



Terms and Formulas Used in Urethane Polymer Preparations

INTRODUCTION

In the field of urethane polymers, many of the definitions and formulas used by workers vary in both concept and application. Assumptions for simplifying the calculations are also not consistent.

Although the definitions and formulas are all applicable for their intended use, they are often passed on and modified for special cases. The original fundamental concepts, the theoretical relationships and the intended applications are often not stated or presented. This inevitably has created confusion and misuse. It has also hampered proper field work evaluations and comparisons.

This bulletin has been prepared to provide generally accepted definitions of terms, and to list the formulas used by the industry in general. The concepts, assumptions and modifications are given. Sample calculations are also shown, for clarification.

DEFINITION OF TERMS

Chemical Nomenclature

Monomer. The fundamental chemical compound which can undergo polymerization and form a polymer chain.

Polymerization. A chemical reaction in which two or more monomers combine to form a polymer. A polymer may be randomly formed or a deliberately planned block polymer.

Polymer. The chemical compound formed by polymerization and consisting essentially of repeating structural units. A polymer chain can be formed from the same — or from more than one — monomer type.

Prepolymer. An intermediate polymer which is not reacted to stoichiometric completion. There is always a deliberate excess of active groups (e.g. -OH, -NCO) which is available for later reaction to form the final polymer.

Homo-polymer. A chain formed by chemically combining the same monomer units.

Block polymer. A chain with a specific planned pattern formed by chemically combining different homo- and/or other polymer chain segments.

Graft polymer. A polymer composed of a main chain, to which other monomeric or polymeric groups are chemically added as side chains. The addition site and the graft are specifically selected to form a desired branch.

Linear polymer. A polymer essentially composed of molecular chains with no radicals, groups or appendages attached along the chains.

Branched polymer. A polymer containing one or more appendages attached to the main chain. These appendages may be small and simple radicals, or they may be rather large and complex chains.

Cross-linked (or three dimensional) polymer. A polymer formed only from monomer and/or polymer units having an average of more than two active centers or groups per molecule. Inter-chain reactions can form a network which can grow infinitely in three dimensions. Cross-linked polymers are of moderate size; normally they are infusible and insoluble.

Mathematical Concepts

Molecular weight (M). The sum of the atomic weights of all the constituent atoms in a molecule. Atomic weight is expressed relative to the arbitrary weight of oxygen (O=16).

Polymers consist of chain molecules of various lengths. When their molecular weights are given, calculated or determined, they are stated as average values. These average molecular weights are based on either of two concepts: *number average or weight average*. Number average and weight average molecular weights cannot be used interchangeably. They are equivalent only when all molecular species are the same, as in the case of pure compounds.

Number average molecular weight M_n . M_n is equal to the total polymer weight, divided by the total number of monomers (molecules). See equation [15].

Since the total weight of a polymer equals the number of monomer molecules, each multiplied by its molecular

KEY TO NOTATION

Symbols and Abbreviations

[]	Reference number for formula
Σ	Summation of
a	amine
b	amine-polyol blend
c	cross-link
d	NCO radical
f	functionality
g	curative and extending agents in general
n	number of molecules
p	polyol
q	water
s	isocyanate
v	prepolymer
A	acid number
Ap	acid number of polyol
D	percent free isocyanates as NCO
E	weight equivalent
Ea	weight equivalent of amine
Eg	weight equivalent of curative or extending agent
Ep	weight equivalent of polyol
Eq	weight equivalent of water
Es	weight equivalent of isocyanate
M	molecular weight
Md	molecular weight of NCO radical (Md = 42)
\bar{M}_n	number average molecular weight
\bar{M}_{nc}	number average molecular weight per cross-link
\bar{M}_w	weight average molecular weight
OH	hydroxyl number
OHp	hydroxyl number of polyol
Q	percent water
R ₁	ratio of amine to polyol or polyester
R ₂	ratio of isocyanate to polyol
R ₃	ratio of isocyanate to amine
R ₄	ratio of isocyanate to amine plus polyol
W	weight
Wa	weight of amine
Wb	weight of amine-polyol blend
Wg	weight of curative or extending agent
Wp	weight of polyol
Wq	weight of water
Ws	weight of isocyanate
Wv	weight of prepolymer
a	fractional weight of first component
(1 - a)	fractional weight of second component
Subscripts	
i	individual molecular species
j, k	individual components in a mixture
m	mixture

weight, \bar{M}_n can also be expressed as in [16]. In other words, \bar{M}_n equals the sum of the number of molecules of each species, multiplied by the molecular weight of the corresponding species, all divided by the total number of molecules.

