

**SYSTEMS, METHODS, AND NON-TRANSITORY COMPUTER-READABLE MEDIUM OF
PREDICTING A COMPATIBILITY OF AN ADHESIVE OR COATING COMPOSITION AND
POLYOLEFIN POLYMERS**

CROSS-REFERENCE TO RELATED APPLICATIONS

[0001] This application claims the benefit of U.S. Provisional Application Serial No. 63/482,099 filed January 30, 2023, the contents of which are incorporated in their entirety herein.

TECHNICAL FIELD

[0002] Embodiments of the present disclosure generally relate to systems, methods, and non-transitory computer-readable mediums for predicting the mechanical recyclability or compatibility of an adhesive or coating composition and polyolefin polymers.

BACKGROUND

[0003] Adhesive or coating compositions are useful for a wide variety of purposes. For instance, adhesive compositions are used to bond together substrates such as polyethylene, polypropylene, polyester, polyamide, metal, paper, or cellophane to form composite films, i.e., laminates. Coating compositions are used to aesthetic, functional, and protective purposes. The use of adhesive or coating compositions in different end-use applications is generally known. For example, adhesives can be used in the manufacture of film and film, film and paper, and film and metal foil laminates used in the packaging industry, especially for food and pharmaceutical packaging. Coatings are applied on plastic films, paper, metal foils, metal parts, and pipes and cables.

[0004] It may be desirable for a number of reasons to predict the mechanical recyclability or interchangeably, compatibility of an adhesive or coating composition and polyolefin polymers. In general, conventional systems and methods determine the mechanical recyclability or compatibility of an adhesive or coating composition and polyolefin polymer by performing experiments. These systems and methods require large investment upfront and are time-consuming and costly. Systems and methods that may predict the mechanical recyclability or

compatibility of an adhesive or coating composition and polyolefin polymer without actual equipment and experiments are not available.

[0005] With the advent of computational modeling methods, it becomes possible to model or simulate many processes, including the mechanical recyclability or compatibility problem. A need exists for systems, methods, and non-transitory computer-readable mediums for predicting the compatibility of an adhesive or coating composition and polyolefin polymers without actual experiments.

SUMMARY

[0006] Embodiments of the present disclosure address meet this need by calculating Hansen's solubility parameter (HSP) of the adhesive or coating composition, the arithmetic distance (R_a) to benchmark materials, such as polyolefin composition, the geometric distance (R_b) to benchmark materials, and the aliphatic carbon ratio (ACR) of the adhesive or coating composition; comparing at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value; comparing the ACR of the adhesive or coating composition to an ACR threshold value of benchmark polyolefin polymer; and predicting the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparisons. This provides means to predict the compatibility of the adhesive or coating composition and the polyolefin polymer composition without performing actual recyclability experiments as well as reducing the time of predicting the compatibility of the adhesive or coating composition and the polyolefin polymer composition with improved accuracy. This may help to screen the adhesive or coating compositions before recyclability experiments, accelerate discovery and save cost, reveal the rules that govern the mechanical recyclability or compatibility of adhesive or coating compositions, and guide future design of adhesive or coating compositions.

[0007] In one or more embodiments, a system of predicting the compatibility of an adhesive or coating composition and polyolefin polymer comprises a controller. The controller is programmed to: receive a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both, receive a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both, calculate Hansen's solubility parameter (HSP, δ_t), polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition based on the name of the adhesive or

coating composition, the trading name of the adhesive or coating composition, or both, calculate HSP of the polyolefin polymer (δ_{t0}), polar interaction subcomponent (δ_{p0}), hydrogen bonding subcomponent (δ_{h0}), and dispersion forces subcomponent (δ_{d0}) of the polyolefin polymer based on the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both, calculate an arithmetic distance parameter (R_a) between the adhesive or coating composition and the polyolefin polymer, calculate a geometric distance parameter (R_b) between the adhesive or coating composition and the polyolefin polymer, calculate an ACR of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both, compare at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value, compare the ACR of the adhesive or coating composition to a threshold value of the ACR, and predict a compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.

[0008] In another embodiment, a method of predicting the compatibility of an adhesive or coating composition and polyolefin polymer includes receiving a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both, receiving a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both, receiving a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both, calculating HSP (δ_t), polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both, calculating HSP of the polyolefin polymer (δ_{t0}), polar interaction subcomponent (δ_{p0}), hydrogen bonding subcomponent (δ_{h0}), and dispersion forces subcomponent (δ_{d0}) of the polyolefin polymer based on the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both, calculating an arithmetic distance parameter (R_a) between the adhesive or coating composition and the polyolefin polymer, calculating a geometric distance parameter (R_b) between the adhesive or coating composition and the polyolefin polymer, calculating an ACR of the adhesive or coating composition based on the name of the adhesive or

coating composition, the trading name of the adhesive or coating composition, or both, comparing at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value, comparing the ACR of the adhesive or coating composition to a threshold value of the ACR, and predicting a compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.

[0009] In yet another embodiment, a non-transitory computer-readable medium for predicting the compatibility of an adhesive or coating composition and polyolefin polymer that, when executed by a controller, causes the controller to receive a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both, receive a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both, calculate HSP (δ_t), polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both, calculate HSP of the polyolefin polymer (δ_{t0}), polar interaction subcomponent (δ_{p0}), hydrogen bonding subcomponent (δ_{h0}), and dispersion forces subcomponent (δ_{d0}) of the polyolefin polymer based on the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both, calculate an arithmetic distance parameter (R_a) between the adhesive or coating composition and the polyolefin polymer, calculate a geometric distance parameter (R_b) between the adhesive or coating composition and the polyolefin polymer, calculate an ACR of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both, compare at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value, compare the ACR of the adhesive or coating composition to a threshold value of the ACR, and predict a compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.

[0010] Additional features and advantages of the described embodiments will be set forth in the detailed description which follows, and in part will be readily apparent to those skilled in the art from that description or recognized by practicing the described embodiments, including the detailed description which follows and the claims.

BRIEF DESCRIPTION OF THE DRAWINGS

[0011] The following detailed description of specific embodiments of the present disclosure can be best understood when read in conjunction with the following drawings, where like structure is indicated with like reference numerals and in which:

[0012] FIG. 1 depicts a schematic diagram of a system of predicting the compatibility of an adhesive or coating composition and polyolefin polymer, according to one or more embodiments shown and described herein;

[0013] FIG. 2 schematically depicts a plurality of memory modules of the system of FIG. 1, according to one or more embodiments shown and described herein;

[0014] FIG. 3 depicts a flowchart for a method of predicting the compatibility of an adhesive or coating composition and polyolefin polymer, according to one or more embodiments shown and described herein; and

[0015] FIG. 4 depicts a table for values of increments in Hoy's system, for the molar attraction function, according to one or more embodiments shown and described herein. Values in FIG. 4 are reproduced from Table 7.12, of D.W. van Krevelen's book "Properties of Polymers" 4th ed., Completely Revised Edition, available from Elsevier: Amsterdam, 2009, ebook ISBN: 9780080915104.

[0016] Reference will now be made in greater detail to various embodiments of the present disclosure, some embodiments of which are illustrated in the accompanying drawings. Whenever possible, the same reference numerals will be used throughout the drawings to refer to the same or similar parts.

DETAILED DESCRIPTION

[0017] Unless stated to the contrary, implicit from the context, or customary in the art, all parts and percentages are based on weight, all temperatures are in degrees Celsius (°C), and all test methods are current as of the filing date of this disclosure.

