosure relates to methods and devices for rheology-based modeling to identify the molecular weight distribution of linear polymers. The present disclosure may utilize machine learning models to predict molecular weight distributions of unknown polymer samples (e.g., linear polymer samples).

[0014] A machine learning model can be a function or equation for identifying patterns in data. A machine learning model can be a part of a plurality of machine learning models utilized together to identify patterns in data. In a specific example, a machine learning model can be organized as a neural network. A neural network can include a set of instructions that can be executed to recognize patterns in data. Some neural networks can be used to recognize underlying relationships in a set of data in a manner that mimics the way that a human brain operates. A neural network can adapt to varying or changing inputs such that the neural network can generate a best possible result in the absence of redesigning the output criteria.

[0015] Artificial neural networks (ANNs) are networks that can process information by modeling a network of neurons, such as neurons in a human brain, to process information (e.g., stimuli) that has been sensed in a particular environment. Similar to a human brain, neural networks typically include a multiple neuron topology, which can be referred to as artificial neurons. An ANN operation refers to an operation that processes inputs using artificial neurons to perform a given task. The ANN operation may involve performing various machine learning algorithms to process the inputs. Example tasks that can be processed by performing ANN operations can include machine vision, speech recognition, machine translation, social network filtering, and medical diagnosis, among others. In a specific example, a neuron can receive X_k inputs, with k corresponding to an index of inputs. For each input, the neuron can assign a weight vector, W_k, to the input. The weight vectors (e.g., weight value, etc.) can, in some embodiments, make the neurons in a neural network distinct from one or more different neurons in the network. In some neural networks, respective input vectors can be multiplied by respective weight vectors to yield a value, as shown by Equation 1, which shows an example of a linear combination of the input vectors and the weight vectors.

$$f(x_1, x_2) = w_1 x_1 + w_2 x_2$$

Equation 1

[0016] In some neural networks, a non-linear function (e.g., an activation function) can be applied to the value $f(x_1, x_2)$ that results from Equation 1. An example of a non-linear function that can be applied to the value that results from Equation 1 is a rectified linear unit function (ReLU). An illustrated application of the ReLU function is shown by Equation 2. The ReLU function is used here merely as an illustrative example of an activation function and is not intended to be limiting. Other non-limiting examples of activation functions that can be applied in the context of neural networks can include sigmoid functions, binary step functions, linear activation functions, hyperbolic functions, leaky ReLU functions, parametric ReLU functions, softmax functions, and/or swish functions, among others.

$$ReLU(x) = \max(x, 0)$$

Equation 2

[0017] During a process of training a neural network, the weight vectors can be altered to "tune" the network. In at least one example, a neural network can be initialized with random weights. Over time, the weights can be adjusted to improve the accuracy of the neural network. This can, over time, yield a neural network with high accuracy. The present disclosure utilizes machine learning such as neural networks for predicting product properties through modeling of input data. In these embodiments, the weights can be tuned based on a number of factors. For example, the weights can be tuned utilizing a plurality of rheology curves for a plurality of known polymer ensembles with known molecular weight distributions. In this way, the plurality of rheology curves can be utilized as features for training the neural network such that the neural network is able to more accurately identify a molecular weight distribution of an unknown polymer sample based on a measured rheology of the unknown polymer sample (e.g., unknown linear polymer sample).

[0018] Embodiments of the present disclosure include methods and devices for rheology-based modeling to identify the molecular weight distribution of linear polymers. The rheology-based modeling can include generating a data set. Generating the data can include utilizing a rheology model (e.g., reaction model, branch on branch (BoB) model, etc.) to generate a data set for a plurality of polymer ensembles. In some embodiments, the rheology model can include data that can be utilized to generate rheology curves for a plurality of different polymer ensembles that represent a relationship between a strain applied and a resulting stress of the polymer ensembles. In some embodiments, the rheology curves can include a plurality of input features

for the machine learning model from the corresponding polymer ensembles. In these embodiments, the plurality of input features (e.g., strain value, stress value, modulus value, etc.) for the machine learning model can be values generated by the rheology model for the plurality of polymer ensembles to be utilized by the machine learning model.

[0019] In these embodiments, the plurality of input features can be utilized to train a machine learning model such as an artificial neural network (ANN). The machine learning model can be trained to identify patterns between the input features and a molecular weight distribution of a polymer ensemble. In this way, the trained machine learning model can be utilized to determine a molecular weight distribution from a rheology measurement of an unknown polymer sample utilizing the plurality of output features with corresponding values from the data set.