\bar{M}_n is an arithmetic mean. Each molecule contributes equally, independent of its weight. \bar{M}_n is most useful in polyurethane calculations since it is inversely proportional to the functionality (number of active groups) and the hydroxyl number (OH). For a definition of \bar{M}_n in terms of functionality and OH number, see [18].

Weight average molecular weight (M_w). M_w equals the sum of the weights of each species multiplied by the molecular weight of the corresponding species, all divided by the total polymer weight [24]. The contribution of each molecular weight class to M_w is proportional to the weight of the molecules in that class. Weight average molecular weight is seldom used in polyurethane calculations, and then only when the molecular weight is calculated from viscosity, light scattering and ultra-centrifuge sedimentation data.

Molecular weight per cross-link \bar{M}_{nc} . \bar{M}_{nc} is the weight of polymer per active center or group which can form a cross-link [22]. The value does not represent the effective or actual arithmetic mean between cross-links in a three dimensional polymer. It is used simply as a convenient method for comparing effectiveness of available cross-linking factors.

Weight equivalent (W). The molecular weight of compound or polymer per active function for the considered reactions [1]. Weight equivalent is used as an average value for polymers.

Hydrogen equivalent. The weight of hydrogen equal to the reactive groups of 100 unit weights of compound or polymer.

Isocyanate equivalent. The weight of the isocyanate radical, NCO (M = 42), which is equal to the reactive groups of 100 unit weights of compound or polymer.

Free or uncombined isocyanate as -NCO (D). Usually expressed as weight percent of the prepolymer.

Hydroxyl percent. The percent by weight of OH (M = 17) which is equivalent to the active functions of a compound or polymer.

Hydroxyl number (OH)*. The number of milliweights of KOH which is chemically equivalent to the active functions per unit weight of the compound or polymer [30]. When free acidity is measured in these units it is usually called acid number.

Acid number (A). See hydroxyl number, above.

Degree of polymerization. Equals the number of monomeric units chemically combined to form a polymer chain or molecule

Functionality (f). The number of chemically active atoms or groups (e.g., -H, -OH, -NCO) per molecule for the considered reaction [27]. This is used as an average value for polymers.

*The molecular weight of KOH is 56.1. Since hydroxyl number (OH) is expressed in milliweights per unit weight, we must multiply 56.1 by 1000 to convert to OH, and the factor 56,100 appears in the calculations. OH is a dimensionless unit; it can be expressed in any weight system without altering its numerical value.

INDEX TO FORMULAS

Weight Equivalent (E)

- [1] E; given \overline{Mn}, f
[2] E; given OH

Weight of Amine Required for Blending with Polyol (Wa)

- [3] Wa; given Ea, Ep, Wp, R₁

Weight of Isocyanate Required for Blending with Various Components (Ws)

- [4] Ws; given Ep, Es, Wp, R₂ (for polyols)
[5] Ws; given Ea, Es, Wa, R₃ (for amines)
[6] Ws; given Ea, Ep, Es, Wa, Wp, R₄ (for amine-polyol blends)
[7] Ws; given Ep, Es, Wp, R₁, R₄ (for amine-polyol blends)
[8] Ws; given Eq, Es, Wq (for water)
[9] Ws; given Es, Wp, OHp, R₂
[10] Ws; given Ea, Es, Wa, Wp, OHp, R₄
[11] Ws; given Eq, Es, Wp, OHp, Ap, Q
[12] Ws; given Ep, Es, Wp, Md, D
[13] Ws; given Ea, Ep, Es, Wb, a, (1 - a), R₄

Weight of Reactive or Curative Agent Needed (Wg)

- [14] Wg; given Eg, Wv, Md, \overline{Mnc} , D

Number Average Molecular Weight (\overline{Mn})

- [15] \overline{Mn} ; given W_i, n_i (general form)
[16] \overline{Mn} ; given M_i, n_i (usual given form)
[17] \overline{Mn} ; given E, f
[18] \overline{Mn} ; given OH, f

Number Average Molecular Weight of 2-Component Mixture (\overline{Mn}_m)

