U.S. Patent No. 6,406,632 describes rapid characterization and screening of polymer samples to determine average molecular weight, molecular weight distribution and other properties is disclosed.

U.S. Patent No. 6,687,621 describes a computational method for predicting a desired property and/or performance of polymers, and/or identifying and designing polymers that provide the desired property and/or performance, wherein the desired property can be provided by the neat, undiluted polymers, or diluted polymers in a composition. The method is a QSAR approach wherein the descriptors used are structural descriptors which are experimentally generated and/or derived from one or more analytical methods.

Despite the research efforts in developing polymer property prediction models, there is still a need for a method for improving the prediction of polymer properties and a system having improved polymer property prediction capabilities. Furthermore, there is a need for a method for automatically determining the feasibility of laboratory measurements using (1) the expected standard deviation of the sample polymer property measurements and/or (2) process models and estimates of measurement uncertainty.

Summary ~~of the Invention~~

The instant ~~invention~~disclosure is a method for improving the prediction and subsequent control of polymer properties and a system having improved polymer property prediction capabilities. The method for improving the prediction of polymer properties according to instant ~~invention~~disclosure comprises the following steps of: (1) providing a polymer; (2) providing a prediction model; (3) utilizing said prediction model to define an average polymer property prediction value; (4) determining a feasible range; (5) measuring one or more properties of said polymer; (6) determining whether said one or measured polymer properties are within said feasible range; (7) validating said one or more

measured polymer properties if said one or more measured polymer properties fall within the feasible range or invalidating said one or more measured polymer properties if said one or more measured polymer properties fall outside of the feasible range; (8) updating said prediction model; (9) repeating said previous steps at least one or more times; and (10) thereby improving the prediction of polymer properties. The polymerization system having improved polymer property prediction capabilities according to instant ~~invention~~disclosure comprises at least one polymerization reactor; an automated prediction model; means for measuring one or more polymer properties; means for detecting one or more erroneous measured polymer properties; and means for updating said automated predication model.

In one aspect, there is provided a method for improving the prediction of polymer properties comprising the steps of:

providing a polymer;

providing a prediction model based on material balance and polymer properties;

utilizing said prediction model to define an average polymer property prediction value, wherein said average polymer property prediction value is x_p;

determining a feasible range;

measuring one or more properties of said polymer;

determining whether said one or more measured polymer properties are within said feasible range;

validating said one or more measured polymer properties if said one or more measured polymer properties fall within the feasible range or invalidating said one or more measured polymer properties if said one or more measured polymer properties fall outside of the feasible range;

updating said prediction model;

repeating said previous steps at least one or more times until updating said prediction model at least one more time; and thereby

improving the prediction of polymer properties; wherein said feasible range is determined via

$$x_{Low} = x_P\left(1 - \frac{\sigma}{x_p}\sqrt{-2\ln(1-f)}\right) - \frac{ax_p}{dt}T_u;$$

and

$$x_{High} = x_P\left(1 + \frac{\sigma}{x_p}\sqrt{-2\ln(1-f)}\right) + \frac{dx_p}{dt}T_u;$$

wherein said polymer property prediction value is logarithmic, and wherein

x_{Low} is the lowest value expected for the lab value;

x_{High} is the highest value expected for the lab value;

f is the probability that the sample is part of the collection of samples;

σ is the standard deviation of the lab measurement method;

x_p is the model predicted bed average value;

T_u is the amount of time uncertainty in the exact sample time; and

$$\frac{dx_p}{dt}$$

is the derivate of x_p with respect to time.

In one embodiment, the instant ~~invention~~disclosure provides a method for improving the prediction of polymer properties comprising the following steps of: (1) providing a polymer; (2) providing a prediction model; (3) utilizing said prediction model to define an average polymer property prediction value; (4) determining a feasible range; (5) measuring one or more properties of said polymer; (6) determining whether said one or measured polymer properties are within said feasible range; (7) validating said one or more measured polymer properties if said one or more measured polymer properties fall within the feasible range or invalidating said one or more measured polymer properties if said one or more measured polymer properties fall outside of the feasible range; (8) updating said prediction model; (9) repeating said previous steps at least one or more times; and (10) thereby improving the prediction of polymer properties.

In another aspect, there is provided a method for improving the prediction of polymer properties comprising the steps of:

providing a polymer;

providing a prediction model based on material balance and polymer properties;

utilizing said prediction model to define an average polymer property prediction value, wherein said average polymer property prediction value is x_p;

determining a feasible range;

measuring one or more properties of said polymer;

determining whether said one or more measured polymer properties are within said feasible range;

validating said one or more measured polymer properties if said one or more measured polymer properties fall within the feasible range or invalidating said one or more measured polymer properties if said one or more measured polymer properties fall outside of the feasible range;

updating said prediction model;

repeating said previous steps at least one or more times until updating said prediction model at least one more time; and

thereby improving the prediction of polymer properties; wherein said feasible range is determined via

$$x_{Low} = x_P\left(1 - \frac{\sigma}{x_p}\sqrt{-2\ln(1-f)}\right) - \frac{dx_p}{dt}T_u;$$

and

$$x_{High} = x_P\left(1 + \frac{\sigma}{x_p}\sqrt{-2\ln(1-f)}\right) + \frac{dx_p}{dt}T_u;$$

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wherein said polymer property prediction value is non-logarithmic, and wherein

x_{Low} is the lowest value expected for the lab value;

x_{High} is the highest value expected for the lab value;

f is the probability that the sample is part of the collection of samples;

σ is the standard deviation of the lab measurement method;

x_p is the model predicted bed average value;

T_u is the amount of time uncertainty in the exact sample time; and

$$\frac{dx_p}{dt}$$

is the derivative of x_p with respect to time.

