ENVIRONMENTAL AND WASTE MANAGEMENT: ADVANCES THROUGH THE ENVIRONMENTAL MANAGEMENT SCIENCE PROGRAM Metal and Organic Contamination

Cosponsored with the Division of Analytical Chemistry Cosponsored with the Division of Nuclear Chemistry Cosponsored with the Committee on Environmental Improvement

> DIVISION OF ENVIRONMENTAL CHEMISTRY 227<sup>th</sup> American Chemical Society meeting Anaheim, CA Wednesday, March 31, 2004 POSTER SESSION 6:00 – 8:00 p.m.

**Organizers: T. Zachry** 

Presiding: T. Zachry

Paper

Effects of FeS on Cr(III) oxidation mediated by manganese oxidizers. Y. Wu and B. Deng

Comparative analysis for polluted agricultural soils with arsenic, lead and mercury in Mexico. M. Yarto-Ramirez, E. S. Santos, <u>A. Gavilan-Garcia</u>, J. Castro-Diaz, I. G. Gavilan, R. Rosiles and S. Suarez-Torres

Kinetic modeling of oxidative coagulation for arsenic removal. <u>J.-W. Kim</u> and T.A. Kramer

**Influence of pH and redox conditions on copper leaching.** <u>R. Kavanaugh</u>, S.R. Al-Abed, J. Purandare and D. Allen

Effect of EDTA on Pb(II) uptake and translocation by Tumbleweed (Salsola kali): Agar and hydroponics studies. <u>G. De la Rosa</u>, J.L. Gardea-Torresdey, J. Peralta-Videa and M. Aldrich

Microbial flocculant for nature soda. P. Qin, T. Zhang and C. Chen

Reaction mechanism of using bi-metallic nanoparticles to remove chlorinated solvent. J.-J. Horng and S.-H. Hsieh

Reduction of aromatic hydrocarbons by zero-valent iron and palladium catalyst. <u>Y.-H. Kim</u>, W.S. Shin, S.-O. Ko and M.-C. Kim

Effects of organic matter heterogeneity on sorption and desorption of hydrophobic organic chemicals (HOCs) by Pahokee peat soil. <u>W. Huang</u>, Z. Yu, J. Song and P. Peng

**Photooxidation of isopropanol and acetone using TiO<sub>2</sub> suspension and UV light.** M.A. Nanny and <u>T.M. El-Morsi</u>

**Decomposition of perfluorocompounds on an alumina-based catalyst.** <u>S. Kanno</u>, S. Tamata and H. Kurokawa

Kinetic study of OH reactions with *n*-octane and *n*-decane using relative rate combining with discharge fast flow and mass spectrometer technique. <u>Z. Li</u>

On line derivatization gas chromatography ion trap mass spectrometry for determination of endocrine disruptors in surface water. <u>S.H. Tzing, Sr.</u> and Y.C. Ling, Sr.

High throughput screening for the discovery of more efficient catalysts for emissions control. <u>A. Hagemeyer</u>, A.F. Volpe, Jr. and K. Yaccato

**Preparation of clay brick using coal waste.** <u>J.W. Yoo</u>, J.H. Jung, J.M. Kim, S.M. Lee and H.T. Kim

Using STELLA system dynamic model to analyze greenhouse gases' emission from solid waste management in Taiwan. J.-J. Horng, R.F. Lee and K.Y. Liao

## ABSTRACTS

Effects of FeS on Cr(III) oxidation mediated by manganese oxidizers. Youxian Wu and <u>Baolin Deng</u>; Department of Civil and Environmental Engineering, University of Missouri-Columbia, Columbia, MO 65211, Fax: 573-882-4784, <u>wuy@missouri.edu</u>, <u>dengb@missouri.edu</u>.

Reductive immobilization of Cr(VI) has been widely explored as a cost-effective approach for Cr-contaminated site remediation. The long-term stability of the immobilized Cr(III), however, is a concern. Cr(III) is known to be oxidized by Mn oxides chemically and Mn-oxides could be produced through microbially mediated Mn(II) oxidation. This study examined the effect of FeS on Cr(III) oxidation mediated by *Pseudomonas putida*. The results showed that commercial granular FeS did not affect Cr(III) oxidation in the culture of *P. putida* with Mn(II), but freshly precipitated FeS slurry inhibited Cr(III) oxidation. A 10 mg/I of FeS did not inhibit the microbial growth, but delayed the production of Mn oxides, thus postponing potential Cr(III) oxidation. In the presence of excessive FeS slurry, both Cr(VI) and Mn oxides were reduced rapidly. The reduced Cr(III) could not be re-oxidized as long as freshly formed FeS was present, even in the presence of the manganese oxidizers.