[0020] As used herein, the singular forms "a", "an", and "the" include singular and plural referents unless the content clearly dictates otherwise. Furthermore, the word "may" is used throughout this application in a permissive sense (e.g., having the potential to, being able to), not in a mandatory sense (e.g., must). The term "include," and derivations thereof, mean "including, but not limited to."

[0021] As will be appreciated, elements shown in the various embodiments herein can be added, exchanged, and/or eliminated so as to provide a number of additional embodiments of the present disclosure. In addition, as will be appreciated, the proportion and the relative scale of the elements provided in the figures are intended to illustrate certain embodiments of the present invention and should not be taken in a limiting sense.

[0022] Figure 1 illustrates one example flow diagram of a method 100 to generate a rheology-based model to identify the molecular weight distribution of linear polymers. The method 100 can be implemented to train one or more machine learning models or ANN to predict the molecular weight distribution from a rheology measurement of an unknown polymer sample. In some examples, the method 100 can be executed by a computing device as described herein. The method 100 can be utilized to train a neural network or other type of machine learning model to determine a polymer structure of an unknown polymer sample based on a rheology measurement of the unknown polymer sample. In some embodiments, the trained neural network can be utilized to provide information to reverse engineer polymers with a particular rheological behavior, characterizing recycled polymers, and/or designing new polymers or resins.

[0023] In some embodiments, the method 100 can analyze or simulate polymer ensembles to collect data to be utilized to train a machine learning model. As used herein, a polymer ensemble refers to a collection or group of polymer molecules that share certain characteristics or properties. For example, a polymer ensemble can refer to a collection of a particular type of polymer within a particular range of molecular weights. In some embodiments, the polymer ensembles can refer to pseudo polymer ensembles that can be theoretical representations that are generated based on theoretical ensembles of particular polymers. In this way, actual measurements may not need to be performed on a plurality of real polymer ensembles to obtain rheology information related to the plurality of polymer ensembles. For example, a rheology model can be utilized to generate rheology information for a plurality of selected pseudo polymer ensembles. Unless specified otherwise, 'polymer ensembles', as used herein includes 'pseudo polymer ensembles'.

[0024] In some embodiments, at step 101 the method 100 can include data generation. In some embodiments, data generation includes generating a data set of information related to a plurality of polymer ensembles. As described further herein, the data set can include molecular weights and blending ratios for corresponding polymers of the plurality of polymer ensembles. In some embodiments, the data set can be utilized to generate rheology data for the plurality of polymer ensembles. In these embodiments, the rheology data can be utilized to generate rheology curves for each of the plurality of polymer ensembles.

[0025] In some embodiments, the data generation can include generating pseudo polymer ensembles within a particular molecular weight range and generate rheology curves for the pseudo polymer ensembles based on a reaction model. A reaction model refers to a conceptual or mathematical representation of a reaction. For example, a reaction model can describe a transformation of reactants into products or a theoretical result of a particular test (e.g., rheology test, etc.). In some examples, the reaction model can include various steps and intermediates involved in the process. In some embodiments, the reaction model can be based in part on branch-on-branch (BoB) modeling. In a specific example, the pseudo polymer ensembles can be a generated model of a particular polymer ensemble with particular properties. In this way, the pseudo polymer ensemble can be utilized to generate rheology data and/or rheology curves based on the reaction model utilizing the BoB modeling.

[0026] In some embodiments, at step 102 the method 100 can include data preprocessing. In some embodiments, data preprocessing can include selecting a portion of the generated rheology curves to be utilized for training the machine learning model. As described herein, the plurality of polymer ensembles can be pseudo polymer ensembles that are generated by a reaction model or simulation. In a specific example, the reaction model or simulation can generate more than 30,000 polymer ensembles that are each within a molecular weight range. In this example, a portion of the plurality of polymer ensembles can be selected to be utilized for training the machine learning model.

[0027] As described further in reference to Figure 2, the plurality of polymer ensembles can be utilized to generate a graphical representation of a molecular weight versus a blending ratio of a first polymer and a second polymer. For example, the blending ratio can be a ratio of a quantity of different linear low-density polyethylene (LLDPE) within the polymer ensemble. Although LLDPE blending ratios are illustrated in this example, other types of polymers and blending ratios can be utilized in a similar way.

