John DeMar, john_demar@hotmail.com
6/1/2003, rev. 11/09/2005

Curative calculation for polymer binder and additives

The function of the curative is to link the OH of the binder (hydroxyl compound) with a NCO of the curative (isocyanate compound). Other liquid additives in the composite mixture may have OH equivalents and need to be taken into account when calculating the amount of curative.

The calculation is based on the *equivalent weight* (EW) of each compound. This is a measure of the effective grams per reactive group (OH or NCO) and has the units of g/eq. Some manufacturers specify this number directly and others give the *percent NCO* by weight (isocyanates) or the *hydroxyl number* in g-OH/g (polymer resins). Each of these must be converted to an EW to calculate the curative required for the overall mixture.

Equivalent weight for hydroxyl compounds (HTPB, etc.):

$$EW = \frac{56{,}100}{\text{Hydroxyl Number}} = \frac{1000}{\text{Hydroxyl Value}} = \frac{1700}{\%\text{OH}}$$

Equivalent weight for isocyanate compounds (MDI, Isonate, etc.):

$$EW = \frac{4200}{\%\text{NCO}}$$

Some EW's for common compounds used in composite propellants are:

Compound:	***EW***
Sartomer HTPB R45M	1370
Sartomer HTPB R45HTLO	1190
Sartomer HTPB R20LM	555
Tepanol (HX-878)	211
Castor Oil	164
Water	9
Curatives:	
TDI (generic)	87
IPDI (generic)	111
MDI (generic)	125
PAPI 94	131
Mondur MR	133
Isonate 143L	144
Desmodur E 744	179

Note: each batch of HTPB may have a slightly different equivalent weight; check with the supplier for the tested hydroxyl value or %OH. Also, the %NCO of curatives will decrease with age (EW will increase).

The general formula to calculate the amount of curative is as follows:

$$W_{curative} = (IR)(EW_{curative})\left(\sum_n \frac{W_n}{EW_n}\right)$$

where:

$W_{curative}$ = weight (mass) of curative (grams)

$EW_{curative}$ = NCO equivalent weight of curative

W_n = weight (mass) of each liquid compound

EW_n = OH equivalent weight for each liquid

IR = Index Ratio for NCO to OH (1.0 for ideal linkage)

Example:

Given the following portions of binder and other liquid ingredients, find the amount of Isonate 143L curative required for a full cure (index ratio of 1.0):

Ingredient	*grams*
R45HTLO	10
Tepanol	0.4
Castor Oil	0.3

$$W_{curative} = (1.0)(144)\left[\tfrac{10}{1190} + \tfrac{0.4}{211} + \tfrac{0.3}{164}\right] = 1.75 \text{ grams}$$

Reduce the index number to 0.95 to get a slightly softer propellant. Increase the index to 1.05 for a (possibly) harder propellant. Too much curative or too little curative will degrade the hardness by leaving behind unlinked liquids.

To mix two different curatives (for increased pot life, etc.), replace a percentage of one with the equivalent curing capacity of the other by weight. For example, to replace 20% of Isonate with IPDI in the above example:

$$W_{Isonate} = (0.8)(1.75) = 1.4 \text{ grams}$$
$$W_{IPDI} = (0.2)(111/144)(1.75) = 0.27 \text{ gram}$$

Note the ratio of the substitute EW over the original EW (111/144). It takes less IPDI to affect the same hardness as Isonate 143L but it will take much longer to fully cure.

*A trace amount of water in the ingredients will require more curative. In the above example, 0.01% H_2O requires 144 * 0.01/9 = 0.16 gram more curative.*