- [19] \overline{Mn}_m ; given $n_j, n_k, \overline{M}_j, \overline{M}_k$ (general form)
[20] \overline{Mn}_m ; given $\overline{Mn}_j, \overline{Mn}_k, a, (1 - a)$
[21] \overline{Mn}_m ; given $OH_j, OH_k, f_j, f_k, a, (1 - a)$

Number Average Molecular Weight Per Cross-link (\overline{Mnc})

- [22] \overline{Mnc} ; given Eg, Wg, Wv, D, Md

Number Average Molecular Weight of Polyol or Polyester Component of a Prepolymer (\overline{Mnp})

- [23] \overline{Mnp} ; given Es, Md, D

Weight Average Molecular Weight (\overline{Mw})

- [24] \overline{Mw} ; given M_i, W_i (general form)
[25] \overline{Mw} ; given M_i, n_i (usual given form)

Weight Average Molecular Weight of a 2-Component System (\overline{Mw}_m)

- [26] \overline{Mw}_m ; given $\overline{Mw}_j, \overline{Mw}_k, a, (1 - a)$

Functionality (f)

- [27] f; given E, \overline{Mn}

Functionality of a Mixture (f_m)

- [28] f_m ; given \overline{Mn}_m, OH_m
[29] f_m ; given $f_j, f_k, OH_j, OH_k, a, (1 - a)$

Hydroxyl Number of a Mixture (OH_m)

- [30] OH_m ; given $OH_j, OH_k, a, (1 - a)$

Weight of Components (a)

- [31] a; given $\overline{Mn}_j, \overline{Mn}_k, \overline{Mn}_m$
[32] a; given $f_j, f_k, \overline{Mn}_m, OH_j, OH_k$
[33] a; given $\overline{Mw}_j, \overline{Mw}_k, \overline{Mw}_m$

FORMULAS

These formulas have general application. When specific compounds or materials are used continuously, the formulas can be simplified considerably by substituting and combining their numerical values.

Weight Equivalent

Given: Number average molecular weight (\bar{M}_n) and functionality (f)

$$[1] \quad E = \frac{\bar{M}_n}{f}$$

Given: Hydroxyl number (OH) and molecular weight of KOH (=56.1)

$$[2] \quad E = \frac{1000(56.1)}{\text{OH}}$$

Weight of Amine Required for Blending With Polyol

Given: Weight equivalents (E_a , E_p), weight of polyol (W_p), and ratio of amine to polyol (R_1).

$$[3] \quad W_a = \frac{E_a W_p R_1}{E_p}$$

Weight of Isocyanate Required at Various Reacting Ratios or for Blending With Various Components

Given: Weight equivalents (E_p , E_q , E_s), weights (W_a , W_p) and ratios (R_2 , R_3 , R_4).

$$[4] \quad W_s = \frac{E_s W_p R_2}{E_p} \quad (\text{For polyols})$$

$$[5] \quad W_s = \frac{E_s W_a R_3}{E_a} \quad (\text{For amines})$$

$$[6] \quad W_s = \left(\frac{E_s W_p}{E_p} + \frac{E_s W_a}{E_a} \right) R_4 \quad (\text{For polyol-amine blends. Also see Equation [13] and Appendix})$$

Given: Weight equivalents (E_s , E_p), weight (W_p) and ratios (R_1 , R_4).

$$[7] \quad W_s = \left(\frac{E_s W_p}{E_p} \right) (1 + R_1) (R_4)$$

$$[8] \quad W_s = \frac{E_s W_q}{E_q} \quad (\text{For water})$$

Given: Hydroxyl number of polyol (OH_p), weight equivalents (E_a , E_s), weights (W_a , W_p) and ratios (R_2 , R_4).

$$[9] \quad W_s = \frac{E_s W_p \text{OH}_p R_2}{1000(56.1)}$$

$$[10] \quad W_s = \left[\frac{E_s W_p \text{OH}_p}{1000(56.1)} + \frac{E_s W_a}{E_a} \right] R_4$$

$$[11] \quad W_s = E_s W_p R_4 \left[\frac{\text{OH}_p + A_p}{1000(56.1)} + \frac{\text{OH}_p R_1}{1000(56.1)} + \frac{Q}{100E_q} \right]$$

Formula [11] can be simplified to:

$$[11A] \quad W_s = E_s W_p R_4 \left[\frac{\text{OH}_p(1 + R_1) + A_p}{1000(56.1)} + \frac{Q}{100E_q} \right]$$

Weight of isocyanate required to obtain a specified percent free NCO in a prepolymer.