[0028] In some embodiments, step 102 can include rescaling a modulus value of the respective rheology curves for each of the plurality of input features to generate a plurality of output features. As described herein, the plurality of rheology curves can represent a relationship between a strain value and a stress value associated with a particular polymer ensemble. In these embodiments, the modulus value can be rescaled between a value of 0 and 1 to generate a plurality of rescaled rheology curves for the plurality of rheology curves. In some embodiments, the rescaled rheology curves can be utilized as input data for training the machine learning model.

[0029] In some embodiments, step 102 can include calculating a relationship between the rescaled modulus value and a composition identified within the data set. For example, a feature graphical representation can be generated that illustrates the rescaled modulus value versus a composition value. In these embodiments, the composition value can be a blending ratio of a first polymer and a second polymer. In some embodiments, the feature graphical representation or data utilized to generate the feature graphical representation can be utilized to train the machine learning model.

[0030] In some embodiments, at step 103 the method 100 can include initial structure generation. The initial structure generation can include training a machine learning model such

as a neural network utilizing the data processed at step 102. In some embodiments, a neural network can be trained by altering weighting vector values for the neural network based on the data processed at step 102. In this way, the neural network can be trained to identify patterns associated between the rheology of a polymer sample and a molecular weight distribution of the polymer sample. As described herein, the data processed at step 102 can include relationship data between the rheology and molecular weight distribution of pseudo polymer ensembles and/or real polymer ensembles.

[0031] In some embodiments, the processed data from step 102 can be utilized with a mean-squared-logarithm error (MSLE) or other loss type functions. As used herein, MSLE can be a variant of the mean squared error (MSE) that incorporates a mathematical function (e.g., logarithmic function, base ten logarithm, natural logarithm, etc.). The use of the logarithm can be relevant when utilizing values that can span several orders of magnitude. The logarithmic transformation helps to penalize underestimates and overestimates more evenly, making the metric sensitive to the relative differences between predicted and true values.

[0032] In some embodiments, at step 104 the method 100 can include neural network optimization. As used herein, optimizing the neural network can include executing an optimization model on the weight vector values to improve or increase an accuracy of outputs associated with the neural network. For example, a Bayesian optimization model can be utilized to determine optimal weight vector values for the neural network such that the weight vector values generate a weight distribution that is closer to a known weight distribution for a known input sample polymer ensemble.

[0033] In some embodiments, at step 105 the method 100 can include model evaluation. As used herein, a model evaluation can include performing a plurality of iterations by providing rheology data to the neural network to determine an output of a molecular weight distribution and comparing the output to a known molecular weight distribution. In some embodiments, the model evaluation can include performing an evaluation of a portion of test datasets. That is, the rheology information associated with the portion of test datasets can be utilized as inputs and the generated molecular weight distribution outputs can be compared to known molecular weight distributions for the corresponding inputs. In some embodiments, the evaluation can pass when the difference between the generated molecular weight distribution outputs and the known molecular weight distributions are within a threshold difference.

[0034] Figure 2 is one example diagram 210 illustrating an approach to generate a rheology curve for a plurality of polymer ensembles. Diagram 210 illustrates a blending ratio graphical representation 211 and a rheology curve graphical representation 212. In some embodiments, the blending ratio graphical representation 211 can illustrate blending ratio 213 of a polymer compared to a molecular weight 214 of a polymer. The blending ratio graphical representation 211 can be a visual representation of data associated with a plurality of pseudo polymer ensembles that have a fixed molecular weight between the range identified by molecular weight 214 on the X-axis and a corresponding blending ratio blending ratio 213 on the Y-axis.

[0035] In some embodiments, the pseudo polymer ensembles can be representations of polymer ensembles that reflect expected properties of the plurality of polymer ensembles. In some embodiments, a particular range of molecular weight 214 and blending ratio 213 can be utilized based on a type of polymer ensemble to be detected. For example, the machine learning model can be trained for polymer types of LLDPE with different ranges of the blending ratio 213. In these embodiments, the molecular weight 214 range can be based on a common range of molecular weights for LLDPE molecules. In a specific example, the molecular weight 214 range can be 10^3 g/mol to 10^7 g/mol. Although this specific range of molecular weight 214 is utilized in the blending ratio graphical representation 211 other ranges can be selected and utilized in a similar way.