**Comparative analysis for polluted agricultural soils with arsenic, lead and mercury in Mexico.** Mario Yarto-Ramirez<sup>1</sup>, Elvira S. Santos<sup>2</sup>, <u>Arturo Gavilan-Garcia<sup>1</sup></u>, Jose Castro-Diaz<sup>1</sup>, Irma G. Gavilan<sup>2</sup>, Rene Rosiles<sup>3</sup> and Sara Suarez-Torres<sup>2</sup>; <sup>1</sup>Direccion de Investigacion sobre Sustancias Quimicas y Riesgos Ecotoxicologicos, Instituto Nacional de Ecologia, Periferico Sur 5000, Mexico City, Mexico, Fax: 52-555-424-5402, <u>myarto@ine.gob.mx</u>, <u>agavilan@ine.gob.mx</u>; <sup>2</sup>Environmental Division, Chemistry School, UNAM; <sup>3</sup>Nutricion Animal, Facultad de Medicina Veterinaria y Zootecnia.

The use of mercury in Mexico has been associated with the mining industry of Zacatecas. This activity has polluted several areas currently used for agriculture. The main objective of this study was to investigate the heavy metal concentration (Hg, As and Pb) in soil of Guadalupe Zacatecas in order to justify a further environmental risk assessment in the site. A 2X3 km grid was used for the sampling process and 20 soil samples were taken. The analysis was developed using EPA SW 846: 3050B/6010B method for arsenic and metals and EPA SW 846: 7471A for total mercury. It was concluded that there are heavy metals in agricultural soils used for corn and bean farming. For this it is required to make an environmental risk assessment and a bio-availability study in order to determine if there's a risk for heavy metals bioaccumulation in animals or human beings or metal lixiviation to aquifers.

Kinetic modeling of oxidative coagulation for arsenic removal. Jin-Wook Kim and Timothy A. Kramer; Department of Civil Engineering, Texas A&M University, WERC 205X, College Station, TX 77843, <u>waterkim@neo.tamu.edu</u>.

A model of oxidative coagulation consisting of Fenton's reagent (Fe(II)/H<sub>2</sub>O<sub>2</sub> at pH 7.0) was established. The optimum condition was found when the mole ratio of As(III):H<sub>2</sub>O<sub>2</sub>:Fe(II)=1:15:20. In this optimum condition, all of Fe(II) was converted to HFO (am-Fe(OH)<sub>3</sub>) and precipitated to be used as the oxidized arsenic(V) adsorbent and particle coagulant. Two sorption models consisting of a surface complexation model and a kinetic model were developed and coupled. Using the coupled sorption model, the kinetics of HFO surface charge/potential during As(V) sorption was calculated. Further, during arsenic sorption, the colloid stability kinetics resulting from the perikinetic coagulation mechanism was calculated by considering interparticle forces. Colloid surface potential was decreased from 60 mv to 12 mv in proportion to the amount of arsenic adsorbed onto HFO and this surface potential directly affected the colloid stability (collision efficiency) (Figs. 1 and 2).



**Influence of pH and redox conditions on copper leaching.** <u>Rathi Kavanaugh</u><sup>1</sup>, Souhail R. Al-Abed<sup>2</sup>, Jaydeep Purandare<sup>3</sup> and Derrick Allen<sup>2</sup>; <sup>1</sup>University of Cincinnati-Onsite EPA Contractor, 5995 Center Hill Ave., Cincinnati, OH 45224, Fax: 513-569-7879; <sup>2</sup>National Risk Management Research Laboratory, U.S. Environmental Protection Agency; <sup>3</sup>England Geosystem.

