DATASHEET

PIPELINE PILOT POLYMER PROPERTIES (SYNTHIA)

The Pipeline Pilot Polymer Properties (Synthia) collection provides a method for fast estimation of properties of bulk amorphous homopolymers and random copolymers based on repeat unit information, molecular weight and temperature. The collection contains published models from J.Bicerano's Prediction of Polymer Properties (Marcel Dekker, NY, 2002.) as well as extensible models for proprietary compounds or focused training sets.

WITH THE POLYMER PROPERTIES COLLECTION YOU CAN:

- Predict mechanical, transport, thermophysical, and many other properties of polymers, including interfacial tensions and effects of cross-linking.
- Create web applications that make polymer property prediction available on any networked machine.
- Tune the accuracy of the prediction by including supplemental experimental data or by creating statistical models for focused chemistries.

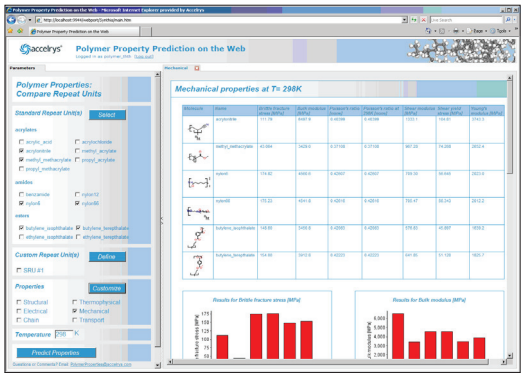

Figure 1: *Pipeline Pilot Polymer Properties (Synthia) can easily be deployed as a web application. In this web interface all you have to do is to sketch or load the monomer repeat units representing your polymer and select the properties you wish to predict.*

PUBLISHED MODELS:

The collection includes components for published models from J.Bicerano's book Prediction of Polymer Properties (Marcel Dekker, NY, 2002.).

Thermophysical Properties

- Glass transition temperature Tg
- Temperature of half decomposition
- Change in molar heat capacity at Tg
- Coefficient of volumetric thermal expansion
- Cohesive energy
- Cp of liquid
- Cp of solid
- Density
- Molar volume
- Solubility parameter
- Surface tension
- Thermal conductivity
- van der Waals volume

Electrical, Optical, Magnetic Properties

- Diamagnetic susceptibility
- Dielectric constant
- Molar refraction
- Refractive index
- Volume resistivity

Mechanical Properties

- Brittle fracture stress
- Bulk modulus
- Poisson's ratio
- Shear modulus
- Shear yield stress
- Young's modulus

Transport Properties

- Activation energy for viscous flow
- Permeability gases (CO2, N2, O2)
- Zero shear viscosity

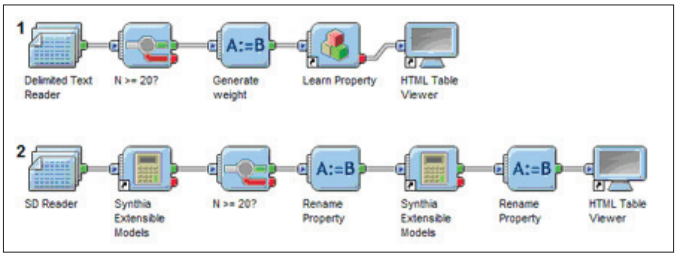

Figure. 2: *Easily replace standard correlations with custom correlations.*

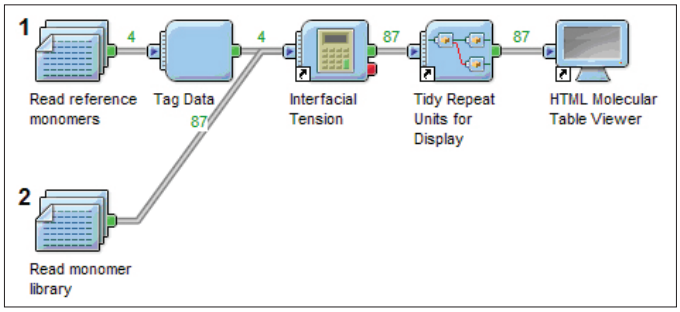

Figure 3: *Prediction of interfacial tension. The data pipeline reads reference monomers together with a library of monomers to run the prediction against.*

EXTENSIBLE MODELS

The extensible models give users access to advanced features that allows tuning the accuracy of the prediction based on supplemental experimental data or research efforts leveraging focused types of chemistry. For example:

- Replace or augment the original experimental data with experimental results from proprietary compounds.
- Recreate the statistical correlations with a focused set of polymer structures that represents a specific chemistry of interest.

Figure 2 shows how this works. The first pipeline reads the data and feeds it into a so-called learner component that generates the custom equation for a focused data set. The second pipeline calculates properties based on standard and custom correlations and compares the results.

INTERFACIAL TENSION

The interfacial tension component calculates the interfacial tension between two polymers. This property depends on the surface tension and the refractive index of each of the polymers.

Larn more about Pipeline Pilot, go to
accelrys.com/pipeline-pilot