[0036] In some embodiments, the blending ratio 213 can be a ratio between a first polymer and a second polymer. As described herein, the blending ratio 213 can be a ratio between different LLDPE polymers within the polymer ensemble, however other polymer blending ratios can be utilized in a similar way. In some embodiments, the values of the blending ratio 213 can be expressed in a plurality of ways to define a percentage of the first polymer and a percentage of a second polymer within the sample of the polymer ensemble.

[0037] In some embodiments, the data associated with the blending ratio graphical representation 211 can be utilized to generate data for the rheology curve graphical representation 212. The data associated with the blending ratio graphical representation 211 can be utilized to determine the plurality of values utilized to generate the rheology curve graphical representation 212. For example, the molecular weight and corresponding blending ratio of a particular sample from the blending ratio graphical representation 211 can be utilized to generate a corresponding value of the rheology curve graphical representation 212. The plurality of values

of the rheology curve graphical representation 212 can represent a rheology value that is predicted utilizing a BoB model with the corresponding blending ratio of the polymer ensemble. The rheology curve graphical representation 212 may also be referred to in the art as a flow curve. The rheology curve graphical representation 212 can be a graphical representation of a relationship between an angular frequency 216 and a modulus 215 of a polymer ensemble. For example, the rheology curve graphical representation 212 can include a modulus value 215 on a first axis (e.g., y-axis) and an angular frequency 216 on a second axis (e.g., x-axis). In this example, the rheology curve graphical representation 212 can represent the modulus values and corresponding retention values.

[0038] In some embodiments, the rheology curve graphical representation 212 can represent the modulus 215 ranging from 10^2 Pa to 10^7 Pa. Although this range is illustrated in the rheology curve graphical representation 212, other ranges are also possible. In these embodiments, rheology curve graphical representation 212 can represent the retention value or angular frequency 216 ranging from 10^{-8} rad/s to 10^8 rad/s. Although this range is illustrated in the rheology curve graphical representation 212, other ranges are also possible. In some embodiments, the rheology curve graphical representation 212 illustrates data from the data set.

[0039] Figure 3 is one example diagram 320 illustrating an approach to rescale a modulus value for a plurality of input features associated with rheology curves to generate a plurality of output features. The diagram 320 can illustrate a rescaled rheology curve graphical representation 321 converted to an output feature representation 322.

[0040] As described herein, the modulus value can be the complex shear modulus value (G*). In these embodiments, the modulus value can be a predicted modulus value for each of the plurality of polymer ensembles as described in reference to Figure 2. In some embodiments, the rescaled modulus value can be rescaled from the modulus 215 of rheology curve graphical representation 212 as illustrated in Figure 2 to a rescaled shear modulus 323 between 0 and 1 as illustrated in the rescaled rheology curve graphical representation 321. In some embodiments, the angular frequency 316 values can be the same values from the rheology curve graphical representation 212 as illustrated in Figure 2 can remain within the same range.

[0041] In this way, the rescaled rheology curve graphical representation 321 can rescale the modulus value within a specific range and maintain the corresponding angular frequency. In some embodiments, a MinMaxScaler can be utilized to rescale the modulus values and/or

predicted modulus values for the plurality of polymer ensembles within a specified range. As used herein, a MinMaxScaler can be a processing technique for transforming a particular feature or value within a specified range. In these embodiments, a maximum value and a minimum value can be selected from the data set. For example, the maximum modulus value and the minimum modulus value can be selected from the data associated with the rheology curve graphical representation 212 as illustrated in Figure 2. The other modulus values from the data set can be rescaled to fall between the maximum modulus value and the minimum modulus value.

[0042] In some embodiments, the rescaled modulus values (e.g., rescaled shear modulus 323 values, etc.) can be utilized as input values for generating corresponding composition 326 values and an output feature representation 322 can be generated based on the rescaled shear modulus 323 and corresponding composition 326. The corresponding composition 326 can be a predicted blending ratio for each of the corresponding rescaled shear modulus 323 values. In this way, the neural network can be trained for a plurality of rescaled shear modulus 323 and corresponding composition 326 or blending ratios. In this way, the neural network can receive a modulus value associated with an unknown sample and convert the modulus value to a rescaled modulus value. The rescaled modulus value can be utilized to determine a corresponding composition as illustrated by the output feature representation 322.