[0018] The term “mechanical recyclability,” “compatibility,” or simply “recyclability,” or “mechanical reprocessability,” or simply “reprocessability,” herein, with reference to a first article having an adhesive or coating, means mechanically recyclable or recyclability; and means the first article with an adhesive or coating is mechanically re-processable to generate a second article having a desirable performance range, wherein the second article has at least a $\leq 33\%$ decreased change in performance relative to the performance of a control article that is without any adhesive or coating and that is reprocessed the same way as the second article. An example, and not to be limited thereby, of testing methods and guidelines for determining recyclability of a plastic article can be found in publication “Critical Guidance Protocol for PE Film and Flexible Packaging,” Document Number FPE-CG-01, Revision date – August 2, 2022, of The Association of Plastic Recyclers (APR).

[0019] In general, the laminate of the present invention, prior to recycling, can be used in a wide range of applications including, for example, packaging applications for manufacturing various packaging materials and products. For example, the laminate can be used for bulk packaging of food grains/pulses, packaging of seeds, packaging of lentils and cereals, packaging of fertilizer, packaging of oilseed, packaging of sugar, packaging of salt, packaging of pharmaceuticals, packaging of other food stuff, and personal care items such as bath salts, detergent pods and the like. The film may also be used as a wrapper for baby wipes, feminine hygiene products, cereal bars, protein bars, cheese, and confectionary products. When used for heavy duty packaging of food grain/pulses, the packaging article shows no signs of tunneling/delamination/deformation in the laminate after the adhesive cures for 24 hours. Also, other advantageous features and applications for the recyclable laminate when used for packaging articles include, for example, resistance to severe weathering conditions, high tensile strength, robust drop test resistance, excellent optical appearance, and resistance to spills. The recycled materials of the present invention can also be used to reproduce non-packaging materials.

[0020] One of the advantages of the present invention is that a used virgin article (first article) made from the laminate of the present invention can be reprocessed, i.e., processed through a recycling process. After recycling, the recycled material from the previous virgin article can be used to make a subsequent recycled laminate, and in turn a recycled article (i.e., a second article), with properties and performances very close to the previous virgin article. One objective of the present invention is to produce a second article that performs as well as, or better than, the first article, i.e. the properties of the second article performs 100 % the same as, or greater than, the properties of the first article. At a minimum, the properties of the second article are maintained at a sufficient level of performance to provide a second article that is useful in another application.

[0021] The first article includes a combination of: (a) at least one polyolefin polymer; and (b) at least an adhesive or coating composition. It has been surprisingly found that the recyclability property of the adhesive or coating composition (according to the publicly recognized mechanical recycling protocols, such as APR FPE-CG-01) can be predicted by some readily observable, calculatable, and measurable physiochemical properties of the same composition; and thus, in some embodiments, the first article is mechanically recyclable, or said to be compatible with polyolefins, and can be used to produce the second article for various other applications.

[0022] The polyolefin polymer, component (a), useful for making the first article of the present invention can include one or more polyolefins. The first article can be, for example, a polyolefin film. Generally, the polymeric portion of the film can be comprised of at least 80 % of a polyolefin polymer, or at least 85 % of a polyolefin polymer, or at least 90 % of a polyolefin polymer. In one embodiment, the polyolefin polymer is at least one PE polymer. For example, the PE polymer, can include one or more of HDPE, LDPE, LLDPE, and mixtures thereof. The polyolefin film may be a monolayer or a multilayer film or may be an oriented film, oriented by machine direction orientation (MDO) or biaxial orientation processes. In another preferred embodiment, the polyolefin is polypropylene (PP), oriented PP (OPP), biaxially oriented PP (BOPP), and mixtures thereof. The non-polyolefin portion of the film may be comprised of polymers such as poly (vinyl alcohol) (EVOH) or a polyamide (e.g., nylon), functionalized tie layer polymers and compatibilizers as described in U. S. Patent No. 10,300,686.

[0023] The thickness of the polyolefin film web used to form the recyclable laminate of the present invention can be, typically, from 10 microns (μm) to 200 μm . For this model to be valid, the weight percentage of the adhesive or coatings in the laminate films or the coated films is less than 15%, preferably less than 10%, more preferably less than 8%, and still more preferably less than 5%.

[0024] The embodiments disclosed herein include systems, methods, and non-transitory computer-readable mediums for predicting the compatibility of an adhesive or coating composition and polyolefin polymer. The systems, methods, and non-transitory computer-readable mediums accurately predict the compatibility of an adhesive or coating composition and polyolefin polymer, without actual experiments, by calculating the HSP of the adhesive or coating composition, the arithmetic distance (R_a), the geometric distance (R_b), and the aliphatic carbon ratio (ACR) of the adhesive or coating composition; comparing at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value of the benchmark polymers; comparing the ACR of the adhesive or coating composition to an ACR threshold value of the benchmark polymers; and predicting the compatibility of the adhesive or coating composition and the polyolefin polymer based on the results of comparisons.

[0025] The term “polymer” may refer to a polymeric compound prepared by polymerizing monomers, whether of the same or a different type. The generic term polymer thus embraces the term homopolymer (employed to refer to polymers prepared from only one type of monomer, with the understanding that trace amounts of impurities can be incorporated into the polymer structure), and the term interpolymer as defined hereinafter. Trace amounts of impurities (for example, catalyst residues) may be incorporated into and/or within the polymer. A polymer may be a single polymer, a polymer blend or a polymer mixture, including mixtures of polymers that are formed in situ during polymerization. The terms “olefin-based polymer” or “polyolefin,” as used herein, refer to a polymer that comprises, in polymerized form, a majority amount of olefin monomer, for example ethylene or propylene or isoprene (based on the weight of the polymer), and optionally may comprise one or more comonomers.

[0026] The term “copolymer” or “interpolymer” may refer to polymers prepared by polymerizing at least two different types of monomers. The generic term interpolymer thus

includes copolymers and other polymers prepared by polymerizing more than two different monomers, such as terpolymers.

[0027] The terms “adhesive or coating” or “adhesive or coating composition” may refer to a composition that adheres to at least one substrate. The adhesive composition may be used as an adhesive layer in between two or more substrates in a multilayer laminate structure. The coating may be used on one substrate.

[0028] The term “polyurethane” may generally refer to a polymer with polyurethane linkages that are derived from chemical reaction between isocyanate groups and polyols. The chemical entities bearing the isocyanate groups and polyols can have many different compositions. For example, one or more isocyanate-terminated polymers may react with small molecule polyols, such as ethylene glycol, propylene glycol, butylene glycol, neopentyl glycol, 1,6-hexane diol, and their combinations, to afford polyurethane polymers. Alternatively, one or more hydroxyl-terminated polymers may react with small molecule isocyanates, such as toluene diisocyanates (TDI), 4,4'-methylenbisphenylisocyanate (MDI), hexamethylene diisocyanate (HMDI), isophorone diisocyanate (IPDI), 4,4'-methylenedicyclohexyldiisocyanate, 1,5-naphthylene diisocyanate, 1,3-bis(isocyanatomethyl)benzene, the dimers and trimers of these isocyanates, and their combinations, to yield polyurethane polymers. Still alternatively, one or more hydroxyl-terminated polymer can react with one or more isocyanate-terminated polymers to afford polyurethane polymers. Common backbones of the hydroxyl- and isocyanate-terminated polymers used for the synthesis of polyurethanes include polyesters, polyethers, polycarbonates, poly(meth)acrylates, polyamides, nylon, and silicones. The polyurethanes can be linear or crosslinked.

