Nuclear Energy Research Initiative (NERI) Program
DE-FG03-99SF21923/A00
Technical Progress Report

Narrative:

Task 1. (Investigator: Simon M. Pimblott, NDRL)

1. Task Status

A methodology for calculating the inelastic energy loss properties of non-relativistic light ions such as H^+, He^{2+} and C^{6+} in liquid water is being developed. This treatment is based on the same formalism used previously to evaluate the stopping power, mean free path and inelastic collision cross-section of electrons and positrons in a variety of condensed media.

Simulations of the kinetics and of the yields of the radicals and molecular products formed by gamma- and fast electron radiolysis of heavy water are being. The results of these simulations will be compared with the available experimental data and with similar calculations already made for light water.

2. Issues / Concerns

None

Task 2. (Investigator: Jay A. LaVerne, NDRL)

1. Task Status

A high temperature cell for the examination of water radiolysis has been constructed and tested to 200 °C. Dosimetry studies will soon be performed, followed by the determination of hydrogen peroxide production at elevated temperatures. A homogeneous kinetic model of water radiolysis has been developed for predicting the dependence of hydrogen peroxide yields on the concentration of dissolved molecular hydrogen.

2. Issues / Concerns

None

Task 3. (Investigator: Dani Meisel, NDRL)

1. Task Status

The rate of H_2 generation from heavily loaded ZrO_2 suspensions has been determined as a function of particle concentration. Several observations are worthy of note:

a) H_2 adsorbs on the particles. Once the particle surface is saturated (at what is believed to be a monolayer of H_2) the amount that is extracted from the solution is linear with dose. This behavior is not observed on SiO_2.

b) b) In spite of the observations reported in our previous quarterly report of escape of electrons, the yield of H_2 does not increase with ZrO_2 concentration provided e^-_{aq} is scavenged. On the contrary, the yield of molecular hydrogen is then decreased proportionately with the decrease in the volume fraction occupied by water upon increasing particle concentrations. On one hand it resembles our observations in SiO_2 suspensions. On the other hand, the back reaction observed in silica, of holes reacting with hydrogen, is not observed in ZrO_2. Probably because little charge separation across the particle interface occurs in zirconia.

Issues / Concerns

None

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Task 4: (Investigator: Thom Orlando, GT)

1. Task Status

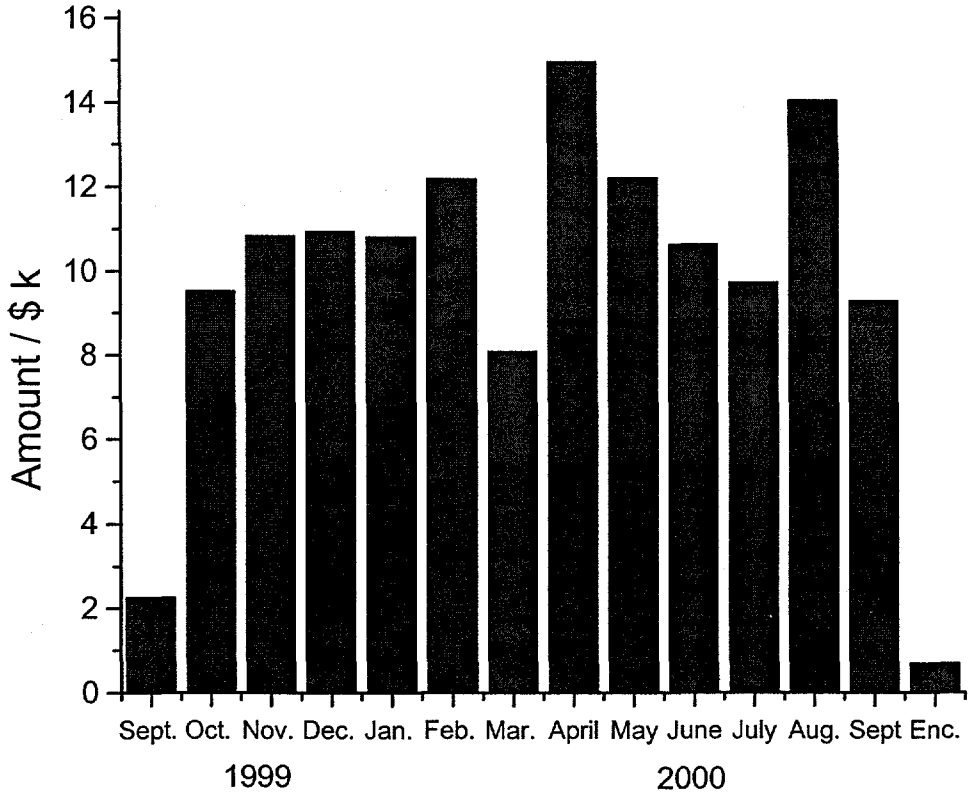
   Co-PI based responsible for this project task took a position as a T&R professor in the Chemistry Department at the Georgia Technical Institute in August 2000. The equipment on which the project task is being performed has been moved Georgia Tech, and is being rebuilt.