[0043] Figure 4 illustrates an example of a method 440 for rheology-based modeling. The method 440 can be implemented to train one or more machine learning models or ANN to predict a molecular weight distribution from a rheology measurement of an unknown polymer sample. In some examples, the method 440 can be executed by a computing device as described herein. The method 440 can be utilized to train a neural network or other type of machine learning model to determine a polymer structure, composition, and/or blending ratio of an unknown polymer sample based on a rheology measurement of the unknown polymer sample. In some embodiments, the trained neural network can be utilized to reverse engineer polymers with a particular rheological behavior, characterizing post-consumer recycles, and/or designing new polymers or resins.

[0044] At step 441, the method 440 can include generating a data set for a plurality of polymer ensembles. In these embodiments, each of the plurality of polymer ensembles comprise a respective plurality of polymers within a defined range of molecular weights. As described herein, the data set can be generated through pseudo polymer ensembles that exhibit predicted

properties. As described herein, the predicted properties can be determined based on modeling. For example, the BoB modeling can be utilized to predict the rheology properties of the plurality of polymer ensembles. In this way, a group of polymer ensembles can be selected, and a data set can be generated utilizing the predicted properties of the selected polymer ensembles. In some embodiments, the polymer ensembles can be selected based on predicted properties or expected properties of potential unknown polymer ensembles to be analyzed.

[0045] In some embodiments, a polymer ensemble refers to a collection or group of polymer molecules that share certain characteristics and/or properties. As used herein, polymers are relatively large molecules composed of repeating structural units called monomers. The polymer ensemble concept acknowledges an inherent variability that can exist within a group of polymer molecules, which may have differences in terms of chain lengths, molecular weights, and/or conformations.

[0046] In some embodiments, the plurality of polymer ensembles are compositions of linear low-density polyethylene (LLDPE). In these embodiments, the method 440 can include generating a rheology curve for one or more of the plurality of polymer ensembles based on a blending ratio of the LLDPE. As described herein with reference to Figure 2, a blending ratio 213 with corresponding molecular weight 214 can be utilized to generate a predicted rheology curve graphical representation 212.

[0047] At step 442, the method 440 can include generating a respective rheology curve for each of the plurality of polymer ensembles. In these embodiments, the respective rheology curve comprises a plurality of features for a corresponding polymer ensemble. As described herein, the rheology curve can represent a modulus value versus angular frequency for the plurality of polymer ensembles.

[0048] As described herein, the respective rheology curves are representations of a relationship between a strain value and a resulting stress value of the plurality of polymer ensembles. As described herein, this can be a predicted relationship based on a predictive model utilized to analyze the selected polymer ensembles.

[0049] At step 443, the method 440 can include rescaling a modulus value of the respective rheology curves for each of the plurality of input features to generate a plurality of output features. As described herein, the rescaled modulus value can be utilized as an input for training the neural network and the output features can be composition features. The output

features and/or input features can be utilized to train a neural network to alter the weighting vectors such that a rescaled modulus value of an unknown polymer ensemble can be utilized to accurately predict the composition and/or molecular weight distribution of the unknown polymer ensemble.

[0050] In some embodiments, the method 440 can include generating a rescaled rheology curve for one or more of the plurality of polymer ensembles based on the plurality of output features. As described herein, the rescaled rheology curve can be a representation of the rescaled modulus value versus the angular frequency value. In this way, the rescaled modulus value can be utilized to generate a composition value that can be utilized to train a machine learning model as described further herein.

[0051] At 444, the method 440 can include training a machine learning model to determine a molecular weight distribution from a rheology measurement of an unknown polymer sample utilizing the plurality of output features with corresponding values from the data set. In some embodiments, the machine learning model can be a neural network that can be trained utilizing the rescaled modulus values and corresponding composition values as described herein. In these embodiments, the determined composition values can be utilized to accurately determine a molecular weight distribution and/or other properties of the unknown polymer sample.

[0052] As described herein, the modulus value from a rheology measurement of an unknown polymer sample can be rescaled and utilized as an input value for the machine learning model to determine an output composition value. The output composition value can be a blend ratio of the unknown polymer sample or a blend ratio of a proposed polymer sample that includes a desired modulus value. As described herein, a correlation can exist between the composition value and a molecular weight distribution. In this way, the machine learning model can utilize the composition value to determine the molecular weight distribution of the unknown polymer sample.

[0053] In some embodiments, the method 440 can include evaluating the machine learning model by providing a known rheology curve for a known polymer ensemble to the machine learning model to generate an output molecular weight distribution graph and comparing the output molecular weight distribution graph to a graphical representation of the known polymer sample. In some examples, evaluating the machine learning model can include performing a plurality of test data inputs to the machine learning model to determine when the

outputs provided by the machine learning model are within a particular threshold or range output values. In this way, the machine learning model can be further tuned to increase accuracy of determining the molecular weight distribution of unknown polymer samples.

