

Autodesk® Moldflow® Insight 2012

AMI Materials Properties

Autodesk®

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Thermoplastic material characteristics

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The important material characteristics to consider when selecting a thermoplastic material grade are described.

Crystallinity

The crystallinity of a material identifies the state of the polymer at processing temperatures, and can range from amorphous to crystalline states. Amorphous polymers are devoid of any stratification and retain this state at ambient conditions. Crystalline polymers have an ordered arrangement of plastic molecules, enabling the molecules to fit closer together.

The extent of crystallinity is a function of temperature and time. Rapid cooling rates are associated with lower levels of crystalline content and vice versa. In injected molded parts, thick regions cool slowly relative to thinner regions, and therefore have a higher crystalline content and volumetric contraction.

Mold and melt temperature

The mold temperature is the temperature of the surface of the mold that comes in contact with the polymer. Mold temperature affects the cooling rate of the plastic, and it cannot be higher than the ejection temperature for a particular material.

The temperature of the molten plastic is the melt temperature. Increasing the melt temperature reduces the viscosity of a material. Additionally, a hotter material will decrease the frozen layer thickness. Decreasing the frozen layer reduces shear stress because flow constriction is less. This results in less material orientation during flow.

Thermal properties

The **specific heat (Cp)** of a material is the amount of heat required to raise the temperature of a unit mass of material by one degree Celsius. Essentially, it is a measure of the ability of a material to convert heat input to an actual temperature increase which is measured at atmospheric pressure and a range of temperatures up to the maximum processing temperature of the material.

The **Thermal Properties** tab of the **Thermoplastic material** dialog shows the specific heat data in tabular format, as follows:

- Each row of the table shows the specific heat data at a given temperature.
- **T** is the test temperature, and the unit of measure is **C**, Celsius.
- **Cp** is the specific heat at the given temperature. The unit of measure is **J/kg-C**, joules per kilogram Celsius.

- The **Heating/cooling rate** is the rate at which the material was heated or cooled when tested. Typically it is cooled and this is represented by a negative value, usually -0.3333. The unit of measure is **C/s**, the temperature change in degrees Celsius per second.

The **thermal conductivity (k)** of a material is the rate of heat transfer by conduction per unit length per degrees Celsius. Thermal conductivity is a measure of the rate at which a material can dissipate heat. This rate is measured under pressure and at a range of temperatures. The unit of measure is **W/m-C**, watts per meter Celsius.

The **Thermal Properties** tab of the **Thermoplastic material** dialog also shows the thermal conductivity data of the material in tabular format, as follows:

- Each row of the table shows the thermal conductivity data at a given temperature.
- **T** is the test temperature. The unit of measure is **C**, Celsius.
- **k** is the thermal conductivity at the given temperature. The unit of measure is **W/m-C**, watts per meter Celsius.
- The **Heating/cooling rate** is the rate at which the material was heated or cooled when tested. Typically this value is zero. The unit of measure is **C/s**, the temperature change in degrees Celsius per second.

Viscosity

The viscosity of a material is a measure of its ability to flow under an applied pressure. Polymer viscosity is dependent on temperature and shear rate. In general, as the temperature and shear rate of the polymer increases, the viscosity decreases, indicating a greater ability to flow under an applied pressure. The material database provides a viscosity index for materials in the **Rheological Properties** tab to enable you to compare ease of flow. The viscosity index assumes a shear rate of 1000 reciprocal seconds and shows the viscosity at the temperature that is specified in parentheses.

pvT data

Autodesk provides pvT models to account for material compressibility during a Fill or Fill+Pack analysis. A pvT model is a mathematical model using different coefficients for different materials, providing a curve of pressure against volume against temperature.

An analysis based on pvT data is more accurate but the iterations for temperature and pressure at each point in the model increase computational intensity. However, this suits complex models that have sudden and large changes in thickness.

Shrinkage

As plastics cool, volumetric shrinkage causes their dimensions to change significantly. The main factors that affect shrinkage are cool orientation, crystallinity, and heat concentrations.

Optical properties

Transparent plastic under stress can exhibit stress birefringence, where the speed of light through the part depends on the polarization of the light. Birefringence can result in double images and the transmission of unevenly-polarized light. Some materials are more prone to stress birefringence than others.

Composite materials

Composite materials contain fillers that are added to polymers for injection molding. Fillers increase the strength of the polymer and help ensure that good quality parts are produced. Most commercial composites contain 10 to 50 percent of fibers by weight. These are regarded as being concentrated suspensions where both mechanical and hydrodynamic fiber interactions apply. In composites that are injection molded, the fiber orientation distributions show a layered nature and are affected by the filling speed, the processing conditions, and the behavior of the material.