[0029] The term “polyethylene (PE)” or “polyolefin polymer polymer” may refer to a polymer comprising a majority amount (> 50 mol %) of units which have been derived from ethylene monomer. This includes polyethylene homopolymers, ethylene/a-olefin interpolymers, and ethylene/a-olefin copolymers. Common forms of polyethylene known in the art include low density polyethylene (LDPE); linear low-density polyethylene (LLDPE); ultralow density polyethylene (ULDPE); very low-density polyethylene (VLDPE); medium density polyethylene (MDPE); high density polyethylene (HDPE); enhanced polyethylene; polyethylene elastomers; and polyethylene plastomers. These PE materials are generally known in the art; however, the

following descriptions may clarify the differences between some of these different PE resins. The term “LDPE” may also be referred to as “high pressure ethylene polymer” or “highly branched polyethylene” and is defined to mean that the polymer is partly or entirely homopolymerized or copolymerized in autoclave or tubular reactors at pressures above 14,500 pounds per square inch (psi) (100 megapascal [MPa]) with the use of free-radical initiators, such as peroxides (see for example U.S. Patent Nos. 8,916,667; 8,871,887; 8,822,601; 9,228,036; and 9,765,160). LDPE resins typically have a density in the range of 0.916 grams per cubic centimeter (g/cm^3) to 0.935 g/cm^3 . The term “MDPE” refers to polyethylenes having densities from 0.926 g/cm^3 to 0.940 g/cm^3 . The term “HDPE” refers to polyethylenes having densities greater than 0.940 g/cm^3 and up to 0.970 g/cm^3 . The term “ULDPE” refers to polyethylenes having densities of 0.880 g/cm^3 to 0.912 g/cm^3 . Polyethylene plastomers/elastomers have a density from 0.870 to 0.917 g/cm^3 .

[0030] The term “composition” may refer to a mixture of materials that comprises the composition, as well as reaction products and decomposition products formed from the materials of the composition. The terms “comprising,” “including,” “having,” and their derivatives, are not intended to exclude the presence of any additional component, step or procedure, whether or not the same is specifically disclosed. In order to avoid any doubt, all compositions claimed through use of the term “comprising” may include any additional additive, adjuvant, or compound, whether polymeric or otherwise, unless stated to the contrary. In contrast, the term, “consisting essentially of” excludes from the scope of any succeeding recitation any other component, step or procedure, excepting those that are not essential to operability. The term “consisting of” excludes any component, step or procedure not specifically delineated or listed.

[0031] FIG. 1 depicts a schematic diagram of a system 100 of predicting the compatibility of an adhesive or coating composition and polyolefin polymer, according to one or more embodiments shown and described herein. Referring to FIG. 1, the system 100 may include one or more processors 102, a communication path 104, one or more memory modules 106, a data storage component 108, and network interface hardware 110. In some embodiments, the system 100 may be a remote computing device (e.g., a cloud computing device) or a local computing device.

[0032] Each of the one or more processors 102 may be any device capable of executing machine readable and executable instructions. Accordingly, each of the one or more processors

102 may be a controller, an integrated circuit, a microchip, a computer, or any other physical or cloud-based computing device. The algorithms, including the trained models, signal preprocessing, and noise removal methods discussed below, may be executed by the one or more processors 102. The one or more processors 102 are coupled to a communication path 104 that provides signal interconnectivity between various modules of the system 100. Accordingly, the communication path 104 may communicatively couple any number of processors 102 with one another, and allow the modules coupled to the communication path 104 to operate in a distributed computing environment. Specifically, each of the modules may operate as a node that may send and/or receive data. As used herein, the term “communicatively coupled” means that coupled components are capable of exchanging data signals with one another such as, for example, electrical signals via conductive medium, electromagnetic signals via air, optical signals via optical waveguides, and the like.

[0033] Accordingly, the communication path 104 may be formed from any medium that is capable of transmitting a signal such as, for example, conductive wires, conductive traces, optical waveguides, or the like. In some embodiments, the communication path 104 may facilitate the transmission of wireless signals, such as WiFi, Bluetooth®, Near Field Communication (NFC) and the like. Moreover, the communication path 104 may be formed from a combination of mediums capable of transmitting signals. In one embodiment, the communication path 104 comprises a combination of conductive traces, conductive wires, connectors, and buses that cooperate to permit the transmission of electrical data signals to components such as processors, memories, sensors, input devices, output devices, and communication devices. Additionally, it is noted that the term “signal” means a waveform (e.g., electrical, optical, magnetic, mechanical or electromagnetic), such as DC, AC, sinusoidal-wave, triangular-wave, square-wave, vibration, and the like, capable of traveling through a medium.

[0034] The system 100 includes one or more memory modules 106 coupled to the communication path 104 and may contain non-transitory computer-readable medium comprising RAM, ROM, flash memories, hard drives, or any device capable of storing machine readable and executable instructions such that the machine readable and executable instructions can be accessed by the one or more processors 102. The machine readable and executable instructions may comprise logic or algorithm(s) written in any programming language of any generation (e.g., 1GL,

2GL, 1GL, 4GL, or 5GL) such as, for example, machine language that may be directly executed by the processor, or assembly language, object-oriented programming (OOP), scripting languages, microcode, etc., that may be compiled or assembled into machine readable and executable instructions and stored on the one or more memory modules 106. Alternatively, the machine readable and executable instructions may be written in a hardware description language (HDL), such as logic implemented via either a field-programmable gate array (FPGA) configuration or an application-specific integrated circuit (ASIC), or their equivalents. Accordingly, the methods described herein may be implemented in any conventional computer programming language, as pre-programmed hardware elements, or as a combination of hardware and software components. The memory modules 106 are discussed in more detail below in connection with FIG. 2.

[0035] Still referring to FIG. 1, the system 100 includes a data storage component 108. The data storage component 108 may store data used by the various components of the system 100. In particular, the data storage component 108 may store a threshold value of the HSP, a threshold value of the ACR, a threshold value of the arithmetic distance, a threshold value of the geometric distance, parameters for calculating at least one of the HSP, the ACR, the arithmetic distance, and the geometric distance, or combinations thereof.

[0036] Still referring to FIG. 1, the system 100 comprises network interface hardware 110 for communicatively coupling the system 100 to other devices. In embodiments, the network interface hardware 110 may be send data to and/or receive data from other computing devices that may be used by the various components of the system 100. The network interface hardware 110 can be communicatively coupled to the communication path 104 and can be any device capable of transmitting and/or receiving data via a network. Accordingly, the network interface hardware 110 can include a communication transceiver for sending and/or receiving any wired or wireless communication. For example, the network interface hardware 110 may include an antenna, a modem, LAN port, Wi-Fi card, WiMax card, mobile communications hardware, near-field communication hardware, satellite communication hardware and/or any wired or wireless hardware for communicating with other networks and/or devices.

[0037] FIG. 2 schematically depicts a plurality of memory modules of the system of FIG. 1, according to one or more embodiments shown and described herein.

[0038] Referring to FIG. 2, the one or more memory modules 106 may include an adhesive or coating composition data reception module 202, a first calculation module 204, a first comparison module 206, an polyolefin polymer data reception module 212, a second calculation module 214, an arithmetic distance calculation module 222, a comparison of the arithmetic distance module 224, a geometric distance calculation module 232, a comparison of the geometric distance module 234, an ACR of the adhesive or coating composition calculation module 242, a comparison of ACR module 244, and a predict module 252.

[0039] The adhesive or coating composition data reception module 202 may receive data of a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both. In some embodiments, a user may provide the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both. The data of the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both may be transmitted to the adhesive or coating composition data reception module 202.

[0040] The adhesive or coating composition may include, but not limited to, polyurethane, acrylics, poly (ethylene-vinyl acetate), polystyrene, natural rubber, synthetic rubber, polyesters, polycarbonates, polyolefins, or combinations thereof.