The Toxicity Characteristic Leaching Procedure (TCLP) is a regulatory leach test in the RCRA programs. It was developed to determine the leaching potential of landfilled waste in order to assess the hazards associated with the leachates. The test was developed to study concentration of hazardous materials in leachates, under a mismanagement scenario, when they are co-disposed with municipal waste. The test uses leaching of waste at either of two acidic pH values *i.e.*, 2.8 and 4.93. While low pH leachant can extract many metals, some metals soluble at higher pH values are either underestimated or totally unaccounted for. The method also has limitations for application to different waste matrices. The procedure does not take into account the effect of redox conditions on leaching. Leaching studies are, therefore, being conducted to determine the effect of combinations of Eh and pH on the leaching potential of mineral and organic wastes. The goal of this study is to propose alternate methods applicable for a variety of waste matrices. The presentation will discuss the effects of combinations of pH and redox conditions on the leaching behavior of copper from a mineral processing waste.

Effect of EDTA on Pb(II) uptake and translocation by Tumbleweed (*Salsola kali*): Agar and hydroponics studies. <u>Guadalupe De la Rosa</u><sup>1</sup>, Jorge L. Gardea-Torresdey<sup>2</sup>, Jose Peralta-Videa<sup>2</sup> and Mary Aldrich<sup>1</sup>; <sup>1</sup>Environmental Science and Engineering, The University of Texas at El Paso, 500 W. University, El Paso, TX 79968, Fax: 915-747-5748, <u>gdelarosa@utep.edu</u>; <sup>2</sup>Department of Chemistry, University of Texas at El Paso.

Environmental accumulation of Pb represents a worldwide health hazard. While conventional cleanup techniques are generally expensive and soil disturbing, phytoremediation represents an inexpensive friendly option for the removal of contaminants from soil and water. In this research, tumbleweed (*Salsola kali*) plants exposed for 15 days to Pb(NO<sub>3</sub>)<sub>2</sub> at 80 and 125 ppm in hydroponics and agar media, demonstrated a high capacity to uptake lead. The results showed that the plants cultivated in agar accumulated 25563, 5534 and 2185 mg Pb kg<sup>-1</sup> DW in roots, stems and leaves, respectively. Moreover, Pb concentrations found in hydroponically grown tumbleweed plants tissues were 30744, 1511 and 1421 mg kg<sup>-1</sup> DW in roots, stems and leaves, respectively. It was observed that EDTA enhanced Pb translocation. No Pb phytotoxic effects were observed during the experimental time period. Cellular structural features were also observed using TEM.

**Microbial flocculant for nature soda.** <u>Peiyong Qin</u><sup>1</sup>, Tong Zhang<sup>2</sup> and Cuixian Chen<sup>1</sup>; <sup>1</sup>Department of Chemical Engineering, Tsinghua University, Beijing 100084, China; <sup>2</sup>Institute of Chemical Engineering, Inner Mongolia Polytechnic University.

Microbial flocculant for nature soda has been studied. *Lactobacillus* TRJ21, which was able to produce an excellent biopolymer flocculant for nature soda, was obtained in our lab. The microbial flocculant was mainly produced when the bacteria laid in stationary growth phase. Fructose or glucose, as carbon sources, were more favorable for the bacterial growth and flocculant production. The bacteria was able to use ammonium sulfate or Urea as nitrogen to produce flocculant, but was not able to use peptone effectively. High C/N ratio was more favorable to *Lactobacillus* TRJ21 growth and flocculant production than low C/N ratio. The biopolymer flocculant was mainly composed of polysaccharide and protein with a molecular weight 1.38x10<sup>6</sup> by gel permeation chromatography. It was able to be easily purified from the culture medium by acetone. Protein in the flocculant was tested for the flocculating activity ingredient by heating the floccuant.

**Reaction mechanism of using bi-metallic nanoparticles to remove chlorinated solvent.** Jao-Jia Horng and Su-Hwei Hsieh; Department of Safety, Health and Environment, National Yulin University of Science and Technology, 123 University Road Section 3, Touliou 640, Taiwan, Fax: 886-5-532-6202, <u>horngij@yuntech.edu.tw</u>.

Abstract not available.

**Reduction of aromatic hydrocarbons by zero-valent iron and palladium catalyst.** <u>Young-Hun Kim</u><sup>1</sup>, Won Sik Shin<sup>2</sup>, Seok-Oh Ko<sup>3</sup> and Myung-Chul Kim<sup>4</sup>; <sup>1</sup>School of Environmental Science, Pusan Catholic University, #9 Pugok 3-dong, Keumjeong-gu, Pusan 609-757, South Korea, Fax: 82-51-510-0638, <u>youngkim@cup.ac.kr</u>; <sup>2</sup>School of Civil and Environmental Engineering, Kumoh National Institute of Technology; <sup>3</sup>Department of Civil Engineering, Kyunghee University; <sup>4</sup>School of General Education, Kyungil University.

