temp
gas rate - HCl recirculation
liq rate
cat - amt
conc of K_2CO_3

MONSANTO COMPANY

Monsanto, Illinois

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SUBJECT: Distribution of Chlorinated Aromatic Compounds

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This is to summarize qualitatively the reaction mechanism in the chlorinators and orient plant experiments to obtain more uniform products.

The distribution of the chlorinated compounds is important for production of Aroclors and Monochlorophenols. The undesired under- and over-chlorinated products affect the thermochemical stability of Aroclors and the economics of phenol chlorination.

In an endeavor to analyze these chlorination processes, the following assumptions are made:

1. The chlorination takes place in the liquid phase as a homogeneous, bimolecular and irreversible reaction. The "bimolecular' implies that the reaction rates are proportional to the concentrations of chlorine and the particular aromatic compound in the liquid.

2. The chlorine first dissolves in the liquid and reacts only thereafter. The solution rate of chlorine is high enough so that it will not introduce a significant resistance to mass transfer.

3. Under plant conditions the chlorine concentration in the liquid is controlled by the chlorine feed rate. This assumption is supported by almost 100% chlorine utilization.

4. The local chlorine concentration in the liquid is controlled by the liquid mixing. This is accomplished by gas sparged agitation and by recirculation of the liquid around the reactor.

5. The heat of reaction is easily removed from the chlorinator.

It is worthwhile to note that the implication of assumption 3 is that presently plant capacity is limited by the chlorine feed rate. This in turn is restricted by the chlorine absorption capacity of the reactor. Because increase in production rate is not required, this aspect is not elaborated on.

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The above given assumptions allow the following conclusions to be drawn:

1. The distribution of the chlorinated compounds is governed by the relative-reaction-kinetic constants and the local concentration of the reactants. The relative-reaction-kinetic constants can be altered by temperature or catalysts only. Therefore; under the plant conditions they are not variables.

2. The relative-reaction-kinetic constants are not known, which means that limiting distribution cannot be computed for comparison with plant performance. The only apparent means to improve present distribution of the chlorinated products, if the limiting distribution has not yet been reached, is to increase liquid mixing.

ACTION:

The recommended action is to double the liquid recirculation rates around the Aroclor and Monochlorophenol reactors. Liquid and chlorine charge should remain the same. The results of these tests will indicate, whether or not present plant conditions provide adequate liquid mixing to approach the limiting distribution.

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