Environmental Impact

Different materials can have different environmental impacts. The polymer family to which a material belongs to can provide an initial indication of processibility and potential recyclability of a material. The Resin Identification code of a selected material is provided to help identify the polymer family.

Minimizing the energy consumption of the injection molding process provides both cost and environmental benefits. Based on the predicted Injection Pressure and Cooling Time for a suite of part geometries and thickness, an Energy usage indicator has been developed for each material in the thermoplastic material database. This provides an indication of the relative energy requirements to produce a part from any given material.

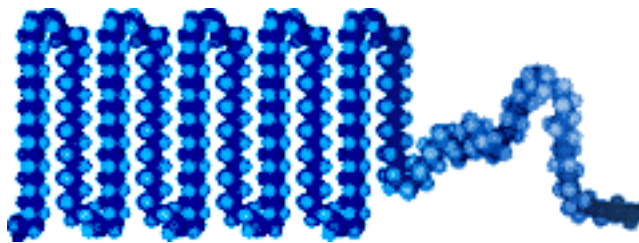
The Resin identification code and the Energy usage indicator are both stored in the thermoplastic material data.

Material crystallinity

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Material crystallinity is the process whereby liquid material solidifies into a transparent crystal-like state.

The molecules in plastics are long chains of atoms, as shown in the following diagram. These long molecular chains may be regularly aligned, which create a crystalline structure; or randomly arranged chains, which create an amorphous structure; or a combination of crystalline and amorphous sections which creates a semi-crystalline structure.



Shrinkage, warpage, and crystallinity

A part will not warp if it shrinks uniformly in all directions and in all areas of the mold.

Crystalline materials have a naturally higher shrinkage than amorphous materials. This means that a part with variations in crystallinity will also have variations in shrinkage, and therefore will probably warp.

How crystallinity develops

Semi-crystalline materials have a tendency to crystallize, but their degree of crystallinity present is affected by the cooling rates of the melt. The faster the melt freezes, the less time there is available for the crystalline sections of the plastic to form.

If parts of the molding cool at a slower rate, these areas will have a higher crystalline content, hence higher shrinkage.

Two main factors affect how fast the melt freezes:

Mold temperature	The higher the mold temperature, the longer the temperature will be maintained, which delays the cooling of the melt.
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Mold geometry Thick regions tend to cool slower than thinner sections and therefore have higher crystalline content and higher volumetric shrinkage than thin sections that cool quickly and so are more amorphous. Thin regions can have a lower volumetric shrinkage than that predicted from equilibrium pVT data.

Semi-crystalline material families

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Semi-crystalline materials have both crystalline and amorphous regions.

The Autodesk Moldflow materials database contains the following semi-crystalline materials:

HDPE
HTN
LDPE
LLDPE
LMDPE
PA
PA12
PA46
PA6
PA610
PA612
PA66
PA666
PA66T
PA6T
PA6T/61
PA6T/66
PBT
PE
POM
POM-HI
PP
PP/EPDM
PP/EPR
PP/PE
TPE
TPO
TPR
UHMWPE
VHMWPE

Thermoset materials

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Cross-linking is a chemical process in which chemical bonds form among molecules of thermosetting materials, resulting in an interconnected network. This cross-linking process is the principal difference between thermoplastics and thermosets.

Prior to molding, the chain-like structure of thermosets is similar to thermoplastics. During processing, with the activation of heat and/or chemical means, thermosets polymerize (react or cure) into a cross-linked microstructure. Once the reaction is completed, the polymer chains are bonded (cross-linked) together to form a three-dimensional network. These cross bonds among molecules prohibit the slippage of individual molecular chains.

Consequently, a thermoset becomes an infusible and insoluble solid that cannot be re-softened and reprocessed by the application of heat, without degrading some linkages. Thermosets are analogous to hard-boiled eggs, where the yolk has turned from a liquid to a solid and cannot be converted back to a liquid.

The table below compares the structure and properties of thermosets and thermoplastics.

Material	Thermoplastics	Thermosets
Microstructure	Linear or branch molecules. No chemical bonds among the molecules.	Cross-linking network with chemical bonds among molecules after the chemical reaction.
Reaction to Heat	Can be re-softened (physical phase change).	Cannot be re-softened after cross-linking without degradation.
General Properties	Higher impact strength. Easier processing. Better adaptability to complex designs.	Greater mechanical strength. Greater dimensional stability. Better heat and moisture resistance.

Material properties required for analysis

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Specific analyses use different material properties in their calculations. The material properties that are required or optional for an analysis are listed.