Permeable reactive barrier (PRB) is an alternative technology for soil and groundwater remediation. Zero valent iron, which is the most popular PRB material, is only applicable to halogenated aliphatic organics and some heavy metals. The objective of this study was to investigate reductive dechlorination of halogenated compounds and reduction of non-halogenated aromatic hydrocarbons using zero valent metals (ZVMs) and catalysts as reactive materials for PRBs. A group of small aromatic hydrocarbons such as monochlorophenols, phenol and benzene were readily reduced with palladium catalyst and zero valent iron. Poly-aromatic hydrocarbons (PAHs) were also tested with the catalysts and zero valent metal combinations. The aromatic rings were reduced and partly reduced PAHs were found as the daughter compounds. The current study demonstrates reduction of aromatic compounds by ZVMs and modified catalysts and

implicates that PRB is applicable not only for halogenated organic compounds but nonhalogenated aromatic compounds such as PAHs.

Effects of organic matter heterogeneity on sorption and desorption of hydrophobic organic chemicals (HOCs) by Pahokee peat soil. Weilin Huang<sup>1</sup>, Zhiqiang Yu<sup>2</sup>, Jianzhong Song<sup>2</sup> and Ping'an Peng<sup>2</sup>; <sup>1</sup>Department of Environmental Sciences, Rutgers University, New Brunswick, NJ 08901-8551, whuang@envsci.rutgers.edu; <sup>2</sup>Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou 510640, China.

Previous studies have shown that isotherm nonlinearity, varied sorption capacity and sorption-desorption hystersis relate primarily to the heterogeneity of soil organic matter (SOM). A comprehensive wet chemical isolation procedure was used to isolate and quantify into four fractions from Pahokee peat soil: (1) demineralized pahokee peat soil, (2) humic acids + kerogen + BC (HKB), (3) kerogen and (4) humic acid (HA). The major physical and chemical properties of each fraction were characterized using different techniques, such as Scanning Electron Microscopy, <sup>13</sup>C-Nuclear Magnetic Resonance Spectroscopy, etc. The impact of SOM heterogeneity on sorption and desorption equilibria by isolated fractions and original soil was conducted using phenanthrene, naphthalene, 1,2-dichlorobenzene and 1,3,5-trichlorobenzene as sorbates. The data indicated that isolated HKB and kerogen fractions exhibit more nonlinear isotherms, greater sorption capacities and desorption hysteresis than that of HA and their original soil. The role of HA to the overall sorption by soil is less significant compared to HKB and kerogen. The sorption capacity and nonlinearity of demineralized Pahokee Peat soil is greater than original soil which suggested that SOM particle may enwrap up by the inorganic and clay materials, therefore sorbate molecules are not accessible to the surface of SOM particle. The results suggested that kerogen and BC may dominate the overall nonlinear sorption by soil and sediments. The contribution of HA in the overall sorption is different from previous studies. It may be caused by different chemical isolation procedures and needs further investigation.

Photooxidation of isopropanol and acetone using TiO<sub>2</sub> suspension and UV light. Mark A. Nanny and <u>Taha M. El-Morsi</u>; School of Civil Engineering and Environmental Science, University of Oklahoma, 202 West Boyd, Room 334, Norman, OK 73019, Fax: 405- 325-4217, <u>nanny@ou.edu</u>, <u>telmorsi@ou.edu</u>.

Small polar organic compounds such as alcohols, ketones and aldehydes are highly soluble and do not adsorb strongly to the  $TiO_2$  surface and, therefore, may be fairly resistant to photocatalytic degradation. Photodegradation of an aqueous solution of isopropanol and its resulting photodegradation product acetone was investigated as a function of  $TiO_2$  substrate concentrations and solution ionic strength and pH. In the presence of 2g/L TiO<sub>2</sub>, isopropanol completely disappeared within 3 hrs, resulting in the nearly complete transformation into acetone. Subsequent photodegradation of acetone occurred at a much slower rate and resulted in complete mineralization. Increasing the

pH slightly decreased the photodegradation rate. Conversely, the degradation rate was enhanced slightly by increasing the ionic strength. The presence of tetranitromethane decreased the isopropanol degradation significantly. This result, combined with the minimal degree of adsorption of isopropanol and acetone onto the surface of the photocatalyst, suggests that the photodegradation pathway occurs *via* free •OH radicals in bulk solution rather than on the catalyst surface.