In an alternative embodiment, the instant ~~invention~~disclosure provides a method for improving the prediction of polymer properties, in accordance with any of the preceding embodiments, except that the average polymer property prediction value is x_p.

In an alternative embodiment, the instant ~~invention~~disclosure provides a method for improving the prediction of polymer properties, in accordance with any of the preceding embodiments, except that the feasible range is determined via

$$x_{Low} = x_P\left(1-\frac{\sigma}{x_p}\sqrt{-2\ln(1-f)}\right)-\frac{dx_p}{dt}T_u\text{; and}$$

$$x_{High} = x_P\left(1+\frac{\sigma}{x_p}\sqrt{-2\ln(1-f)}\right)+\frac{dx_p}{dt}T_u\text{;}$$

wherein the polymer property prediction value is logarithmic;

or the feasible range is determined via

$$x_{Low} = x_P-\sigma\sqrt{-2\ln(1-f)}-\frac{dx_p}{dt}T_n\text{; and}$$

$$x_{High} = x_P+\sigma\sqrt{-2\ln(1-f)}+\frac{dx_p}{dt}T_u\text{;}$$

wherein the polymer property prediction value is non-logarithmic;

and wherein

x_{Low} is the lowest value expected for the lab value;

x_{High} is the highest value expected for the lab value;

f is the probability that the sample is part of the collection of samples;

σ is the standard deviation of the lab measurement method;

x_p is the model predicted bed average value;

T_u is the amount of time uncertainty in the exact sample time; and

$\frac{dx_p}{dt}$ is the derivative of x_p with respect to time.

In another aspect, there is provided a method for improving the prediction of polymer properties comprising the steps of:

providing a polymer;

providing a prediction model based on material balance and polymer properties;

utilizing said prediction model to define an average polymer property prediction value, wherein said average polymer property prediction value is x_p;

determining a feasible range;

measuring one or more properties of said polymer;

determining whether said one or more measured polymer properties are within said feasible range; validating said one or more measured polymer properties if said one or more measured polymer properties fall within the feasible range or invalidating said one or more measured polymer properties if said one or more measured polymer properties fall outside of the feasible range;

updating said prediction model;

repeating said previous steps at least one or more times until updating said prediction model at least one more time; and thereby improving the prediction of polymer properties;

wherein said feasible range is determined via $x_{Low}=x_p(1-\text{delta})_n$; and $x_{High}=x_p(1+\text{delta})$; wherein x_p is the model predicted bed average value.

In an alternative embodiment, the instant ~~invention~~disclosure provides a method for improving the prediction of polymer properties, in accordance with the preceding embodiment, except that the $\frac{dx_p}{dt}$ is determined via $\frac{x_p^k - x_p^{k-1}}{t^k - t^{k-1}}$; wherein

k represents the current time; and

k-1 represents the time one calculation interval previously.

In an alternative embodiment, the instant ~~invention~~disclosure further provides a polymerization system having improved polymer property prediction capabilities comprising at least one polymerization reactor; an automated prediction model; means for measuring one or more polymer properties; means for detecting one or more erroneous measured polymer properties; and means for updating said automated predication model.

In an alternative embodiment, the instant ~~invention~~disclosure further provides a method and a system for detecting erroneous polymer property measurement values before these values are used to manipulate reactor conditions.

In an alternative embodiment, the instant ~~invention~~disclosure provides a polymerization system having improved polymer property prediction capabilities, in accordance with the preceding embodiment, except that the means for measuring one or more polymer properties is an automated device.

In an alternative embodiment, the instant ~~invention~~disclosure provides a polymerization system having improved polymer property prediction capabilities, in accordance with any of the preceding embodiments, except that the means for detecting one or more erroneous measured polymer properties is an automated device.

In an alternative embodiment, the instant ~~invention~~disclosure provides a polymerization system having improved polymer property prediction capabilities, in accordance with any of the preceding

embodiments, except that the means for updating said automated predication model is an automated device.

In an alternative embodiment, the instant ~~invention~~disclosure provides a polymerization system having improved polymer property prediction capabilities, in accordance with any of the preceding embodiments, except that the automated predication model is a computer model.

Brief Description of the Drawings

For the purpose of illustrating the invention, there is shown in the drawings a form that is exemplary; it being understood, however, that this invention is not limited to the precise arrangements and instrumentalities shown.

Fig. 1 is a flow chart illustrating how the instant invention operates;

Fig. 2 is flow chart illustrating how one or more erroneous measured polymer properties are detected; and

Fig. 3 is a graphical illustration of automated detection of one or more erroneous measured polymer properties to improve the prediction of such polymer properties.

Detailed Description of the Invention

The instant invention is a method for improving the prediction of polymer properties and a system having improved polymer property prediction capabilities. The method for improving the prediction of polymer properties according to instant invention comprises the following steps of: (1) providing a polymer; (2) providing a prediction model; (3) utilizing said prediction model to define an average polymer property prediction value; (4) determining a feasible range; (5) measuring one or more properties of said polymer; (6) determining whether said one or measured polymer properties are within said feasible range; (7) validating said one or more measured polymer properties if said one or more measured polymer properties fall within the feasible range or invalidating said one or