

WEDNESDAY, AUGUST 24, 2005, A.M.

SESSION 32: INTERNATIONAL SYMPOSIUM ON COMPUTATIONAL ANALYSIS IN HYDROMETALLURGY (35TH ANNUAL HYDROMETALLURGY MEETING)

CHEMICAL AND PHYSICAL MODELING I

Sponsor(s): Hydrometallurgy Section, The Metallurgical Society of CIM

Room: Herald

Chairmen: D. DIXON, University of British Columbia, Canada and
D. BERKLEY, H.G. Engineering, Canada

PAPER 32.1—8:30

A COMPREHENSIVE MODEL FOR CALCULATING PHASE EQUILIBRIA AND THERMOPHYSICAL PROPERTIES OF ELECTROLYTE SYSTEMS.

P. WANG, A. ANDERKO, R.D. YOUNG and R.D. SPRINGER, OLI Systems Inc., U.S.A.

A thermodynamic model has been developed for calculating phase equilibria and other properties of multicomponent electrolyte systems. The model has been designed to reproduce the properties of both aqueous and mixed-solvent electrolyte systems ranging from infinite dilution to solid saturation or pure solute limit. The model incorporates formulations for the excess Gibbs energy and standard-state properties coupled with an algorithm for detailed speciation calculations. The excess Gibbs energy model consists of a long-range interaction contribution represented by the Pitzer-Debye-Hückel expression, a second virial coefficient-type term for specific ionic interactions and a short-range interaction term expressed by the UNIQUAC equation. The accuracy of the model has been demonstrated for common acids and bases and for multicomponent systems containing aluminum species in various environments.

PAPER 32.2—8:55

CHEMICAL MODELLING IN HYDROMETALLURGY USING OLI.

H. LIU, V.G. PAPANGELAKIS and J.F. ADAMS, University of Toronto, Canada

Chemical modelling is becoming increasingly useful in the development, analysis, design, and control of hydrometallurgical processes. The paper presents the development of reliable databases for chemical modelling of selected hydrometallurgical systems using state-of-the-art software, such as OLI. The modelling strategies are also demonstrated. The high pressure acid leaching (HPAL) of laterites, oxygen solubility in the oxidative leaching process of zinc sulfide, gypsum solubility and lead chemistry in mixed sulfate-chloride solutions are presented as case studies. This on-going work attempts to bridge the gap between theoretical research and industry needs.

PAPER 32.3—9:20

SPECIATION FOR AQUEOUS SYSTEMS – AN EQUILIBRIUM CALCULATION APPROACH.

H.-H. HUANG, L.G. TWIDWELL and C.A. YOUNG, Montana Tech, U.S.A.

Equilibrium calculational software programs can be effectively utilized to model important parameters in aqueous and aqueous/solid systems, e.g., activity or concentration, solubility, temperature, solution pH, solution potential, and ligand complexation. In this regard, the calculational program STABCAL will be demonstrated. Illustrative examples for the creation of diagrams such as potential-pH, and activity or concentration-pH will be presented to demonstrate the fundamentals in real hydrometallurgical systems. Speciation, titration and mixing will be used to simulate or predict operational processes. Berkeley Pit water from a flooded abandoned copper open-pit mine will be used to illustrate the modeling process. According to analytical results the water contains about 20 important constituents. In addition to measured potential and dissolved oxygen, there are two distinctive oxidation/reduction couples. Concentration and other experimental parameters are seldom matched to each other and 12 different conditions have been identified. Water for each condition must be speciated in order to find the best-fit model. The STABCAL program will be used for the modeling calculations and the implication of the water chemistry to defining treatment opportunities will be discussed.

PAPER 32.4—9:45

THERMODYNAMICALLY CONSISTENT VERSUS COMPLETELY EMPIRICAL PROPERTY MODELS IN PROCESS SIMULATION.

M.W. WADSLEY, Austherm Pty. Ltd., Australia

Physical and chemical property models are widely used in process engineering. There exist, in the published literature, completely empirical models of “thermodynamic properties”, that is, property models that are not consistent with the laws of thermodynamics. There also exist property models that purport to be thermodynamically consistent

but are flawed in their implementation. There are also published property models that are consistent with the laws of thermodynamics but that do not reproduce property values with an acceptable accuracy. A practicing engineer might be asked to assess very different property models for which there are a variety of claims. This paper discusses features of thermodynamic and empirical property models that may assist in their practical evaluation and implementation.

COFFEE BREAK—10:10-10:40

PAPER 32.5—10:40

MODELLING OF PHASE TRANSFORMATIONS AND EQUILIBRIA OF CALCIUM SULFATE HYDRATES IN CONCENTRATED AQUEOUS CHLORIDE SOLUTIONS USING THE OLI SOFTWARE.

Z. LI and G.P. DEMOPOULOS, McGill University, Canada

The solubilities of calcium sulfate in HCl-CaCl₂-H₂O solutions up to 100°C were successfully modelled with the aid of OLI software after bringing proper modification to it. Modelling, more specifically, was carried out with the help of the Environmental Simulation Program, V-6.6.0.4 (www.olisystems.com). New model parameters were obtained by regressing the solubility data. A private databank was established by adding the newly defined model parameters and the calcium sulfate hemihydrate phase that is not included in the original OLI database. The McGill-modified OLI software was successfully applied not only to modelling solubilities but also the transformation of the various CaSO₄ phases, namely dihydrate, hemihydrate and anhydrite. In this paper, the modelling methodology will be discussed along with a comparison of the capabilities of the newly developed model vs the original OLI model.

PAPER 32.6—11:05

MODELLING THE HIGH PRESSURE LEACHING OF LATERITE USING ASPEN PLUS AND OLI.

M. DRY, V. PAPANGELAKIS and M. CHEUNG, University of Toronto, Canada

The high pressure acid leaching of laterite was modelled and simulated using a combination of two commercially available software packages, namely Aspen Plus 11.1 and the OLI Stream Analyzer. New kinetic parameters for the acid-controlled metal dissolution and precipitation reactions at temperature were first determined from previous experimental data on the leaching of limonite. A grain model with cylindrical pellets was used to model the solid-liquid dissolution reactions. Precipitation reactions were modeled via aqueous equilibrium chemistry. A dedicated thermodynamic database previously developed at the University of Toronto was used in conjunction with the OLI software to model the solution chemistry and calculate the concentration of hydrogen ions in solution at the leaching temperature. Mass balances were handled by Aspen Plus. The simulation gave good predictions of nickel dissolution under industrial and laboratory conditions, for the dissolution of limonite and limonite/saprolite blends.

PAPER 32.7—11:30

CHEMICAL TITRATION SIMULATION – AN EQUILIBRIUM CALCULATION APPROACH.

H.-H. HUANG, L.G. TWIDWELL, C.G. ANDERSON and C.A. YOUNG, Montana Tech, U.S.A.

An equilibrium calculational computer program (STABCAL) can be used for titration simulation. The program can handle various forms of titrants: solid, aqueous, gaseous or another solution, and various type of reactions: reductive, oxidative and adsorption. Background chemistry, mathematical considerations, and program development will be illustrated. Also, simple titration applications such as how to determine the acidity of aqueous solutions and alkaline sulfide leaching of gold are presented. Processing of an acid mine water from the Berkeley Pit in Butte, Montana has been used for illustration purposes. The treatment studies included: cementation, sulfidization, and neutralization. The calculational results for the neutralization treatment using various alkaline reagents are compared to actual experimental data and potentially appropriate processes are discussed.