[0054] Figure 5 illustrates an example of a machine readable medium 550 for rheology-based modeling. The machine readable medium 550 can be communicatively connected to a processor resource 552 by a communication path 554. In some examples, a communication path 554 can include a wired or wireless connection that can allow communication between devices and/or components within a single device. As used herein, the processor resource 552 can include, but is not limited to: a central processing unit (CPU), an application specific integrated circuit (ASIC), a field programmable gate array (FPGA), a metal-programmable cell array (MPCA), a semiconductor-based microprocessor, or other combination of circuitry and/or logic to orchestrate execution of instructions 556, 558, 560, 562. In a specific example, the processor resource 552 utilizes a non-transitory computer-readable medium storing instructions 556, 558, 560, 562, that, when executed, cause the processor resource 552 to perform corresponding functions.

[0055] The machine readable medium 550 may be electronic, magnetic, optical, or other physical storage device that stores executable instructions. Thus, a non-transitory machine-readable medium (MRM) (e.g., machine readable medium 550) may be, for example, a non-transitory MRM comprising Random-Access Memory (RAM), read-only memory (ROM), an Electrically Erasable Programmable ROM (EEPROM), a storage drive, an optical disc, and the like. The machine readable medium 550 may be disposed within a controller and/or computing device. In this example, the executable instructions 556, 558, 560, 562, can be "installed" on the device. Additionally, and/or alternatively, the machine readable medium 580 can be a portable, external, or remote storage medium, for example, which allows a computing system to download the instructions 556, 558, 560, 562, from the portable/external/remote storage medium. In this situation, the executable instructions may be part of an "installation package".

[0056] The machine readable medium 550 includes instructions 556 to provide a data set for a plurality of polymer ensembles. In these embodiments, each of the plurality of polymer ensembles comprise a respective plurality of polymers within a defined range of molecular weights and a blending ratio of the respective plurality of polymers.

[0057] The machine readable medium 550 includes instructions 558 to generate a respective rheology curve for the plurality of polymer ensembles based on a strain applied to the respective plurality of polymers and a resulting stress of the respective plurality of polymers for each of the plurality of polymer ensembles. As described herein, the plurality of polymer ensembles can include pseudo polymer ensembles that can represent a polymer ensemble within a particular molecular weight range. In this way, the applied strain value, predicted modulus value, and/or predicted stress value of the plurality of polymer ensembles can be based on predictive modeling, such as, but not limited to BoB modeling.

[0058] In these embodiments, the rheology curve comprises a plurality of input features based on the applied strain and predicted stress of the plurality of polymer ensembles. In some embodiments, the respective rheology curves are linear rheology curves. As used herein, a linear rheology curve can refer to a portion of rheological behavior of a material that exhibits a linear relationship between stress and strain. In some embodiments, the machine readable medium 550 can include instructions to generate the respective rheology curves utilizing a correlation of features under different frequencies of oscillation. In these embodiments, the features can be a modulus that can be based on the blending ratio and the different frequencies can be different levels of angular frequency. In this way, the respective rheology curve can be generated for each of the plurality of polymer ensembles that utilize different predicted modulus values and corresponding angular frequency values.

[0059] In some embodiments, the machine readable medium 550 can include instructions to map nonlinear relationships between a molecular structure of the polymer ensembles and rheology behavior of the polymer ensembles. In some embodiments, the machine readable medium 580 can include instructions to train the machine learning model to identify nonlinear relationships within the rheology measurement and compare the identified nonlinear relationships to the rheology curve for the plurality of polymer ensembles. In rheology, a relatively high stress and/or a relatively high strain of the polymer material can result in nonlinear behavior. Nonlinear behavior in the rheology curve indicates that the response of the material has deviated from a simple, proportional relationship between stress and strain. Some types of nonlinear relationships observed in rheology include nonlinear elasticity, yield stress, thixotropy and rheopexy, strain hardening and strain softening, viscoelasticity, among other nonlinear relationships.

[0060] The machine readable medium 550 includes instructions 560 to rescale a modulus value (e.g., shear modulus value, etc.) for the plurality of input features of the respective rheology curves to generate a plurality of output features. In these examples, the modulus value is a numerical value representing the ratio of the predicted stress and applied strain. That is, the shear modulus represents the material's resistance to deformation under shear stress. A higher shear modulus indicates greater stiffness and resistance to shear deformation, while a lower shear modulus suggests a more compliant and deformable material.