[0041] The adhesive or coating composition may optionally include one or more ingredients such as fillers, dyes and pigments, tackifiers, plasticizers, rheology modifiers, polymers (including, for example, thermoplastic resins other than those discussed herein above), dehydrating agents (including, for example, silanes), benzoyl chloride, other polyols (including, for example, fatty polyols), ultraviolet indicators, solvents, etc.

[0042] In some embodiments, the adhesive or coating composition may be included in an external coating layer in a laminate structure. The adhesive or coating layer may improve interlayer adhesion between functional layers and prevent delamination of the layers. In some embodiments, the adhesive or coating composition may be included in an external layer, such as a coating layer, of the laminate structure. The external layer may provide mechanical support and protection of the other layers of the laminate structure. Furthermore, the external layer film may be particularly well suited for protection, inscribing, or printing.

[0043] In some embodiments, in response to receiving the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both, the first calculation module 204 may list ingredients of the adhesive or coating composition. The first calculation module 204 may remove solvents from the list of ingredients of the adhesive or coating composition. The first calculation module 204 may remove any ingredients having a concentration of less than or equal to 1 weight percent (wt.%) based on a total amount of the adhesive or coating composition. ADCOTE® 102E/Coreactant CT (the “/” means “with”), a solvent-based polyurethane adhesive system, is used to illustrate the calculation of HSP of the adhesive or coating composition, the arithmetic distance (R_a), the geometric distance (R_b), and the ACR of the adhesive or coating composition. The values against those of polyolefin polymers are used to define boundaries of mechanic recyclability of the polyurethane adhesive system and the polyolefin polymers. The boundaries are valid for the polyurethane adhesives and coatings. Adhesive or coating compositions based on other chemistries may have different set of values and boundaries. For example, in response to receiving the trading name of the adhesive or coating composition, such as “ADCOTE® 102E/Coreactant CT,” the first calculation module 204 may list ingredients of the adhesive or coating compositions without solvents and ingredients having a concentration of less than or equal to 1 wt.% based on a total amount of the adhesive or coating composition, such as isophthalic acid, terephthalic acid, azelaic acid, ethylene glycol, and ISONATE® 125m pure MDI.

[0044] The first calculation module 204 may determine a weight, a molecular weight, the number of moles, and a molecular formula of each ingredient on the list of the adhesive or coating composition. For example, in response to listing ingredients of “ADCOTE® 102E/ Coreactant CT” at a mix weight ratio of 100:5.2, the first calculation module 204 may determine a weight, a molecular weight, the number of moles, and a molecular formula of each ingredient as shown in Table 1.

Table 1

	Formula	Weight (grams)	Molecular weight (MW)	Moles= Weight/ MW

Isophthalic acid	$(\text{C}_6\text{H}_4)(\text{COOH})_2$	4.73	166.13	0.028
Terephthalic acid	$(\text{C}_6\text{H}_4)(\text{COOH})_2$	9.20	166.13	0.055
Azelaic acid	$(\text{CH}_2)_7(\text{COOH})_2$	15.95	188.22	0.085
Ethylene glycol	$(\text{CH}_2)_2(\text{HO})_2$	13.51	26.07	0.52
ISONATE [®] 125m pure MDI	$(\text{CH}_2)(\text{C}_6\text{H}_4)(\text{NCO})_2$	3.15	250.25	0.0126
Total		46.54		0.7006

[0045] The first calculation module 204 may calculate values of group contributions of each ingredient based on the weight, the molecular weight, the number of moles, and the molecular formula of each ingredient. In embodiments, the group contributions may include molar attraction function (F_t), polar component (F_p), molar volume (V), Lydersen correction for solvents (Δ_T), and Lydersen correction for polymers ($\Delta_T^{(p)}$), or combinations thereof. All numerical values are in FIG. 4.

[0046] For example, in response to listing ingredients of “ADCOTE[®] 102E/Coreactant CT,” the first calculation module 204 may calculate values of group contributions of isophthalic acid. Isophthalic acid may have 0.028 moles of disubstituted benzene (4 aromatic C-H and 2 aromatic carbon) and 0.056 moles of carboxylic acid. The molar attraction function (F_t) and the polar component (F_p) of isophthalic acid may be calculated as follows:

[0047]
$$F_t = 0.028 \times (4 \times 241 + 2 \times 201) + 0.056 \times 565 = 69.89$$

[0048]
$$F_p = 0.028 \times (4 \times 62.5 + 2 \times 65) + 0.056 \times 415 = 33.88$$

[0049] The first calculation module 204 may calculate molar volume (V), Lydersen correction for solvents (Δ_T), and Lydersen correction for polymers ($\Delta_T^{(p)}$) of isophthalic acid. The first calculation module 204 may calculate values of group contributions including molar attraction function (F_t), polar component (F_p), molar volume (V), Lydersen correction for solvents (Δ_T), and

Lydersen correction for polymers($\Delta_T^{(p)}$), or combinations thereof, of each of terephthalic acid, azelaic acid, ethylene glycol, and ISONATE[®] 125m pure MDI .

[0050] The first calculation module 204 may further calculate the HSP, polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition based on the name of the adhesive or coating composition or polyolefins, the trading name of the adhesive or coating composition or polyolefins, or both. In some embodiments, the first calculation module 204 may calculate the HSP, polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition or polyolefins using a table in FIG. 4. FIG. 4 shows values of increments in Hoy's system for the molar attraction function. Each of the HSP, polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) may be calculated using the following Equations 3-6 respectively. All equations required by the calculation can be obtained from Chapter 7, of D.W. van Krevelen's book "Properties of Polymers" 4th ed., Completely Revised Edition, available from Elsevier: Amsterdam, 2009, ebook ISBN: 9780080915104.

$$\text{[0051]} \quad \delta_p = \sqrt{\frac{\delta_t * F_{p,i}}{777 * \Delta_{T,j}^{(p)}}} \quad - \quad \text{Equation 3}$$

$$\text{[0052]} \quad \delta_h = \left[\delta_t \sqrt{1 - \frac{1}{\alpha}} \right] \quad - \quad \text{Equation 4}$$

[0053] Where $\alpha = 1.433045685$ for polymers and 2.40 for small molecules. Small molecules may refer to molecules with molecular weight equal or less than 800 Daltons and constant and well-defined molecular formula (i.e., the ratios of the number of moles of each element in the molecule to the number of moles of the molecule are non-negative integers). Polymers may refer to macromolecules with n repeated monomer units, where n is a positive integer and $n \geq 10$.

$$\text{[0054]} \quad \delta_d = \sqrt{\delta_t^2 - \delta_p^2 - \delta_h^2} \quad - \quad \text{Equation 5}$$

$$\text{[0055]} \quad \delta_t = \frac{F_{t,j} + 554 * \Delta_{T,j}^{(p)}}{V_i} \quad - \quad \text{Equation 6}$$

[0056] The first comparison module 206 may compare the HSP of the adhesive or coating composition to a threshold value of the HSP. The threshold value of the HSP may be stored in the first comparison module 206 prior to activating the system 100 (shown in FIG. 1) of predicting the compatibility of the adhesive or coating composition and the polyolefin polymer. In some embodiments, the threshold value of the HSP of the polyurethane adhesive or coating composition may be 22.7. The term “polyurethane adhesive or coating composition” may refer to an adhesive or coating composition comprises polyurethane. In some embodiments, polyurethane adhesive or coating composition may consist of or consist essentially of polyurethane. For adhesive or coating composition based on chemistries other than polyurethanes, the HSP value may be different than 22.7.