Table 1: Material property requirements by analysis type

Fill+Pack analysis	Required/Optional
Viscosity	Required
Transition temperature	Required
Thermal conductivity	Required
Specific heat	Required
p _v T	Required
Mechanical constants	Required
Mold coefficient of thermal expansion (CTE) data	Required
Ejection temperature	Required if automatic cooling time is used
Juncture loss	Optional
Shrinkage data (CRIMS/Strain)	Optional
Matrix properties	Optional
Recommended melt/mold temperatures and ranges	Optional
Optical properties	Optional
Filler weight percentage	Required for Fiber analysis
Filler aspect ratio	Required for Fiber analysis
Filler mechanical properties data	Required for Fiber analysis
Filler coefficient of thermal expansion (CTE) data	Required for Fiber analysis
Cool analysis	Required/Optional
Melt density of polymer	Required
Specific heat of polymer	Required

Cool analysis	Required/Optional
Thermal conductivity of polymer	Required
Thermal conductivity of mold material	Required
Warp analysis	Required/Optional
Mechanical properties	Required
Insert (metal or polymer) mechanical properties	Required if model includes part insert
Anisotropic matrix properties	Required if using the Mori-Tanaka micro-mechanics model
Stress analysis	Required/Optional
Mechanical properties	Required
Coefficient of thermal expansion (CTE) data	Required for thermal analysis
Insert (metal or polymer) mechanical properties and coefficient of thermal expansion (CTE) data	Required if model includes part insert
Solid density of polymer and / or metal	Required for modal frequency analysis
Stress-strain curve data	Required for creep analysis

Environmental impact

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Users have the option to consider the environmental aspects of the materials being used.

Materials will typically be selected on criteria such as strength and functionality of the finished part. Once these primary considerations have been met, environmental factors can help finalize material selection.

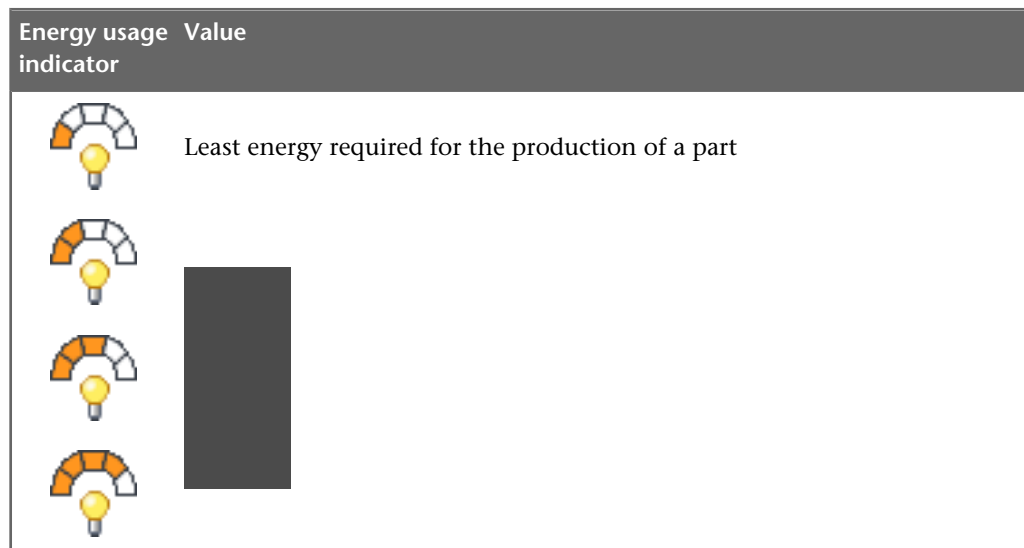
NOTE: The classifications are for the base polymer only. The effect of fillers and additives should be reviewed separately.



Energy usage indicator

The Energy usage indicator is a relative assessment of the energy requirements of the molding phase of a part, based on the material selected. The result of this assessment is a relative value derived from the injection pressure and cooling time predictions for a suite of typical geometries and thicknesses using the material's recommended conditions and processing inputs determined by an optimization calculation.

These results were standardized and an Energy usage indicator value was applied.

It is expected that existing polymer Energy usage indicator ratings will change as more environmentally efficient polymers are developed.



Energy usage indicator	Value
	Most energy required for the production of a part
	Not available







NOTE: The Energy usage indicator may not available for two reasons:



- Legacy material data from a personal database or a previous study may not include environmental information. Reload the material from the current database to view these parameters.
- The calculations for a small number of materials cannot return an injection pressure or cooling time for all the geometries tested.

Resin identification code

This code identifies the resin family to which the material belongs.

NOTE: Any materials that are a blend or contain fillers have been included in the *Other* category.

Icon	Plastic family
	Polyethylene terephthalate (PET, PETE)
	High density polyethylene (HDPE)
	Polyvinyl chloride (PVC)
	Low density polyethylene (LDPE)
	Polypropylene (PP)
	Polystyrene (PS)

Icon	Plastic family
	Other. Includes any resin not specifically listed. This category also includes all materials that are blends or contain fillers.
	Undetermined, for example, legacy data

Material Quality Indicators

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Because of the importance of quality material data on analysis accuracy, Autodesk Moldflow Plastics Labs have developed Material Quality Indicators.