Given: Weight equivalents (E_p , E_s), weight (W_p), molecular weight of NCO radical ($M = 42$), and percent free NCO in a prepolymer (D).

$$[12] \quad W_s = \frac{E_s W_p}{E_p} \left[\frac{100(42) + D E_p}{100(42) - D E_s} \right]$$

Given: Weight equivalents (E_a , E_p), weight (W_b), ratio (R_4), fractional weight of polyol in blend (a) and fractional weight of amine in blend ($1-a$).

$$[13] \quad W_s = E_s W_b R_4 \left[\frac{a}{E_p} + \frac{(1-a)}{E_a} \right]$$

Weight of a Reactive or Curative Agent Needed to give a cross-linked product from a linear isocyanate prepolymer, with a predetermined molecular weight per cross-link. (See Definition of \bar{M}_{nc} for significance and limitations.)

Given: Weight equivalent (E_g) of reactive or curative agent, weight (W_v), molecular weight of NCO radical ($\bar{M}_d = 42$), number average molecular weight per cross-link (\bar{M}_{nc}), and percent free isocyanates as NCO (D).

$$[14] \quad W_g = \frac{E_g W_v}{100(42)} \left[\frac{\bar{M}_{nc} D - 100(42)}{\bar{M}_{nc} + E_g} \right]$$

To solve Equation [14] for \bar{M}_{nc} when weight equivalent (Wg) is given, see Equation [22].

Number Average Molecular Weight

$$[15] \quad \bar{M}_n = \frac{\sum_i W_i}{\sum_i n_i} \quad (\text{General form})$$

$$[16] \quad \bar{M}_n = \frac{\sum_i n_i M_i}{\sum_i n_i} \quad (\text{Usual given form})$$

Given: Weight equivalent (E) and functionality (f)

$$[17] \quad \bar{M}_n = E f$$

Given: Hydroxyl number (OH) and functionality (f)

$$[18] \quad \bar{M}_n = \frac{1000(56.1) f}{\text{OH}}$$

Number Average Molecular Weight Of 2-Component Mixture

$$[19] \quad \bar{M}_{n_m} = \frac{n_j M_j + n_k M_k}{n_j + n_k} \quad (\text{General form})$$

Given: Number average molecular weights ($\bar{M}_{n_j}, \bar{M}_{n_k}$) and fractional weights of components (a), (1 - a).

$$[20] \quad \bar{M}_{n_m} = \frac{\bar{M}_{n_j} \bar{M}_{n_k}}{\bar{M}_{n_k} a + \bar{M}_{n_j} (1 - a)}$$

To solve Equation [20] for a when \bar{M}_{n_m} is given, see Equation [31].

Given: Hydroxyl numbers (OH_j, OH_k), functionalities (f_j, f_k) and fractional weights of components (a) and (1 - a).

$$[21] \quad \bar{M}_{n_m} = \frac{1000(56.1) f_j f_k}{\text{OH}_j f_k a + \text{OH}_k f_j (1 - a)}$$

Number Average Molecular Weight Per Cross-link

Given: Weight equivalent (Eq) of curative per given prepolymer, weights (Wg, Wv), molecular weight of NCO radical (Md = 42), and percent free isocyanate as NCO (D).

$$[22] \quad \bar{M}_{nc} = 100(42) \text{Eg} \left[\frac{W_v + W_g}{W_v \text{Eg} D - 100(42) W_g} \right]$$

To solve Equation [22] for (Wg) when (Mnc) is given, see Equation [14].

Number Average Molecular Weight of Polyol or Polyester Component of a Prepolymer
(Approximation for a difunctional system.)

Given: Weight (Es), molecular weight of NCO radical (Md = 42), and percent free isocyanate as NCO (D).

$$[23] \quad \bar{M}_{np} = \frac{200(42) - 4 \text{Es} D}{D}$$

NOTE: Valid only when there are no free (OH) groups, no free isocyanate and most (OH) groups are combined with one isocyanate.