[0061] The machine readable medium 550 includes instructions 562 to train a machine learning model utilizing the plurality of output features with corresponding molecular weights and blending ratios for the plurality of polymer ensembles from the data set. In these examples, the machine learning model is configured to determine an unknown molecular weight distribution for an unknown polymer based on a rheology measurement of the unknown polymer based on the training. In these embodiments, the rheology measurement is a measured rheology of the unknown polymer utilizing small-amplitude oscillatory shear (SAOS) data. As used herein, the SAOS data is obtained by subjecting a material to a controlled oscillatory shear deformation with a small amplitude. In a more general case, SAOS experiments can be performed by applying either a sinusoidal strain or a sinusoidal stress to the material, and by measuring the resulting response (stress or strain, respectively). When strain is the input, the amplitude of the applied strain is kept small enough to ensure that the material responds linearly to the deformation. This means that the material's response is directly proportional to the applied strain, allowing for the characterization of its linear viscoelastic behavior.

[0062] As described herein, the machine learning model can be a neural network that can be trained utilizing the input data and corresponding output data associated with the plurality of polymer ensembles. As described herein, this data can be generated by utilizing predictive modeling such as BoB or other types of predictive modeling associated with polymer structure. In this way, the quantity of the plurality of polymer ensembles and corresponding data can be relatively high compared to utilizing actual measured data.

[0063] In addition, the data can be more cohesive since the data was collected utilizing the same or similar predictive modeling techniques. In some embodiments, the machine learning model can be tuned based on the linear relationships and nonlinear relationships of the data set. The machine learning model can be utilized to predict a plurality of features of an unknown

polymer sample including, but not limited to a molecular weight distribution and/or a blending ratio.

[0064] Figure 6 illustrates an example of a device 670 for rheology-based modeling. In some examples, the device 670 is a computing device that includes a processor resource 652 and a machine readable medium 650 to store instructions 671, 672, 673, 674, 675, 676 that are executed by the processor resource 652 to perform particular functions. Figure 6 illustrates how a computing device can execute instructions to perform functions described herein.

[0065] The device 601 includes instructions 671 stored by the machine readable medium 650 that is executed by the processor resource 652 to generate a data set utilizing a rheology model (e.g., reaction model, etc.) for a plurality of polymer ensembles. In these embodiments, the rheology model can be a predictive model such as a BoB model that can be utilized to predict rheology data based on the properties of the plurality of polymer ensembles. In these examples, the data set includes molecular weights and blending ratios for corresponding polymers of the plurality of polymer ensembles. As described herein, the data set can be generated using pseudo polymer ensembles that represent different blending ratios of polymers and/or different molecular weights. In this way, the data set can be generated without having to perform corresponding experiments on the polymer ensembles.

[0066] The device 670 includes instructions 672 stored by the machine readable medium 650 that is executed by the processor resource 652 to combine experimental data with the data set. In these examples, the experimental data includes rheology measurements of additional polymer ensembles. As described herein, the plurality of polymer ensembles can be pseudo polymer ensembles. In this way, a plurality of additional experimental data can be added to the data set. The additional experimental data can be data collected from experiments conducted on real polymer ensembles. In some embodiments, the experimental data can be utilized to improve the data set by adding real world data that is not based on a particular model. In some embodiments, the experimental data can help identify outliers of the particular model utilized to generate the data set.

[0067] The device 670 includes instructions 673 stored by the machine readable medium 650 that is executed by the processor resource 652 to generate a respective rheology curve for the plurality of polymer ensembles based on a modulus value from an applied strain and a resulting stress for corresponding polymers of each of the plurality of polymer ensembles. In these

embodiments, the respective rheology curves each comprise a plurality of input features that include a modulus value and strain value (e.g., angular frequency, etc.) for the plurality of polymer ensembles.

[0068] In some embodiments, the device 601 includes instructions to generate a rheology curve for one or more of the plurality of polymer ensembles based on a blending ratio of LLDPE within the polymer ensembles. The device 601 includes instructions 674 stored by the machine readable medium 650 that is executed by the processor resource 652 to rescale the modulus value for the plurality of input features of the respective rheology curves to a scale of a value of 0 to 1 to generate a plurality of output features.