[0057] The polyolefin polymer data reception module 212 may receive data of a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both. In some embodiments, a user may provide the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both. The data of the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both may be transmitted to the polyolefin polymer data reception module 212.

[0058] The polyolefin polymer may include polyethylene, polypropylene (PP), oriented PP (OPP), biaxially oriented PP (BOPP), or combinations thereof. The non-polyolefin portion of the film may be comprised of polymers such as poly(vinyl alcohol) (EVOH) or polyamides (e.g., nylon), functionalized tie layer polymers and compatibilizers as described in U. S. Patent No. 10,300,686.

[0059] In some embodiments, similar to the adhesive or coating composition, in response to receiving the name of the polyolefin polymer composition, the trading name of the polyolefin polymer composition, or both, the second calculation module 214 may list ingredients of the polyolefin polymer composition. The second calculation module 214 may remove solvents from the list of ingredients of the polyolefin polymer composition. The second calculation module 214 may remove any ingredients having a concentration of less than or equal to 1 wt.% based on a total amount of the polyolefin polymer composition.

[0060] The second calculation module 214 may determine a weight, a molecular weight, the number of moles, and a molecular formula of each ingredient on the list of the polyolefin polymer composition.

[0061] The second calculation module 214 may calculate values of group contributions including molar attraction function (F_i), polar component (F_p), molar volume (V), Lydersen correction for solvents (Δ_T), and Lydersen correction for polymers ($\Delta_T^{(p)}$), or combinations thereof, of each ingredient on the list. All numerical values are in FIG. 4.

[0062] The arithmetic distance calculation module 222 may calculate an arithmetic distance (R_a) between the adhesive or coating composition and the polyolefin polymer. In some embodiments, the arithmetic distance calculation module 222 may calculate an arithmetic distance (R_a) between the adhesive or coating composition and the polyolefin polymer using the following Equation 1. The equations required by the calculation can be obtained from Chapter 7, of D.W. van Krevelen's book "Properties of Polymers" 4th ed., Completely Revised Edition, available from Elsevier: Amsterdam, 2009, ebook ISBN: 9780080915104.

$$\mathbf{[0063]} \quad R_a = \sqrt{4(\delta_p - \delta_{p0})^2 + (\delta_h - \delta_{h0})^2 + (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 1}$$

[0064] A R_a calculation of "ADCOTE[®] 102E/ Coreactant CT" at a mix weight ratio of 100:5.2 with polyethylene polymers as the benchmark is illustrated as following. For polyethylene that is composed of infinite number of ethylene groups (CH_2), $\delta_{p0} = 0$, $\delta_{h0} = 10.67$, $\delta_{d0} = 14.51$, as calculated by the model. For "ADCOTE[®] 102E/Coreactant CT" at a mix weight ratio of 100:5.2, $\delta_p = 17.09$, $\delta_h = 16.70$, $\delta_d = 14.94$. Plug in all the value into Equation 1, R_a is 18.14, the arithmetic distance parameter that can be used to describe the mechanical recyclability or compatibility of the adhesive or coating compositions and polyolefin polymers. The smaller the distance, the higher the chemical similarity of the adhesive or coating compositions to polyolefin polymers, such as PE, the more likely the adhesive or coating compositions to be mechanically recyclable in polyolefin polymers.

[0065] The comparison of the arithmetic distance module 224 may compare the arithmetic distance (R_a) to a threshold value of the arithmetic distance. The comparison of the arithmetic distance module 224 may compare the arithmetic distance (R_a) to a threshold value of the

arithmetic distance of a polymer of comparison, such as polyolefin polymers. The threshold value of the arithmetic distance (R_a) may be stored in the comparison of the arithmetic distance module 224 prior to activating the system 100 (shown in FIG. 1) of predicting the compatibility of the adhesive or coating composition and the polyolefin polymer. In some embodiments, the threshold value of the geometric distance (R_a) of polyurethane adhesive or coating composition for recyclability in polyolefin polymers may be less than or equal to 12. For adhesive or coating composition based on chemistries other than polyurethanes, the R_a value may be different than 12.

[0066] The geometric distance calculation module 232 may calculate a geometric distance (R_b) between the adhesive or coating composition and the polyolefin polymer. The geometric distance (R_b) is different from the arithmetic distance (R_a) in that mathematically it is a geometric average. In some embodiments, the arithmetic distance calculation module 222 may calculate a geometric distance (R_b) between the adhesive or coating composition and the polyolefin polymer using the following Equation 2.

$$\text{[0067]} \quad R_b = \sqrt[6]{(\delta_p - \delta_{p0})^2 (\delta_h - \delta_{h0})^2 (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 2}$$

[0068] A R_b calculation of “ADCOTE® 102E/ Coreactant CT” at a mix weight ratio of 100:5.2 with polyethylene polymers as the benchmark is illustrated as following. For polyethylene, $\delta_{p0} = 0$, $\delta_{h0} = 10.67$, $\delta_{d0} = 14.51$, as calculated by the model. For “ADCOTE® 102E/ Coreactant CT” at a mix weight ratio of 100:5.2, $\delta_p = 17.09$, $\delta_h = 16.70$, $\delta_d = 14.94$. Plug in all the value into Equation 2, R_b of 10.15 is obtained, the geometric distance parameter that can be used to describe the mechanical recyclability or compatibility of the adhesive or coating composition and polyolefin polymers. The smaller the distance, the higher the chemical similarity of the adhesive or coating compositions to polyolefin polymers, such as PE, the more likely the adhesive or coating compositions to be mechanically recyclable in polyolefin polymers.

[0069] The comparison of the geometric distance module 234 may compare the geometric distance (R_b) to a threshold value of the geometric distance. The comparison of the geometric distance module 234 may compare the geometric distance (R_b) of the adhesive or coating composition to a threshold value of the geometric distance of a polymer of comparison, such as

polyolefin polymers. The threshold value of the geometric distance (R_b) may be stored in the comparison of the geometric distance module 234 prior to activating the system 100 (shown in FIG. 1) of predicting the compatibility of the polyurethane adhesive or coating composition and the polyolefin polymer. In some embodiments, the threshold value of the geometric distance (R_b) may be less than or equal to 6. For adhesive or coating composition based on chemistries other than polyurethanes, the R_b value may be different than 6.

[0070] The ACR of the adhesive or coating composition calculation module 242 may calculate an ACR (ACR) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both. Aliphatic carbon may refer to carbon atoms in methyl (CH_3), methylene (CH_2), methine (CH), quaternary carbon (C), and alkenic carbon ($\text{C}=\text{C}$). The term “ACR (ACR) of the adhesive or coating composition” may refer to the ratio of the number of moles of aliphatic carbon in the adhesive or coating composition to the number of moles of total substances in the adhesive or coating composition. The higher the ACR, the more chemically similar of the adhesive or coating composition to hydrocarbons, the more likely the composition to be mechanically recyclable in polyolefin polymers. For instance, for 0.034 mole of 2-phenylethanol ($\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{OH}$), there is 0.068 mole of aliphatic carbon (two CH_2 functional groups in one molecule). The ACR of the compound is therefore $0.068/0.034 = 2$. The same calculation is applied to “ADCOTE® 102E/ Coreactant CT” at a mix weight ratio of 100:5.2 and yields an ACR of 2.48.

