Polyurethanes

Polyurethanes are versatile polymers which provide products ranging from soft, thermoplastic elastomers to hard, thermosetting coatings and rigid insulating foams. The basic building blocks for polyurethanes are di-isocyanates and glycols.

We have the following categories

1)These single package urethane coatings are cured by reaction with atmospheric moisture. The applied urethane prepolymer reacts with atmospheric moisture to form a substituted urea polymer network. The byproduct of this curing mechanism is CO2 which escapes to the atmosphere. A minimum relative humidity of 30% is required to achieve a good cure.

2)These coatings are characterized by the absence of any significant quantity of free isocyanate groups. The isocyanate component has been prereacted with oils to produce single package air-dry coatings that are commonly called "uralkyds."

3)These are single package heat-cured polyurethanes. The reactive isocyanate group is inactivated or "blocked," but becomes reactive when subjected to elevated temperatures.

4)These are two package catalyzed polyurethanes. An isocyanate terminated prepolymer is cured by reaction with a catalyst at room temperature.

5)These two package ambient-cured polyurethanes are the most common urethane coatings. An isocyanate terminated prepolymer, which may be "aromatic" or "aliphatic," is cured by reaction with glycols (polyols). The polyol component of the coating usually consists of hydroxylated acrylic, polyester, or polyether resins. Aromatic polyurethanes provide excellent toughness and abrasion resistance but have poor weatherability

6)One package, nonreactive lacquer polyurethane with no reactive isocyanate groups. These cure via solvent evaporation only.

Guide to Urethane Calculations

Equivalent weight:
The equivalent weight (eq. wt.) tells you how many grams of a product you need to have for one equivalent of reactive groups. For an isocyanate, the reactive group is -N=C=O (NCO), and its concentration is measured by weight percent NCO.

Isocyanate equivalent weight = 4,200 ÷ NCO (unit: g/eq)

Example:
Isocyanate eq. wt. of pure MDI = 4,200 ÷ 33.6 = 125 g/eq

For a polyol, the reactive group is -O-H (OH).
The OH concentration is measured by the OH value (mg KOH/g sample):

Equivalent weight of a polyol = 56100 ÷ OH Value (unit: g/eq)

Example:
Eq. wt. of ethylene glycol = 56,100 ÷ 1810 = 31.0 g/eq

Molecular weight of a polyol:
The molecular weight (mol. wt.) of a polyol is approximated by the polyol equivalent weight (eq. wt.) multiplied by the nominal functionality (fn).

Polyol mol. wt. = (eq.wt.) *x* (fn) = [56,100 ÷ OH value] *x* (fn) (unit: g/mol)

Mol. wt. of any diol = [56,100 ÷ OH value] *x* 2 g/mol

Mol. wt. of any triol = [56,100 ÷ OH value] *x* 3 g/mol

Example:
Mol. wt. of ethylene glycol = [56,100 ÷ 1,810] *x* 2 = 62.0 g/mol

Total weight of MDI required for reaction:
MDI = Diphenylmethane Diisocyanate

When reacting an isocyanate with one or more polyols to form a polyurethane, one NCO group reacts with one OH group. When the number of NCO groups equals the number of OH groups, you have a stoichiometric NCO : OH ratio of 1.0. This ratio is commonly referred to as the index. To determine the amount of MDI required to react with a given polyol blend, you must know the desired index (often 1.0), the MDI equivalent weight (MDI eq. wt.), and the weight fractions (pbw) and equivalent weights of the polyols and any water present in the blend.

Total weight of MDI required =

index *x* MDI eq. wt. *x* {(pbw polyol A ÷ eq. wt. polyol A) + (pbw polyol B ÷ eq. wt. polyol B) + ... + (pbw polyol N ÷ eq. wt. polyol N) + (pbw water ÷ eq. wt. water)

Example formulation:
Say you have the following polyol blend and would like to determine the amount of pure MDI to add to achieve a fully reacted polyurethane with a slight excess of isocyanate (target index = 1.05)

Polyol A (OH value = 490)	100.00
1,4 Butanediol (BD) (eq. wt. = 45)	20.00
Water	0.15
pure MDI (% NCO = 33.6)	X

X = pbw MDI = index *x* MDI eq. wt. *x* {[100 ÷ (56100 ÷ 490)] + (20 ÷ 45) + (0.15 ÷ 9)}
X = 1.05 *x* (4200 ÷ 33.6) *x* {0.873 + 0.444 + 0.017}
X = 1.05 *x* 125 *x* 1.334
X = 175 pbw MDI

Equivalent Weight

The equivalent weight (eq. wt.) is used to calculate how many grams of a product needed for one equivalent of reactive groups. For an **isocyanate**, the reactive group is -N=C=O (NCO. Its concerntration is measured by weight percent NCO.

$$\textit{Isocyanate equivalent weight} = \frac{4{,}202}{NCO}\ g/eq$$

The reactive group for a **polyol** is -O-H (OH).

$$\textit{Equivalent weight of a polyol} = \frac{56{,}100}{\textit{OH Value}}\ g/eq$$

Molecular Weight of a Polyol

The molecular weight (mol. wt.) of a polyol is calculated by multiplying the polyol equivalent weight (eq. qt.) by the nominal funcationality (fn).

$$\textit{Polyol mol. wt.} = (\textit{eq. wt.})(fn) = \left(\frac{56{,}100}{\textit{OH value}}\right)\ (fn)\ g/mole$$

Total Weight of MDI Required for Reaction

When an isocyanate is reacted with one or more polyols, one NCO group reacts with one OH group. When the number of NCO groups is equal is to the number of OH groups, the result is a stoichioetric NCO : OH ratio of 1.0. A ratio of 1.0 is commonly known as the index.

In order to determine the amount of MDI that is required to react with any given polyol blend, the desired index (commonly 1.0) must be known, as well as the MDI equivalent weight (MDI eq. wt.), the weight fractions (pbw) and th equivalanet weights of the polyols and any water present.

Total weight of MDI required =

$$(\textit{index})(\textit{MDI eq. wt.})(fn) = \left(\frac{\textit{pbw polyal A}}{\textit{eq. wt. polyol A}} + \frac{\textit{pbw polyal B}}{\textit{eq. wt. polyol B}} + \ldots + \frac{\textit{pbw polyal E}}{\textit{eq. wt. polyol E}} + \frac{\textit{pbw H2O}}{\textit{eq. wt. H2O}}\right)$$

Calculation for Formulating a Prepolymer to a Specific Percent NCO

MDI Prepolymer calculation:

Where N = Desired NCO
Where X = Equivalent weight of the diisocyanate
Where Y = Equivalent weight of the polyol

$$MDI = X + \left(\frac{N\,(X+Y)}{(42/X) - N}\right)$$