[0069] The device 601 includes instructions 675 stored by the machine readable medium 650 that is executed by the processor resource 652 to generate a rescaled rheology curve for each of the respective rheology curves based on the plurality of output features. In some embodiments, the device 601 includes instructions to calculate a relationship between the rescaled modulus value and a composition identified within the data set. In these examples, the composition is a blending ratio between a first polymer and a second polymer of the plurality of polymer ensembles.

[0070] The device 601 includes instructions 676 stored by the machine readable medium 650 that is executed by the processor resource 652 to train a machine learning model to determine an unknown molecular weight distribution for an unknown polymer based on a rheology measurement of the unknown polymer utilizing the rescaled rheology curve with corresponding molecular weights and blending ratios for the plurality of polymer ensembles from the data set. As described herein, the trained machine learning model can be a neural network that includes trained weight vectors to identify patterns between the rheology measurement and the molecular weight distribution of a polymer sample.

[0071] In some embodiments, the device 601 includes instructions to calculate a composition of the plurality of polymer ensembles based on the rescaled rheology curve. As described herein, the composition of the plurality of polymer ensembles can be utilized to determine a molecular weight distribution and/or other properties associated with the unknown polymer sample. The composition can be a blending ratio of two or more polymers within the polymer ensemble.

[0072] Although specific embodiments have been described above, these embodiments are not intended to limit the scope of the present disclosure, even where only a single embodiment is described with respect to a particular feature. Examples of features provided in the disclosure are intended to be illustrative rather than restrictive unless stated otherwise. The above description is intended to cover such alternatives, modifications, and equivalents as would be apparent to a person skilled in the art having the benefit of this disclosure.

[0073] The scope of the present disclosure includes any feature or combination of features disclosed herein (either explicitly or implicitly), or any generalization thereof, whether or not it mitigates any or all of the problems addressed herein. Various advantages of the present disclosure have been described herein, but embodiments may provide some, all, or none of such advantages, or may provide other advantages.

[0074] In the foregoing Detailed Description, some features are grouped together in a single embodiment for the purpose of streamlining the disclosure. This method of disclosure is not to be interpreted as reflecting an intention that the disclosed embodiments of the present disclosure have to use more features than are expressly recited in each claim. Rather, as the following claims reflect, inventive subject matter lies in less than all features of a single disclosed embodiment. Thus, the following claims are hereby incorporated into the Detailed Description, with each claim standing on its own as a separate embodiment.

Claims

What is claimed is:

1. A method, comprising:

generating a data set for a plurality of polymer ensembles, wherein each of the plurality of polymer ensembles comprise a respective plurality of polymers within a defined range of molecular weights;

generating a respective rheology curve for each of the plurality of polymer ensembles, wherein the respective rheology curve comprises a plurality of input features for a corresponding polymer ensemble;

rescaling a modulus value of the respective rheology curves for each of the plurality of input features to generate a plurality of output features; and

training a machine learning model to determine a molecular weight distribution from a rheology measurement of an unknown polymer sample utilizing the plurality of output features with corresponding values from the data set.

2. The method of claim 1, further comprising generating a rescaled rheology curve for one or more of the plurality of polymer ensembles based on the plurality of output features.

3. The method of claim 1, further comprising evaluating the machine learning model by:

providing a known rheology curve for a known polymer ensemble to the machine learning model to generate an output molecular weight distribution graph; and

comparing the output molecular weight distribution graph to a graphical representation of the unknown polymer sample.

4. The method of claim 1, wherein the respective rheology curves are representations of a relationship between a strain applied and a resulting stress of the plurality of polymer ensembles.

5. The method of claim 1, wherein the plurality of polymer ensembles are compositions of linear low-density polyethylene (LLDPE).

6. The method of claim 5, further comprising generating a rheology curve for one or more of the plurality of polymer ensembles based on a blending ratio of the LLDPE.

7. The method of claim 1, wherein the plurality of input features include a first value to represent an angular frequency applied to a corresponding polymer ensemble and a second value to represent a modulus of the corresponding polymer ensemble at the first value.

8. The method of claim 1, wherein the rheology measurement is a measured rheology of the unknown polymer utilizing small-amplitude oscillatory shear (SAOS) data.

9. The method of claim 1, wherein, comprising instructions to map nonlinear relationships between a molecular structure of the polymer ensembles and rheology behavior of the polymer ensembles.

10. The method of claim 1, the respective rheology curves are linear rheology curv