[0071] The comparison of ACR module 244 may compare the ACR of the adhesive or coating composition to a threshold value of the ACR. The comparison of ACR module 244 may compare the ACR of the adhesive or coating composition to an ACR threshold value of a polymer of comparison, such as polyolefin polymers. The threshold value of the ACR may be stored in the comparison of ACR module 244 prior to activating the system 100 (shown in FIG. 1) of predicting the compatibility of the adhesive or coating composition and the polyolefin polymer. In some embodiments, the threshold value of the ACR of polyurethane adhesive or coating compositions for recyclability in polyolefin polymer may be 6.9. For adhesive or coating composition based on chemistries other than polyurethanes, the ACR value may be different than 6.9.

[0072] The predict module 252 may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.

[0073] The adhesive or coating composition may be experimentally determined as being compatible or recyclable with the polyolefin polymer composition when a laminated or coated structure comprising the adhesive or coating composition satisfies the following requirements. When the adhesive composition is included in the laminated film, the laminate structure may be PE Film A//adhesive //PE Film B, which means that the laminate structure consisting of PE film A, adhesive, and PE film B and the adhesive layer is disposed between two PE films A and B. Film A and B may be the same or different. The laminate is referred to as laminate I. In embodiments, PE films A and B may be granulated together and dried to give pellet C. Laminate I may be granulated and dried to give pellet D. Pellets C and pellet D may be mixed at a 1:1 weight ratio to afford a blended pellet E. In embodiments, Pellet C and E may be blown separately into 50-micron monolayer films. The resultant films, referred to as film C and film E, respectively, may be subjected to the following ASTM tests shown in Table 2, with the former being the control and the basis for comparison.

[0074] When the coating composition is included in the external layer, the coated film structure is coating//PE Film F, which means that the coated film structure consisting of the coating layer and PE film F and the coating layer is disposed on PE film F. The coated film is referred to as laminate II. In embodiments, PE films F may be granulated and dried to give pellet G. Laminate II may be granulated and dried to give pellet H. Pellets G and pellet H may be mixed at a 1:1 weight ratio to afford a blended pellet J. In embodiments, Pellet G and J may be blown separately into 50-micron monolayer films. The resultant films, , referred to as film G and film J, respectively, may be subjected to the following ASTM tests shown in Table 2, with the former being the control and the basis for comparison.

Table 2: ASTM tests for determining the compatibility of the adhesive or coating composition and the polyolefin polymer composition

Tests	ASTM	Units
Tear strength (TD, MD)	ASTM D1922	Psi
Tensile strength (TD, MD)	ASTM D882	Psi
Elongation at yield (TD, MD)	ASTM D882	%
Dart impact	ASTM D1709 A	Wf

[0075] In response to comparing the test results of film E and film C, the adhesive composition in laminate I may be defined that it is compatible or recyclable with the polyolefin polymer composition in PE films A and B, when all test values, such as tear strength, tensile strength, elongation at yield, and dart impact, of film E do not drop more than 33% against those of film C.

[0076] In response to comparing the test results of film G and film J, the coating composition in laminate II may be defined that it is compatible or recyclable with the polyolefin polymer composition in PE films F, when all test values, such as tear strength, tensile strength, elongation at yield, and dart impact, of film J do not drop more than 33% against those of film G.

[0077] In embodiments, the predict module 252 may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of the HSP of the adhesive or coating composition to the threshold value of the HSP and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR. In some embodiments, the predict module 252 may determine that the adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the HSP of the polyurethane adhesive or coating composition is lower than or equal to 22.7 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9. For adhesive or coating composition based on chemistries other than polyurethanes, the HSP and ACR values may be different.

[0078] In embodiments, the predict module 252 may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of the arithmetic distance (R_a) to the threshold value of the arithmetic distance and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR. In some embodiments, the predict module 252 may determine that the polyurethane adhesive or coating

composition is more likely than not to be compatible with the polyolefin polymer when the arithmetic distance (R_a) is lower than or equal to 12 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9. For adhesive or coating composition based on chemistries other than polyurethanes, the ACR and R_a values may be different.

[0079] In embodiments, the predict module 252 may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of the geometric distance (R_b) to the threshold value of the geometric distance and a result of comparison of the ACR of the adhesive or coating composition to the threshold value of the ACR. In some embodiments, the predict module 252 may determine that the adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the geometric distance (R_b) is lower than or equal to 6 and the ACR of the adhesive or coating composition is greater than or equal to 6.9. For adhesive or coating composition based on chemistries other than polyurethanes, the ACR and R_b values may be different.

[0080] FIG. 3 depicts a flowchart for a method 300 of predicting the compatibility of an adhesive or coating composition and polyolefin polymer that may be performed by the system 100 depicted in FIG. 1.

[0081] Referring to FIGS. 1-3, in step S310, the controller, such as the adhesive or coating composition data reception module 202, may receive a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both. In some embodiments, a user may provide the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both.

[0082] In some embodiments, in response to receiving the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both, the controller may list ingredients of the adhesive or coating composition. The controller may determine a weight, a molecular weight, a number of moles, and a molecular formula of each ingredient on the list. The controller may calculate values of group contributions of each ingredient based on the weight, the molecular weight, the number of moles, and the molecular formula of each ingredient. In embodiments, the group contributions may include molar attraction function (F_t), polar component (F_p), molar volume (V), Lydersen correction for solvents (Δ_T), and Lydersen correction for

polymers($\Delta_T^{(p)}$), or combinations thereof, as described in Chapter 7, D.W. van Krevelen's book "Properties of Polymers" 4th ed., Completely Revised Edition, available from Elsevier: Amsterdam, 2009, ebook ISBN: 9780080915104.

[0083] Still referring to FIGS. 1-3, in step S320, the controller, such as the polyolefin polymer data reception module 212, may receive a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both. In some embodiments, a user may provide the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both.

[0084] In some embodiments, similar to the adhesive or coating composition, in response to receiving the name of the polyolefin polymer composition, the trading name of the polyolefin polymer composition, or both, the controller may list ingredients of the polyolefin polymer composition. The controller may determine a weight, a molecular weight, a number of moles, and a molecular formula of each ingredient on the list. The controller may calculate values of group contributions including molar attraction function (F_i), polar component (F_p), molar volume (V), Lydersen correction for solvents (Δ_T), and Lydersen correction for polymers($\Delta_T^{(p)}$), or combinations thereof, of each ingredient on the list.

[0085] Still referring to FIGS. 1-3, in step S330, the controller, such as the first calculation module 204, may calculate the HSP, polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both.

[0086] Still referring to FIG. 3, in step S340, the controller, such as the second calculation module 214, may calculate the HSP, polar interaction subcomponent (δ_{p0}), hydrogen bonding subcomponent (δ_{h0}), and dispersion forces subcomponent (δ_{d0}) of the polyolefin polymer based on the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both.

[0087] Still referring to FIGS. 1-3, in step S350, the controller, such as the arithmetic distance calculation module 222, may calculate an arithmetic distance (R_a) between the adhesive or coating composition and the polyolefin polymer. In some embodiments, the controller, such as the arithmetic distance calculation module 222, may calculate an arithmetic distance (R_a) between the adhesive or coating composition and the polyolefin polymer using the following Equation 1.

$$[0088] \quad R_a = \sqrt{4(\delta_p - \delta_{p0})^2 + (\delta_h - \delta_{h0})^2 + (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 1}$$

[0089] Still referring to FIGS. 1-3, in step S360, the controller, such as the geometric distance calculation module 232, may calculate a geometric distance (R_b) between the adhesive or coating composition and the polyolefin polymer. In some embodiments, the controller, such as the geometric distance calculation module 232, may calculate a geometric distance (R_b) between the adhesive or coating composition and the polyolefin polymer using the following Equation 2.

$$[0090] \quad R_b = \sqrt[6]{(\delta_p - \delta_{p0})^2 (\delta_h - \delta_{h0})^2 (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 2}$$

[0091] Still referring to FIGS. 1-3, in step S370, the controller, such as the ACR of the adhesive or coating composition calculation module 242, may calculate an ACR of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both.

