# Guidelines for Substituting Chlorendic Anhydride for Het® Acid in Esterification Processes such as Polyester or Alkyd Resin Manufacturing

## Stoichiometry

Het® Acid (HA) has a molecular weight of 388.8 g/mol. Chlorendic Anhydride (CA) has a molecular weight of 370.8 g/mol. On a 1:1 molar equivalent basis the mass charge of CA is less than the mass charge of HA. To calculate the charge of CA, multiply the charge of HA by the ratio of CA to HA molecular weights (i.e., 370.8/388.8 = 0.9537). If the HA charge was 1 kg, then the new CA charge is 1 kg * 0.9537 = 0.9537 kg CA.

In the above example the two materials were assumed to be 100% pure. In reality, this is not the case. The following example describes the methodology for using materials that are not 100% pure.

Example

1. HA charge is 1 kg of 99% pure HA. This calculates to 0.99 kg of pure HA.
2. The calculated equivalent charge of CA is 0.99 kg HA * 0.9537 = 0.9442 kg of CA.
3. If the purity of the actual CA is 97%, then the 0.9442 kg must be divided by 0.97 in order to calculate the correct charge. So, 0.9442 kg/0.97 = 0.9734 kg of 97% pure CA = 1 kg of 99% pure HA.

## Rate of Reaction

CA is an anhydride. Anhydrides react in polyesterification by first proceeding through a ring opening reaction and then proceeding through a direct esterification. HA reacts through two direct esterifications. The ring opening reaction occurs readily at temperatures above 60 °C and is mildly exothermic. Direct esterification reactions typically require a temperature above 120 °C and are endothermic.

## Water of Reaction

The ring opening reaction described above is a condensation reaction that does not produce water as a byproduct. As a result, the CA diesterification reaction only produces one mole of water per mole of CA. The diesterification of HA produces two moles of water per mole of HA. This results in the reduction of water production by one half.

## Solvent Content

CA contains approx. 3 weight % occluded hydrocarbon solvent. Accounting for the difference in assay due to the effect of solvents on purity is described in the Stoichiometry section of this document. These solvents are released when the CA is dissolved. It is recommended that the CA be charged to the glycol at a glycol temperature between 20 to 80 °C in order to minimize the rate of solvent release during charging.

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