**Decomposition of perfluorocompounds on an alumina-based catalyst.** <u>Shuichi</u> <u>Kanno</u><sup>1</sup>, Shin Tamata<sup>2</sup> and Hideaki Kurokawa<sup>3</sup>; <sup>1</sup>Power & Industrial Systems R & D Laboratory, Hitachi, Ltd., 832-2 Horiguchi, Hitachinaka-shi Ibaraki-ken 312-8507, Japan, Fax: 81-29-276-5783, <u>shuuichi kanno@pis.hitachi.co.jp</u>; <sup>2</sup>Hitachi Works, Hitachi, Ltd.; <sup>3</sup>Power & Industrial Systems Environmental Systems Business Div, Hitachi, Ltd.

The control of the atmospheric release of PFCs (perfluorocompounds) is an important environmental problem worldwide. PFCs are powerful greenhouse gases used by the semiconductor and liquid crystal industries as etching and cleaning agents. We developed a catalyst that decomposes PFCs with only water. Al<sub>2</sub>O<sub>3</sub> was selected from the survey of some single metal-oxide catalysts. Addition of another metal-oxide improved the decomposition ratio and durability. The Al<sub>2</sub>O<sub>3</sub>-based catalyst decomposed  $CF_4$ ,  $C_2F_6$ ,  $C_3F_8$ ,  $C_4F_8$ ,  $NF_3$  and  $SF_6$  by more than 99% at 750 degrees Celsius. Furthermore, our catalyst retained a high decomposition ratio as demonstrated by a continuous run for about 4000 hours at 700-750 degrees Celsius. The influence of chlorine as an impurity with regard to the SF<sub>6</sub> decomposition ratio on the catalyst was examined. SF<sub>6</sub> was decomposed at more than 99% during 8 hours in the presence of 400 ppm chlorine. Chlorine concentration in the outlet gas was less than TLV. No chlorine compounds were found by X-ray diffraction analysis of the used catalyst. That is, the hydrogenation of chlorine did not inhibit the surface catalytic reaction for PFC. Also, CF<sub>4</sub> was decomposed at the condition of 1.4% of high concentration. The conversion remained higher than 99% throughout during a durability test. Furthermore, we investigated a large-scale decomposition system in the paper.

Kinetic study of OH reactions with *n*-octane and *n*-decane using relative rate combining with discharge fast flow and mass spectrometer technique. Zhuangjie Li; Department of Chemistry and Biochemistry, California State University, Fullerton, 800 N. State College, Fullerton, CA 92834, Fax: 714-626-8010, zli@exchange.fullerton.edu.

The combination of the relative rate method with the discharge fast flow/mass spectrometer technique (RR/DF/MS) has been developed to measure the rate constants for gas phase reactions involving OH radicals. The RR/DF/MS technique was used to measure the rate constant for reactions of the OH radical with *n*-octane (k<sub>3</sub>) and cyclohexane (k<sub>5</sub>) using 1,4-dioxane as a reference compound and with *n*-decane (k<sub>6</sub>) using *n*-octane and 1,4-dioxane as reference compounds. At 298 K, these rate constants were determined to be k<sub>3</sub>=(8.88 ± 0.31) x 10<sup>-12</sup>, k<sub>5</sub>=(6.95 ± 0.20) x 10<sup>-12</sup> and

 $k_6$ =(1.38 ± 0.08) x 10<sup>-11</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>, respectively, which are in very good agreement with those measured using different techniques. The features of the RR/DF/MS technique are discussed.

On line derivatization gas chromatography ion trap mass spectrometry for determination of endocrine disruptors in surface water. Shin Hwa Tzing, Sr. and Young Chien Ling, Sr.; Chemistry, National Tsing Hua University, 101, Section 2 Kuang Fu Road, Hsinchu, Taiwan 300, Republic of China, Hsinchu 300, Taiwan, Fax: 886-03-5711082, tzing@gmlab.chem.nthu.edu.tw.

