Memo 7

DIVERSIFIED CHEMICAL PRODUCTS
Research and Product Development Division
Blacksburg VA

TO: U. R. Engineer
FROM: Phil D. Chemist
DATE: 2006 Sep 22
SUBJECT: Physical Property Data for Lucretex Components

This memo provides physical property data for all the components in the case-study. Table 1 contains pure-component property values.

Models for Temperature-Dependent Pure-Component Properties (see Table 2)

Ideal Gas Heat Capacity (J kmol^{-1} K^{-1}):

$$C_{p,ig} = A_1 + A_2T + A_3T^2 + A_4T^5 + A_5T^4 + A_6T^5 \qquad A_7 \le T \le A_8$$
$$= A_9 + A_{10}T^{A_{11}} \qquad T < A_7$$

Extended-Range Antoine Equation for Vapor Pressure (N m^{-2}):

$$\ln P_s = B_1 + \frac{B_2}{T + B_3} + B_4T + B_5 \ln T + B_6T^{B_7} \qquad B_8 \le T \le B_9$$

Binary Wilson Model for Activity Coefficients (see Table 3)
The liquid interactions between components i and j are represented by the Wilson liquid solution model in the following form:

$$\ln \gamma_i = 1 - B_i - \sum_{j=1}^{n} e^{a_{ji} + \frac{b_{ji}}{T} - B_j} x_j$$

$$B_i = \ln\left[\sum_{j=1}^{n} e^{a_{ij} + \frac{b_{ij}}{T}} x_j\right]$$

where γ_i denotes the activity coefficient of component i, a_{ij} and b_{ij} represent binary interaction parameters between component pairs (i, j), and T denotes the temperature (in kelvins) of the system. All available binary interaction parameters are shown in Table 3.