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FOREIGN TRIP REPORT

ORNL/FTR-2620

DATE: July 26, 1987

SUBJECT: Report of Foreign Travel of Charles H. Byers, Group Leader, Chemical Technology Division

TO: Herman Postma

FROM: C. H. Byers

PURPOSE: To participate in the NATO Advanced Study Institute on the Electrical Properties of Liquids at Sintra, Portugal, July 5-17, 1987.

SITES VISITED:

7/5-17/1987	NATO Advanced Study Institute Sintra, Portugal	
7/9 and 7/15	Universidade Nova de Lisboa Chemical Engineering Department Lisbon, Portugal	M. Carrondo

ABSTRACT: The traveler attended the NATO Advanced Study Institute on the Electric Properties of Liquids and presented a paper entitled "The Use of Pulsed Electric Fields in the Emulsification and Coalescence of Liquids." The conference was of particular interest to the ORNL program on multiphase separations in that papers were presented which bear directly on the phenomena with which the program is currently dealing. Internationally known experts presented papers on the properties of electric fields in liquids and the breakdown of such fields, which will have immediate applicability to our ongoing programs. The visits to the Universidade Nova de Lisboa established important international contacts in the areas of sorption and simulation (Professors Carrondo and Lobo). The traveler presented two seminars at the university and ensured the establishment of continuing contacts with Portuguese chemical engineers.

REPORT OF TRAVEL TO PORTUGAL

July 5–17, 1987

C. H. Byers

The primary purpose of the NATO Advanced Study Institute on the Electric Properties of Liquids was to provide a forum for presentations by world authorities on the interactions of electric phenomena and liquids and to present this body of knowledge in a semitutorial manner so that all participants could discuss the current state of the field and needs for research and development. This is of particular importance to the mission of the Department of Energy because of the applications in transformer technology and safety aspects of fluid transport, as well as the fundamental aspects relating to theory of the liquid phase. The institute was of special interest because of our local program developments in the use of high voltage fields to enhance mass transport. The background and current status of international research on the influence of electric fields upon fluid behavior forms a foundation for our future work.

The conference was divided into five sessions, each of which consisted of several lectures, discussion, and some appropriate poster papers. These sessions included:

1. Theories of Liquid Structure
2. Ionic and Electronic Processes
3. Interfacial Phenomena
4. Breakdown and Conduction
5. Research in the Liquid State

The conference was arranged so that the viewpoints of chemists, physicists, and engineers were represented in a balanced fashion.

Advances in the theory of the liquid state have centered upon the spatial analog of the harmonic oscillator model and the limited use of nonlinear models to explain such phenomena as freezing. The use of supercomputers has facilitated the complex computations which are characteristic of this approach. The solvated electron, which is of considerable importance to the theoretical studies of the electrical behavior of liquids, may be approached by the Feynman path integral approach. A review of the mathematics of molecular and electron transport was particularly interesting because the current work in that area forms the basis for much of the work in our group at ORNL. An excellent review of the mathematics of scattering completed the background and theories session. The new insights gained here on potential data treatments may also be useful for the research conducted by the laser-light scattering group.

The traveler presented a paper entitled "The Use of Pulsed Electric Fields in the Emulsification and Coalescence of Liquids," which elicited considerable interest and comment from the chemical community. The paper discussed our development of a separations concept that allows the simultaneous emulsification and coalescence of the dispersed phase in a liquid-liquid system. The implications for the use of this technology in hazardous liquid-liquid extraction work were explored. This application of pulsed fields was a novel departure from most of the work presented at the conference.

The theory of electron motion under various circumstances formed the bulk of the conference subject matter during the first week of the conference. Results of both theoretical and experimental work in this area were presented by an international group of experts. Most of the studies were for simple liquid systems and are not sufficiently sophisticated for use in our area. However, some of the theoretical treatments may help to explain some of the phenomena we have observed.

During the second week of the conference, the breakdown of electric fields was discussed. Here the implications useful for the work of our group involved the shaping of electrodes, concerns for impurities, and the nature of the continuous phase. The methods explored by Professor M. Zahn of Massachusetts Institute of Technology may have application in our video approach to flow and field visualization. A useful contact has been established there.

The findings presented from research work with very fast reactions, such as isomerizations where picoseconds and even shorter times are involved, show great promise for our work with surface interactions.

During the conference the traveler made two visits to the Department of Chemical Engineering at the Universidade Nova de Lisboa, at the invitation of Dr. Manuel Carrondo. My primary contacts were with Dr. Carrondo and with Dr. Maria Lobo, chairman of the department. The traveler also presented seminars to the department entitled: "An ASPEN Simulation Approach to Current Modeling Problems — The Hydrolysis of Woody Biomass," and "Vacuum Sorption Pumping Studies of Pure Gases on 4A Molecular Sieves." As a result of the first seminar, a tentative

arrangement has been made for a joint effort in which a student from Lisbon would come to ORNL to work, with the objective of implementing that ASPEN technology use in Lisbon. Details are currently being investigated.

APPENDIX A. ITINERARY

July 1–2, 1987	Travel from Oak Ridge to London, England.
July 3–4, 1987	Personal travel.
July 5, 1987	Travel to Sintra, Portugal.
July 5–17, 1987	Participate in the NATO Advanced Study Institute on the Electric Properties of Liquids, Hotel Trivoli, Sintra, Portugal.
July 17, 1987	Travel to London, England.
July 18, 1987	Personal travel.
July 19, 1987	Travel from London to Oak Ridge.

APPENDIX B. PERSONS CONTACTED

Professor K. G. Spears	Department of Chemistry Northwestern University Evanston, IL 60201
Discussion Topic:	Solvent effects in the hydrolysis of tetra-ethoxysilane. Hydrogen bonding theory.
Professor Alan Watson:	Department of Electrical Engineering University of Windsor Windsor, Ontario, Canada
Discussion Topic:	Electrode shape effects on the disruption of two-phase systems.
Dr. O. B. Nagy	Universite Catholique de Louvain Laboratoire de Chimie Organique Physique Louvain la Neuve, Belgium
Discussion Topic:	Emulsion phase contactors and their potential in industrial practice.
Professor Aysen Turkman	Department of Environmental Engineering Dokuz Eylul University Bornova, Izmir, Turkey
Discussion Topic:	The use of anionic exchange resins for the removal of nitrates from drinking water.
Professor Markus Zahn	Department of Electrical Engineering Massachusetts Institute of Technology Cambridge, MA
Discussion Topic:	Potential methods for improving our pulsed field generator. Photographing electric field effects in high fields.
Professor Manuel Carrando	Department of Chemical Engineering Universidade Nova de Lisboa Lisbon, Portugal
Discussion Topic:	The use of the ASPEN simulator to model bio-reactors.
Professor Mario Lobo	Department of Chemical Engineering Universidade Nova de Lisboa Lisbon, Portugal
Discussion Topic:	The use of the ASPEN simulator to model catalytic reactors. Sorption pumping.