A method has been developed for the determination of endocrine disruptors (EDs) (containing hydroxyl groups) in surface water from different sources. The surface water samples from different sites including school and local dormitory sewage effluents. lake water and river water were collected and analyzed. In this method, the pretreated sample is directly analyzed by GC-MS using on-line derivatization, where tetramethylammonium hydroxide (TMA-OH) was used as the derivatizing agent. Use of large-volume direct sample introduction (DSI) and co-injection of the sample and TMA-OH avoids external contaminations as observed in conventional derivatization protocols. Additionally, the use of chemical ionization (CI) and CI-MS/MS could enable detection of EDs at lower concentrations and reduce the matrices' interference thereby enhancing detection sensitivity of EDs for quantification. In this work, the use of dichloromethane as CI reagent for EDs is reported for the first time and could detect EDs to concentrations as low as 0.5 pg/mL. The recovery ranged from 74 to 112 % and the relative standard derivations for replicate analyses ranged from 5 to 17 %. We hope that this method will be applicable for routine analysis of EDs with hydroxyl functional groups.

High throughput screening for the discovery of more efficient catalysts for emissions control. <u>Alfred Hagemeyer</u>, Anthony F. Volpe, Jr. and Karin Yaccato; Heterogeneous Catalysis, Symyx Technologies, 3100 Central Expressway, Santa Clara, CA 95051, Fax: 408-748-0175, <u>ahagemeyer@symyx.com</u>.

High-throughput synthesis and screening methods have been developed for the discovery of highly active catalysts for the control of emissions from stationary and mobile sources. Low temperature CO oxidation, CO methanation, NO<sub>x</sub> abatement and the destruction of Volatile Organic Compounds (VOCs) will be discussed. The discovery libraries for primary screening consisted of both 11x11 and 16x16 catalyst arrays on 3" and 4" quartz wafers, respectively. Catalysts were prepared by robotic liquid dispensing techniques and screened for catalytic activity in Symyx's Scanning Mass Spectrometer. The screening protocols encompassed mixed metal oxides, perovskites and supported base and noble metals. Active hits were further optimized in focus libraries using shallower compositional gradients. The ScanMS is a fast serial screening tool that uses flat wafer catalyst surfaces, local laser heating, a scanning/sniffing nozzle and a quadrupolar mass spectrometer to compare relative catalytic activities. The temperature

range from 200C to 600C is accessible. Typically, 256 catalysts can be screened per day and about 100,000 experiments conducted annually.

**Preparation of clay brick using coal waste.** Jung W. Yoo, Jin H. Jung, Jae M. Kim, Sung M. Lee and Hyung T. Kim; Material Team, Korea Institute of Chemical Engineering & Technology, 233-5, Gasan-Dong, Guemcheon-Gu, Seoul 153-801, South Korea, Fax: 82-2-867-6251, jwyoo@kicet.re.kr.

A great deal of coal waste produced during the development of a mine was accumulated around the mine, which caused many problems such as traffic, acid mine drainage and damage of forest and scenery. Carbon in the coal waste helps calcination of the brick even at low temperature. Considering the reuse of natural waste and energy saving, clay brick was prepared using coal waste under various conditions, including particle size, amount of coal waste mixed, calcination temperature and pressing pressure. The specimens were characterized by XRD, SEM and TG-DTA and interpreted in terms of water absorption and compressive strength.

Using STELLA system dynamic model to analyze greenhouse gases' emission from solid waste management in Taiwan. Jao-Jia Horng, R. F. Lee and K. Y. Liao; Department of Safety, Health and Environment, National Yulin University of Science and Technology, 123 University Road Section 3, Touliou 640, Taiwan, Fax: 886-5-532-6202, horngji@yuntech.edu.tw.

Using a system dynamic model (SDM), such as STELLA, to analyze the waste management policy is a new trial for Taiwan's research communities. We have developed an easy and relatively accurate model for analyzing the greenhouse gases' emission for the wastes from animal farming and municipalities. With the local research data of the past decade, we extract the most prominent factors and assemble the SDM. The results and scenarios were compared with the national inventory. By comparing to the past data, we found these models reasonably represent the situation in Taiwan. However, SDM can program many scenarios and produce a lot of prediction data. With the development of many program control tools on STELLA, we believe the models could be further used by researchers or policy-makers to find the needed research topics, to set the future scenarios and to determine the management tools.