Weight Average Molecular Weight

$$[24] \quad \bar{M}_w = \frac{\sum_i W_i M_i}{\sum_i W_i} \quad (\text{General form})$$

$$[25] \quad \bar{M}_w = \frac{\sum_i n_i M_i^2}{\sum_i n_i M_i} \quad (\text{Usual given form})$$

Weight Average Molecular Weight of 2-Component System

Given: Weight average molecular weights ($\bar{M}_{w_j}, \bar{M}_{w_k}$), and fractional weights of components (a), (1 - a).

$$[26] \quad \bar{M}_{w_m} = \bar{M}_{w_j} a + \bar{M}_{w_k} (1 - a)$$

NOTE: Number average molecular weight (\bar{M}_n) or hydroxyl number (OH) cannot be used.

To solve Equation [26] for (\bar{M}_{w_m}) when (a) is given, see Equation [33].

Functionality

Given: Number average molecular weight (\bar{M}_n) and equivalent weight (E).

$$[27] \quad f = \frac{\bar{M}_n}{E}$$

Functionality of a Mixture

Given: Number average molecular weight of mixture (\overline{Mn}_m) and hydroxyl number of mixture (OH_m).

$$[28] \quad f_m = \frac{\overline{Mn}_m \cdot OH_m}{1000(56.1)}$$

Given: Functionality of components (f_j, f_k), hydroxyl numbers of components.

$$[29] \quad f_m = \frac{OH_m f_j f_k}{OH_j f_k a + OH_k f_j (1-a)}$$

Hydroxyl Number of Mixture

Given: Hydroxyl numbers of compounds (OH_j, OH_k) and fractional weights of each component (a) and $(1 - a)$.

$$[30] \quad OH_m = OH_j a + OH_k (1 - a)$$

Weight of Components

Given: Number of average molecular weights of components ($\overline{Mn}_j, \overline{Mn}_k$) and number average molecular weight of mixture (\overline{Mn}_m).

$$[31] \quad a = \frac{\overline{Mn}_j}{\overline{Mn}_m} \left(\frac{\overline{Mn}_k - \overline{Mn}_m}{\overline{Mn}_k - \overline{Mn}_j} \right)$$

To solve Equation [31] for number average molecular weight of mixture (\overline{Mn}_m) when weight of component (a) is given, see Equation [20].

Given: Number average molecular weight of mixture (\overline{Mn}_m), functionality of components (f_j, f_k) and hydroxyl numbers of components (OH_j, OH_k).

$$[32] \quad a = \frac{f_j}{\overline{Mn}_m} \left[\frac{1000(56.1) f_k - \overline{Mn}_m}{OH_j f_k - OH_k f_j} \right]$$

Given: Weight average molecular weights of mixture and components ($\overline{Mw}_m, \overline{Mw}_j, \overline{Mw}_k$).

$$[33] \quad a = \frac{\overline{Mw}_m - \overline{Mw}_k}{\overline{Mw}_j - \overline{Mw}_k}$$

To solve Equation [33] for weight average molecular weight of mixture (\overline{Mw}_m) when component weight (a) is given, see Equation [26].

APPENDIX

In Equation [6]

$$\frac{Es \cdot Wp}{Ep}$$

... equals the isocyanate equivalent for the charged polyol. Similarly,

$$\frac{Es \cdot Wa}{Ea}$$

... equals the isocyanate equivalent for the amine. It is convenient to base the ratio (R_4) on the sum of the isocyanate weight equivalences. We prefer this, but the ratio of isocyanate to polyol, plus the ratio of isocyanate to amine, may also be used. Equation [6] then becomes:

$$Ws = \frac{Es \cdot Wp \cdot R_2}{Ep} + \frac{Es \cdot Wa \cdot R_3}{Ea}$$

SAMPLE CALCULATIONS

NOTE: In a number of the following examples MBCA is used as the amine. MBCA is a DuPont trademark for 4,4'-methylene-bis-(2-chloroaniline).

