pH-Meter Simulation with Sensitivity Analysis (PH-METER)

DESCRIPTION:

This seemingly simple job demonstrates ChemCAD's Electrolyte package and Sensitivity Analysis. By simple assumption we simulate neutralization of phosphoric acid with sodium hydroxide.

NOTES:

- 1. The electrolyte system works in Apparent Component Approach mode (separate lists are kept for regular components and for electrolytes.) To build the ionic system for NaOH/H3PO4, it is enough to select Sodium Hydroxide, Phosphoric Acid and Water to the Component List, launch the Comp/ Electrolytes option, and accept all defaults by pressing ESC for several times. As we operate with dilute solutions, there is no need to select any hydrate nor solid component to the system.
- 2. A simple assumption was made to simulate pH-meter operation: when two streams are mixed together, and the ionic reaction is instantaneous, then the time factor can be neglected, and the stream flowrates will represent mass. The stream #1, the phosphoric acid solution is kept at fixed

rate. The stream of sodium hydroxide is added at increasing rate by Sensitivity Analysis (SA).

3. Please open our SA by Run/Sensitivity/Run Old Analysis option, and review the X-Y Data. The SA is increasing the NaOH solution flowrate to achieve molar ratio of NaOH:H3PO4 = 3.01, and it is recording stream parameter 22, the pH-value of the product stream. Display X-Y Plot of pH-value of the product as a function of NaOH added. The changes in pH-value are buffered by phosphate equilibria:

$$H_3PO_4 = H^+ + H_2PO_4^-$$

 $H_2PO_4^- = H^+ + HPO_4^{-2}$
 $HPO_4^{-2} = H^+ + PO_4^{-3}$

4. The chemist's flask and the pH-meter symbol were made as Unit Icons, for MIXEr and PRODuct respectively. User-Added Unit Icons are stored in file ICONS.UF, in the directory CC3DATA. We moved this specific file to the job's subdirectory, PH-METER, so it would not get in conflict with Icons you have made so far.

