To: Brinkhuis, Randall[Brinkhuis.Randall@epa.gov]
Cc: Henry, Tala[Henry.Tala@epa.gov]; Krasnic, Toni[krasnic.toni@epa.gov]; Kennedy, Amuel[Kennedy.Amuel@epa.gov]; Blunck, Christopher[Blunck.Chris@epa.gov]; Fritz, Greg[Fritz.Greg@epa.gov]; Engler, Richard[Engler.Richard@epa.gov]; Townsend, Mark[Townsend.Mark@epa.gov]; Lee, Doyoung[Lee.Doyoung@epa.gov]; Fehrenbacher, Cathy[Fehrenbacher.Cathy@epa.gov]
From: Williamson, Tracy
Sent: Fri 1/24/2014 4:00:14 PM
Subject: RE: MCHM and other chemicals

Thanks Randy.

None of this is very sophisticated chemistry.

Reaction processes used to make an MCHM surfactant (34885-03-5, "Cyclohexanemethanol, 4-methyl-") are not very clean, so there are likely left over starting materials as well as byproducts in the mix that is the crude end product. Since this is used in coal processing (coal washing step), which is of course not at all sophisticated processing, the end product surfactant doesn't need to be cleaned up first (it can be used in crude form). So there are a number of chemicals in the crude product being used so there will be a number of chemicals in the spill. There are no mystery chemicals as the press is reporting.

From: Brinkhuis, Randall
Sent: Friday, January 24, 2014 10:39 AM
To: Williamson, Tracy; Fehrenbacher, Cathy
Cc: Henry, Tala; Krasnic, Toni; Kennedy, Amuel; Blunck, Christopher; Fritz, Greg; Engler, Richard; Townsend, Mark
Subject: MCHM and other chemicals

Tracy and Cathy,

Based on the information in the MSDS for Crude MCHM (the product) I looked up some of the chemicals in Kirk-Othmer and Ullmann's. If you already have this info, please disregard.

Kirk-Othmer didn't really have much of significance, but in Ullmann's I discovered that the last chemical listed on the MSDS, 1,4-cyclohexanedimethanol (CHDM) [CASRN 105-08-8], is a precursor for MCHM, with DMT [CASRN 120-61-6] and possibly DMHT [CASRN 94-60-0] being intermediates. CHDM was listed as a source for polyesters, so I assume that it's probably an HPV chemical.

I also noticed that two of the chemicals on the MSDS were carboxylates. Not being a chemist I don't know if these are related, but two cyclohexane carboxylic acids were referenced [CAS RNs 98-89-5 and 1076-97-7]. (I didn't look any further for info on those.)

Doing this the old-fashioned way (I looked up the chemicals in the indexes) I also noticed mention of a number of cyclohexane amines. While those wouldn't appear to be directly related to MCHM and CHDM, Ex. 5 - Deliberative Ex. 5 - Deliberative I mention that only because of one of the texts mentioning that liquid cycloaliphatic amines and diamines possibly being isocyanate precursors. Not being a chemist I don't know, but figured those of you who are chemists would know if that was possible and, if so, whether it is significant.

Neither of the texts went into detail about breakdown products of MCHM. Oh, and I did check the Merck Index for the three non-water chemicals that were listed as being 5% or greater on the MSDS (I thought there might be mention of a patent), but none of the three [CAS RNs 34885-03-5, 98955-27-2, or 51181-40-9] were listed in Merck.

Randy

"Knowing is not enough; we must apply. Willing is not enough; we must do." —Goethe

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