There are three different indicators that reflect the confidence you can have in the material data, for different analysis requirements.

- Fill Quality Indicator** Investigates the quality of the Viscosity, Specific Heat Capacity and Thermal Conductivity data.
- Packing Quality Indicator** Incorporates the quality of the Fill Quality Indicator results and the pvT data. The Packing Quality Indicator cannot exceed the Fill Quality Indicator.
- Warpage Quality Indicator** Incorporates the suitability of the Packing Quality Indicator along with the Mechanical Property and Shrinkage data. The Warpage Quality Indicator cannot exceed the Packing Quality Indicator.

Each indicator can be assigned a Gold, Silver or Bronze rating based on the following criteria.

- Testing method employed to generate the value of each material property.
- Completeness of the range of material properties needed for the analysis type.
- How recently the testing was completed.

Table 2: Material Quality Indicator icons

	Gold	Silver	Bronze	Unknown
Fill Quality				
Packing Quality				
Warpage Quality				

A Gold rating indicates a high confidence in the quality of the material data for the analysis type. When accurate analysis results are critical, it is recommended that a material with a Gold rating should be used.

A Silver rating can result from a combination of well tested, and supplemental¹ material data. For example, a material might have a Gold Packing Quality rating but use supplemental Mechanical Properties data. This could result in a Silver Warpage Quality Indicator rating.

Bronze ratings can reflect problems such as incomplete data sets, the extensive use of supplemental data and untested material properties. The use of Bronze-rated materials can still generate good results, but these results should not be relied upon to determine critical requirements such as precise warpage or shrinkage allowances used for the cutting of molds.

An unknown rating indicates a material that has been used in an earlier version of the software. Re-selecting the same material will update the Material Quality Indicators.

The rating for a material is displayed in the **Study Tasks** pane of a study. Hover the mouse over an icon for the rating to be displayed.

This information is also in the **Quality Indicators** tab of the **Thermoplastics material** dialog (**Home** tab > **Molding Process Setup** panel > **Select Material** > **Details**).

The **View Details** button on the Quality Indicators tab of the Thermoplastic material dialog outlines the parameters considered in assigning a rating. Other tabs on the Thermoplastic material dialog further define the material testing data.

Material Quality Indicators

Three different material quality indicators have been provided to help you choose an appropriate material for your analysis.

Filling Data Quality Details

The factors that contribute to the specific material Filling Quality Indicator are outlined.

The confidence in the results of an analysis depends on the quality of the material data used to generate these results.

The Filling Data Quality Details dialog identifies the major material properties that contribute to a Fill analysis and gives a weighted rating of the reliability of that data.

The resulting Filling quality indicator takes into account the reliability of the viscosity, specific heat and thermal conductivity data that are associated with this material.

A material can have a Gold , Silver  or Bronze  filling data quality rating.

¹ Supplemental data are untested parameter values that are typical for that material family. In the Thermoplastic material dialog, any group of parameters (e.g. Mechanical properties data) that are highlighted in red, indicate that the values used are supplemental.

The parameters considered in assessing the filling quality indicators are listed in this dialog. The more factors that are checked, the more reliable the indicator. There are three sets of data that contribute to the quality rating:

- Viscosity data
- Specific heat data
- Thermal conductivity data

Packing Data Quality Details

The factors that contribute to the specific material Packing Quality Indicator are listed in this dialog.

The confidence in the results of an analysis depends on the quality of the material data used to generate these results.

The Packing Data Quality Details dialog lists the major material properties that contribute to a Fill + Pack analysis and gives a weighted rating of the reliability of that data.

The resulting Pack quality indicator takes into account the reliability of the pVT data along with the Filling quality indicator result that is associated with this material.

A material can have a Gold , Silver  or Bronze  packing data quality rating.

Warpage Data Quality Details

The factors that contribute to the specific material Warpage Quality Indicator are listed in this dialog.

The confidence in the results of an analysis depends on the quality of the material data used to generate these results.

The Warpage Data Quality Details dialog identifies the major material properties that contribute to a Warpage analysis and gives a weighted rating of the reliability of that data.

The resulting Warpage quality indicator takes into account the reliability of the mechanical properties and shrinkage data along with the Pack quality indicator result that is associated with this material.

A material can have a Gold , Silver  or Bronze  warpage data quality rating.

The parameters considered in assessing the warpage quality indicators are listed in this dialog. The more factors that are checked, the more reliable the indicator. There are two sets of data that contribute to the quality rating:

- Mechanical property data
- Shrinkage data