

Interoffice Communication

To A. J. Lundeen
From R. B. Merriam
Date September 23, 1983
Subject PVC Polymerization Kinetics--Initiator Parameter Evaluation

Summary

PED requests a pilot plant program be developed to determine kinetic parameters for several initiators used in PVC polymerization reactions. The kinetic parameters are used in a model to simulate reactor relief conditions. The simulations help assure adequate relief system capacity and safe operating conditions. PVC pilot plant tests are necessary because data from other sources (i.e. vendor literature) does not accurately predict actual polymerization rates.

Discussion

Several different initiators are used in our PVC plants. Kinetic parameters consistent with our model are needed for every initiator used in the plants. The kinetic parameters are used in a model to simulate reactor relief conditions. The simulations help assure adequate relief system capacity. The simulations are also used to evaluate safe operating conditions.

Initiator vendors normally supply kinetic data in their literature. However, vendor data is often insufficient to determine all the kinetic parameters needed for simulation. Also, vendor data has usually been determined by decomposing the initiator in various solvents rather than by actually polymerizing VCM. The solvent obtained data does not always accurately predict polymerization characterization factors. Using solvent obtained data rather than actual polymerization data could introduce errors as high as 10 percent in maximum heat release and 20 percent in poly time.

Good kinetic parameters can be obtained from heat release data for actual polymerization runs. PED requests pilot plant tests be run to determine the kinetic parameters for all initiators used in the plants. Additional runs should be performed to determine the effect on reaction rates of any Chain Transfer Agent (CTA) or Chain Coupling Agent (CCA) used in the production reactors. Kinetic parameters for L-225 and L-10 have previously been obtained from runs in the 50 gallon reactor. The procedure for these runs is outlined in David Lundeen's Research Report 820-10-1-79. The kinetic parameters for each initiator can be obtained with seven runs. The effect of CTA or CCA on reaction rates can be determined with one or two additional runs for each CTA or CCA.

DTH 000106599

A. J. Lundeen

Page 2

The HP data acquisition system has been used to obtain the heat release data from reactor R-110. It is now operational, but its accuracy is limited by the temperature probe accuracy. The inlet and outlet cooling probes are Resistance Temperature Devices (RTD's) with accuracy of only $\pm .5^{\circ}\text{F}$. Cooling water temperature differences at maximum heat release are only 5 to 6 $^{\circ}\text{F}$. This can lead to errors in predicted heat release rates of ± 15 to 20 percent. At conversions other than maximum heat release, the error can be higher. New probes with 0.001 $^{\circ}\text{F}$ accuracy are being installed to obtain good heat release data. These probes will give a heat release rate accuracy of better than 0.5 percent.

Ambient heat loss from the reactor should be determined to improve heat release data. A water-VCM mixture should be used as recommended in David Lundeen's Research Report 820-19-1-79. Other recommendations given in that report should also be considered.



Russell B. Merriam
Process Engineer
Chemicals Division
Process Engineering Department

em

CC:

GJH:RBQ:PAS:DRW:CRD:JHM:DAB

~~RAF:JPW:RDM:PVC GROUP~~

File: P-28

DTH 000106800