[1]	Molecular weight of polyol (\overline{Mn})	1000
	Functionality of polyol (f)	2
	$E = \frac{1000}{2} = 500$	

[2]	Hydroxyl number of polyol (OH)	58
	$E = \frac{1000(56.1)}{58} = 967.2$	

[3]	Weight equivalent of amine (Ea)	133.5
	Weight of polyol (Wp)	100
	Blending ratio, amine:polyol (R_1)	1
	Weight equivalent of polyol (Ep)	490
	$Wa = \frac{133.5(100)(1)}{490} = 27.2$	

[4]	Weight equivalent of TDI (Es)	87
	Weight of polyol (Wp)	100
	Charging ratio, TDI:polyol (R_2)	1.08
	Weight equivalent of polyol (Ep)	1009
	$Ws = \frac{87(100)(1.08)}{1009} = 9.3$	

[5]	Weight equivalent of TDI (Es)	87
	Weight of MBCA (Wa)	100
	Charging ratio, TDI:MBCA (R_3)	1.04
	Weight equivalent of MBCA (Ea)	133.5
	$Ws = \frac{87(100)(1.04)}{133.5} = 67.8$	

[6]	Weight equivalent of TDI (Es)	87
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Weight of polyol (Wp)	100
Weight of MBCA (Wa)	25
Charging ratio, TDI:MBCA + polyol (R ₄)	1.05
Weight equivalent of polyol (Ep)	504
Weight equivalent of MBCA (Ea)	133.5

$$W_s = \left[\frac{87(100)}{504} + \frac{87(25)}{133.5} \right] 1.05 = 35.2$$

[7]

Weight equivalent of TDI (Es)	87
Weight of polyol in blend (Wp)	100
Charging ratio, MBCA:polyol (R ₁)	0.8
Charging ratio, TDI:MBCA + polyol (R ₄)	1.08
Weight equivalent of polyol (Ep)	510

$$W_s = \left[\frac{100(87)}{510} \right] (1 + 0.8)(1.08) = 33.2$$

[8]

Weight equivalent of TDI (Es)	87
Weight of water (Wq)	1.12
Weight equivalent of water (Eq)	9

$$W_s = \frac{87(1.12)}{9} = 10.8$$

[9]

Weight equivalent of TDI (Es)	87
Weight of polyol (Wp)	100
Hydroxyl number of polyol (OHp)	74
Charging ratio, TDI:polyol (R ₂)	1.05

$$W_s = \frac{87(100)(74)(1.05)}{1000(56.1)} = 12.0$$

[10]

Weight equivalent of TDI (Es)	87
Weight of polyol (Wp)	100
Hydroxyl number of polyol (OHp)	110
Weight of MBCA (Wa)	26.2
Charging ratio, TDI:MBCA + polyol (R ₄)	1.05
Weight equivalent of MBCA (Ea)	133.5

$$W_s = \left[\frac{87(100)(110)}{1000(56.1)} + \frac{87(26.2)}{133.5} \right] 1.05 = 35.8$$

[11]

Weight equivalent of TDI (Es)	87
Weight of polyol (Wp)	100
Charging ratio, TDI:MBCA + polyol (R ₄)	1.05
Hydroxyl number of polyol (OHp)	110
Acid number of polyol (Ap)	1.0
Blending ratio, MBCA:polyol (R ₁)	1.1
Percent of water in polyol (Q)	0.06
Weight equivalent of water (Eq)	9

$$W_s = 87(100)(1.05) \left[\frac{110 + 1.0}{1000(56.1)} + \frac{110(1.1)}{1000(56.1)} + \frac{0.06}{100(9)} \right] = 38.4$$

[12]

Weight equivalent of TDI (Es)	87
Weight of polyol (Wp)	100
Percent free isocyanate as NCO in prepolymer (D)	6.2
Weight equivalent of polyol (Ep)	510

$$W_s = \frac{87(100)}{510} \left[\frac{100(42) + 6.2(510)}{100(42) - 6.2(87)} \right] = 34.3$$

[13]

Weight equivalent of TDI (Es)	87
Weight of amine-polyol blend (Wb)	100
Charging ratio, TDI:MBCA + polyol (R ₄)	1.08
Fractional weight of polyol in blend (a)	0.823
Fractional weight of MBCA in blend (1 - a)	0.177
Weight equivalent of polyol (Ep)	510
Weight equivalent of MBCA (Ea)	133.5

$$W_s = 87(100)(1.08) \left(\frac{0.823}{510} + \frac{0.177}{133.5} \right) = 27.6$$

[14]

Weight equivalent of reactive agent (Eg) = weight equivalent of MBCA (Ea)	133.5
Weight of prepolymer (Wv)	100
Molecular weight of cross-link (\bar{M}_{nc})	5000
Percent free isocyanate as NCO in prepolymer (D)	7.2

$$W_g = \frac{133.5(100)}{100(42)} \left[\frac{5000(7.2) - 100(42)}{5000 + 133.5} \right] = 19.7$$