[0092] Still referring to FIGS. 1-3, in step S380, the controller may compare at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value. The controller may compare at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to HSP of the polyolefin polymer,

[0093] In embodiments, the controller, such as the first comparison module 206, may compare the HSP of the adhesive or coating composition to a threshold value of the HSP. In some embodiments, the threshold value of the HSP of the polyurethane adhesive or coating composition may be 22.7.

[0094] In embodiments, the controller, such as the comparison of the arithmetic distance module 224, may compare the arithmetic distance (R_a) to a threshold value of the arithmetic distance of a polymer of comparison, such as polyolefin polymers. In some embodiments, the threshold value of the arithmetic distance (R_a) of the polyurethane adhesive or coating composition may be 12.

[0095] In embodiments, the controller, such as the comparison of the geometric distance module 234, may compare the geometric distance (R_b) of the adhesive or coating composition to a threshold value of the geometric distance of a polymer of comparison, such as polyolefin polymers. In some embodiments, the threshold value of the geometric distance (R_b) of the polyurethane adhesive or coating composition may be 6.

[0096] Still referring to FIGS. 1-3, in step S390, the controller, such as the comparison of ACR module 244, may compare the ACR of the adhesive or coating composition to an ACR threshold value of a polymer of comparison, such as polyolefin polymers. In some embodiments, the threshold value of the ACR of the polyurethane adhesive or coating composition may be 6.9.

[0097] Still referring to FIGS. 1-3, in step S400, the controller, such as the predict module 252, may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.

[0098] In embodiments, the controller, such as the predict module 252, may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of the HSP of the adhesive or coating composition to the threshold value of the HSP and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR. In some embodiments, the controller may determine that the adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the HSP of the polyurethane adhesive or coating composition is lower than or equal to 22.7 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.

[0099] In embodiments, the controller, such as the predict module 252, may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of the arithmetic distance (R_a) to the threshold value of the arithmetic distance and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR. In some embodiments, the controller may determine that the polyurethane adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when

the arithmetic distance (R_a) is lower than or equal to 12 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.

[00100] In embodiments, the controller, such as the predict module 252, may predict the compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of the geometric distance (R_b) to the threshold value of the geometric distance and a result of comparison of the ACR of the adhesive or coating composition to the threshold value of the ACR. In some embodiments, the controller may determine that the polyurethane adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the geometric distance (R_b) is lower than or equal to 6 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.

[00101] In some embodiments, after predicting the compatibility of the adhesive or coating composition and the polyolefin polymer, the adhesive or coating composition may be mixed with the polyolefin polymer to recycle the adhesive or coating composition. For example, after mixing the adhesive or coating composition with the polyolefin polymer to produce a mixture, the mixture may be reused in a laminate structure. In embodiments, after mixing the adhesive or coating composition with the polyolefin polymer to produce a mixture, the mixture may be reused in coated film structure.

[00102] It is noted that one or more of the following claims utilize the term “wherein,” “where” or “in which” as a transitional phrase. For the purposes of defining the present technology, it is noted that this term is introduced in the claims as an open-ended transitional phrase that is used to introduce a recitation of a series of characteristics of the structure and should be interpreted in like manner as the more commonly used open-ended preamble term “comprising.” For the purposes of defining the present technology, the transitional phrase “consisting of” may be introduced in the claims as a closed preamble term limiting the scope of the claims to the recited components or steps and any naturally occurring impurities. For the purposes of defining the present technology, the transitional phrase “consisting essentially of” may be introduced in the claims to limit the scope of one or more claims to the recited elements, components, materials, or method steps as well as any non-recited elements, components, materials, or method steps that do not materially affect the novel characteristics of the claimed subject matter. The transitional phrases “consisting of” and “consisting essentially of” may be interpreted to be subsets of the open-ended transitional

phrases, such as “comprising” and “including,” such that any use of an open-ended phrase to introduce a recitation of a series of elements, components, materials, or steps should be interpreted to also disclose recitation of the series of elements, components, materials, or steps using the closed terms “consisting of” and “consisting essentially of.” For example, the recitation of a composition “comprising” components A, B, and C should be interpreted as also disclosing a composition “consisting of” components A, B, and C as well as a composition “consisting essentially of” components A, B, and C. Any quantitative value expressed in the present application may be considered to include open-ended embodiments consistent with the transitional phrases “comprising” or “including” as well as closed or partially closed embodiments consistent with the transitional phrases “consisting of” and “consisting essentially of.”

[00103] As used in the Specification and appended Claims, the singular forms “a,” “an,” and “the” include plural references unless the context clearly indicates otherwise. The verb “comprises” and its conjugated forms should be interpreted as referring to elements, components or steps in a non-exclusive manner. The referenced elements, components or steps may be present, utilized or combined with other elements, components or steps not expressly referenced.

[00104] Further, when an amount, concentration, or other value or parameter is given as either a range, preferred range or a list of upper preferable values and lower preferable values, this is to be understood as specifically disclosing all ranges formed from any pair of any upper range limit or preferred value and any lower range limit or preferred value, regardless of whether ranges are separately disclosed. Where a range of numerical values is recited herein, unless otherwise stated, the range is intended to include the endpoints thereof, and all integers and fractions within the range. It is not intended that the scope of the invention be limited to the specific values recited when defining a range. When a component is indicated as present in a range starting from 0, such component is an optional component (i.e., it may or may not be present). When present an optional component may be at least 0.1 weight % of the composition or copolymer.

[00105] When materials, methods, or machinery are described herein with the term “known to those of skill in the art,” “conventional” or a synonymous word or phrase, the term signifies that materials, methods, and machinery that are conventional at the time of filing the present application are encompassed by this description.

[00106] It should be understood that any two quantitative values assigned to a property may constitute a range of that property, and all combinations of ranges formed from all stated quantitative values of a given property are contemplated in this disclosure. The subject matter of the present disclosure has been described in detail and by reference to specific embodiments. It should be understood that any detailed description of a component or feature of one or more embodiments does not necessarily imply that the component or feature is essential to the particular embodiment or to any other embodiment. Further, it should be apparent to those skilled in the art that various modifications and variations can be made to the described embodiments without departing from the spirit and scope of the claimed subject matter.

CLAIMS

1. A system of predicting compatibility of an adhesive or coating composition and polyolefin polymers comprising:

a controller programmed to:

receive a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both;

receive a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both;

calculate Hansen's solubility parameter (HSP; δ_t), polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both;

calculate HSP of the polyolefin polymer (δ_{t0}), polar interaction subcomponent (δ_{p0}), hydrogen bonding subcomponent (δ_{h0}), and dispersion forces subcomponent (δ_{d0}) of the polyolefin polymer based on the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both;

calculate an arithmetic distance parameter (R_a) between the adhesive or coating composition and the polyolefin polymer;

calculate a geometric distance parameter (R_b) between the adhesive or coating composition and the polyolefin polymer;

calculate an aliphatic carbon ratio (ACR) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both;

compare at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value;

compare the ACR of the adhesive or coating composition to a threshold value of the ACR; and

predict a compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the

threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.