Weight of reactive agent (Wg) = weight of MBCA (Wa)

[17]
Weight equivalent of polyol (Ep) 1020
Functionality of polyol (f) 3
 $\bar{M}_n = 1020(3) = 3060$

[18]
Functionality of polyol (f) 3
Hydroxyl number of polyol (OH_p) 55.8
 $\bar{M}_n = \frac{1000(56.1)(3)}{55.8} = 3016.1$

[21]
Functionality of first component (f_j) 2
Functionality of second component (f_k) 2
Hydroxyl number of first component (OH_j) ... 55.4
Fractional weight of first component (a) 0.7
Hydroxyl number of second component (OH_k) . 110
Fractional weight of second component ($1 - a$) . 0.3
 $\bar{M}_n = \frac{1000(56.1)(2)(2)}{55.4(2)(0.7)+110(2)(0.3)} = 1563.1$

[22]
Weight equivalent of curative (Eg)
= weight equivalent of MBCA (Ea) 133.5
Weight of prepolymer (Wv) 100
Weight of reactive agent (Wg)
= weight of MBCA (Wa) 11
Percent free isocyanate as NCO
in prepolymer (D) 5.8
 $\bar{M}_{nc} = \frac{100(42)(133.5)}{100(133.5)(5.8)-100(42)(11)} = 1992.9$

[23]
Weight equivalent of TDI (Es) 87
Percent free isocyanate as NCO (D) 3.8
 $\bar{M}_{np} = \frac{200(42) - 4(87)(3.8)}{3.8} = 1862.5$

[26]
Molecular weight of first component ($\bar{M}w_j$) ... 800
Fractional weight of first component (a) 0.6
Molecular weight of second component ($\bar{M}w_k$) . 1900
Fractional weight of second component ($1 - a$) . 0.4
 $\bar{M}w_m = 800(0.6) + 1900(0.4) = 1240$

[27]
Molecular weight of polyol (\bar{M}_n) 1000
Weight of polyol (Ep) 500
 $f = \frac{1000}{500} = 2$

[28]
Molecular weight of mixture ($\bar{M}n_m$) 2500
Hydroxyl number of mixture (OH_m) 56.5
 $f_m = \frac{2500(56.5)}{1000(56.1)} = 2.52$

[29]
Hydroxyl number of mixture (OH_m) 79
Functionality of first component (f_j) 3
Functionality of second component (f_k) 2
Hydroxyl number of first component (OH_j) ... 58
Fractional weight of first component (a) 0.625
Hydroxyl number of second component (OH_k) . 114
Fractional weight of second component ($1 - a$) . 0.375
 $f_m = \frac{79(3)(2)}{58(2)(0.625) + 114(3)(0.375)} = 2.36$

[30]
Hydroxyl number of first component (OH_j) ... 55.4
Fractional weight of first component (a) 0.645
Hydroxyl number of second component (OH_k) . 110
Fractional weight of second component ($1 - a$) . 0.355
 $OH_m = 55.4(0.645) + 110(0.355) = 74.8$

[31]
Molecular weight of first component ($\bar{M}n_j$) ... 1990
Molecular weight of second component ($\bar{M}n_k$) . 1009
Molecular weight of mixture ($\bar{M}n_m$) 1500
 $a = \frac{1990}{1500} \left(\frac{1009 - 1500}{1009 - 1990} \right) = 0.664$
 $(1 - a) = 0.336$

[32]

Functionality of first component (f_j)	2
Functionality of second component (f_k)	3
Molecular weight of mixture ($\bar{M}n_m$)	2500
Hydroxyl number of second component (OH_k)	57.2
Hydroxyl number of first component (OH_j)	55.4

$$a = \frac{2}{2500} \left[\frac{1000(56.1)(3) - 2500(57.2)}{55.4(3) - 57.2(2)} \right] = 0.391$$

$$(1 - a) = 0.609$$

[33]

Molecular weight of mixture ($\bar{M}w_m$)	1800
Molecular weight of second component ($\bar{M}w_k$)	2100
Molecular weight of first component ($\bar{M}w_j$)	920

$$a = \frac{1800 - 2100}{920 - 2100} = 0.254$$

$$(1 - a) = 0.746$$

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