2. The system of claim 1, wherein the controller is further programmed to:
 - list ingredients of the adhesive or coating composition;
 - determine a weight, a molecular weight, a number of moles, and a molecular formula of each ingredient; and
 - calculate values of group contributions of each ingredient based on the weight, the molecular weight, the number of moles, and the molecular formula of each ingredient.
3. The system of claim 1 or claim 2, wherein the group contributions comprise molar attraction function (Ft), polar component (Fp), molar volume (V), Lydersen correction for solvents (Δ_T), and Lydersen correction for polymers($\Delta_T^{(p)}$), or combinations thereof.
4. The system of any preceding claim, wherein the controller is further programmed to:
 - calculate the arithmetic distance (R_a) between the adhesive or coating composition and the polyolefin polymer using a following Equation 1; and

$$R_a = \sqrt{4(\delta_p - \delta_{p0})^2 + (\delta_h - \delta_{h0})^2 + (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 1}$$

calculate the geometric distance (R_b) between the adhesive or coating composition and the polyolefin polymer using a following Equation 2.

$$R_b = \sqrt[6]{(\delta_p - \delta_{p0})^2 (\delta_h - \delta_{h0})^2 (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 2.}$$

5. The system of any preceding claim, wherein the adhesive or coating composition is a polyurethane adhesive or coating composition, and
 - wherein the controller is further programmed to:
 - compare the HSP of the adhesive or coating composition to a threshold value of the HSP;
 - and
 - determine that the adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the HSP of the polyurethane adhesive or coating composition is lower than or equal to 22.7 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.

6. The system of any preceding claim, wherein the adhesive or coating composition is a polyurethane adhesive or coating composition, and
wherein the controller is further programmed to:
compare the arithmetic distance (R_a) to a threshold value of the arithmetic distance; and
determine that the polyurethane adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the arithmetic distance (R_a) is lower than or equal to 12 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.
7. The system of any preceding claim, wherein the adhesive or coating composition is a polyurethane adhesive or coating composition, and
wherein the controller is further programmed to:
compare the geometric distance (R_b) to a threshold value of the geometric distance; and
determine that the polyurethane adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the geometric distance (R_b) is lower than or equal to 6 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.
8. The system of any preceding claim, wherein the adhesive or coating composition comprises polyurethane, acrylics, poly (ethylene-vinyl acetate), polystyrene, natural rubber, synthetic rubber, polyesters, polycarbonates, polyolefins, or combinations thereof.
9. The system of any preceding claim, wherein the polyolefin polymer comprises polyethylene, polypropylene (PP), oriented PP (OPP), biaxially oriented PP (BOPP), or combinations thereof.
10. A method of predicting compatibility of an adhesive or coating composition and a polyolefin polymer comprising:
receiving a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both;

receiving a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both;

calculating Hansen's solubility parameter (HSP; δ_t), polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both;

calculating HSP of the polyolefin polymer (δ_{t0}), polar interaction subcomponent (δ_{p0}), hydrogen bonding subcomponent (δ_{h0}), and dispersion forces subcomponent (δ_{d0}) of the polyolefin polymer based on the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both;

calculating an arithmetic distance parameter (R_a) between the adhesive or coating composition and the polyolefin polymer;

calculating a geometric distance parameter (R_b) between the adhesive or coating composition and the polyolefin polymer;

calculating an aliphatic carbon ratio (ACR) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both;

comparing at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value;

comparing the ACR of the adhesive or coating composition to a threshold value of the ACR; and

predicting a compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.

11. The method of claim 10, further comprising:

listing ingredients of the adhesive or coating composition;

determining a weight, a molecular weight, a number of moles, and a molecular formula of each ingredient; and

calculating values of group contributions of each ingredient based on the weight, the molecular weight, the number of moles, and the molecular formula of each ingredient.

12. The method of claim 10 or claim 11, wherein the group contributions comprise molar attraction function (Ft), polar component (Fp), molar volume (V), Lydersen correction for solvents (Δ_T), and Lydersen correction for polymers($\Delta_T^{(p)}$), or combinations thereof.

13. The method of any of claims 10-12, further comprising:

calculating the arithmetic distance (R_a) between the adhesive or coating composition and the polyolefin polymer using a following Equation 1; and

$$R_a = \sqrt{4(\delta_p - \delta_{p0})^2 + (\delta_h - \delta_{h0})^2 + (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 1}$$

calculating the geometric distance (R_b) between the adhesive or coating composition and the polyolefin polymer using a following Equation 2.

$$R_b = \sqrt[6]{(\delta_p - \delta_{p0})^2 (\delta_h - \delta_{h0})^2 (\delta_d - \delta_{d0})^2} \quad - \quad \text{Equation 2.}$$

14. The method of any of claims 10-13, wherein the adhesive or coating composition is a polyurethane adhesive or coating composition,

further comprising:

comparing the HSP of the adhesive or coating composition to a threshold value of the HSP;

and

determining that the polyurethane adhesive or coating composition is more likely than not to be compatible with the polyolefin polymers when the HSP of the polyurethane adhesive or coating composition is lower than or equal to 22.7 and the ACR of the adhesive or coating composition is greater than or equal to 6.9.

15. The method of any of claims 10-14, wherein the adhesive or coating composition is a polyurethane adhesive or coating composition,

further comprising:

comparing the arithmetic distance (R_a) to a threshold value of the polyolefin polymers;

and

determining that the polyurethane adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the arithmetic distance (R_a) is lower than or equal to 12 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.

16. The method of any of claims 10-15, wherein the adhesive or coating composition is a polyurethane adhesive or coating composition,

further comprising:

comparing the geometric distance (R_b) to a threshold value of the polyolefin polymers; and

determining that the polyurethane adhesive or coating composition is more likely than not to be compatible with the polyolefin polymer when the geometric distance (R_b) is lower than or equal to 6 and the ACR of the polyurethane adhesive or coating composition is greater than or equal to 6.9.

17. The method of any of claims 10-16, wherein the adhesive or coating composition comprises polyurethane, acrylics, poly (ethylene-vinyl acetate), polystyrene, natural rubber, synthetic rubber, polyesters, polycarbonates, polyolefins, or combinations thereof.

18. The method of any of claims 10-17, wherein the polyolefin polymer comprises polyethylene, polypropylene (PP), oriented PP (OPP), biaxially oriented PP (BOPP), or combinations thereof.

19. A non-transitory computer-readable medium for predicting compatibility of an adhesive or coating composition and polyolefin polymer that, when executed by a controller, cause the controller to:

receive a name of the adhesive or coating composition, a trading name of the adhesive or coating composition, or both;

receive a name of the polyolefin polymer, a trading name of the polyolefin polymer, or both;

calculate Hansen's solubility parameter (HSP; δ_t), polar interaction subcomponent (δ_p), hydrogen bonding subcomponent (δ_h), and dispersion forces subcomponent (δ_d) of the adhesive

or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both;

calculate HSP of the polyolefin polymer (δ_{t0}), polar interaction subcomponent (δ_{p0}), hydrogen bonding subcomponent (δ_{h0}), and dispersion forces subcomponent (δ_{d0}) of the polyolefin polymer based on the name of the polyolefin polymer, the trading name of the polyolefin polymer, or both;

calculate an arithmetic distance parameter (R_a) between the adhesive or coating composition and the polyolefin polymer;

calculate a geometric distance parameter (R_b) between the adhesive or coating composition and the polyolefin polymer;

calculate an aliphatic carbon ratio (ACR) of the adhesive or coating composition based on the name of the adhesive or coating composition, the trading name of the adhesive or coating composition, or both;

compare at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to a threshold value;

compare the ACR of the adhesive or coating composition to a threshold value of the ACR; and

predict a compatibility of the adhesive or coating composition and the polyolefin polymer based on a result of comparison of at least one of the HSP of the adhesive or coating composition, the arithmetic distance (R_a) and the geometric distance (R_b) to the threshold value and a result of comparison of the ACR of the adhesive or coating composition and the threshold value of the ACR.