2. Issues / Concerns

   None

Cost Performance:

NDRL:



GT: Funding provided directly as separate grant to Georgia Tech.

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Status Summary of NERI Tasks - Phases 1-3:

Phase 1:

Milestone/Task Description	Planned Completion Data	Actual Completion
Task 1. 1. Compilation of information on radiation chemistry of water and aqueous solutions at elevated temperatures. 2. Algorithms for TRACKKIN code that include the effects of temperature on energy loss and the results of calculations on hydrogen yields at elevated temperatures.	8/14/2000 8/14/2000	Compilation completed. Web publication in progress. Coding completed. Calculation of chemical kinetics following g irradiation at room and at elevated temperatures (0 – 300oC) completed. Submission for scientific publication in progress
Task 2. 1. Results of hydrogen peroxide yields from gamma and high LET irradiation in the presence of H_2 scavengers at high dose. 2. Schematics for the high temperature cell for gamma irradiation..	8/14/2000 8/14/2000	Experiments completed. Submission for scientific publication in progress Completed
Task 3. 1. Compilation of information on radiation chemistry of water at interfaces of interest. 2. Tested procedures to synthesize (or concentrate dilute suspensions of) iron and zirconium oxide. 3. Results from the irradiation of these oxides.	8/14/2000 8/14/2000 8/14/2000	Literature survey completed Completed Experiments completed for zirconium oxide. Submission for scientific publication in progress
Task 4. 1. Growth and Characterization of Crystalline ZrO_2 Films 2. Characterization of Oxidized Zirconium Metal	8/14/2000 8/14/2000	Completed Completed

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Status Summary of NERI Tasks - Phases 1-3: cont

Phase 2:

Milestone/Task Description	Planned Completion Data	Actual Completion Date
Task 1. 1. Algorithm and testing of code to simulate high-LET heavy-ion track structure in water. 2. Simulate results of H_2 saturated solutions at ambient temperature.	8/14/2001 8/14/2001	In progress.
Task 2. 1. Tested protocol for O_2 measurement from gamma irradiation. 2. Results from the effect of H2 on O_2 yields in gamma irradiated solutions at high doses.	8/14/2001 8/14/2001	
Task 3. 1. Schematics of cell for high temperature pulse radiolysis at elevated temperatures. 2. Results from irradiation of heavy loaded suspensions at ambient temperature. 3. Effect of surface potential on escape depth from narrow bandgap oxide materials. 4. Results from feasibility tests of EPR and conductivity techniques to measure the charge escape of electrons and holes from these oxides.	8/14/2001 8/14/2001 8/14/2001 8/14/2001	In progress. In progress.
Task 4. 1) Electronic band structures of doped zirconia. 2) Results from controlled irradiation of water covered with iron oxide. 3) Results from integrity measurements on the zirconia and iron-oxide/water overlayers.	8/14/2001 8/14/2001 8/14/2001	

Status Summary of NERI Tasks - Phases 1-3: cont

Phase 3:

Milestone/Task Description	Planned Completion Data	Actual Completion Date
Task 1. 1. Results from simulations of irradiation at various temperatures. 2. Comparison between simulations and experimental results of Task 2 and 3. 3. Incorporation of Task 4 into the model.	8/14/2002 8/14/2002 8/14/2002	
Task 2. 1. Results from the effect of H_2 on O_2 yields in high LET irradiated solutions at high dose. 2. Results from the effect of H_2 on O_2 yields in gamma irradiated solutions at elevated temperatures. 3. Measurements of the effect of H_2 on H_2O_2 yields from gamma irradiation.	8/14/2002 8/14/2002 8/14/2002	
Task 3. 1. Results from the irradiation of suspensions at elevated temperatures. 2. Flat band potentials of the relevant oxides at various temperatures. 3. Results from the effects of core-shell structures on yields of water radiolysis.	8/14/2002 8/14/2002 8/14/2002	
Task 4. 1. Hydrogen yield profiles as a function of depth within doped zirconia. 2. Quantitative comparison of low-energy with high energy radiolysis.	8/14/2002 8/14/2002	

NERI Progress Chart

ID	Task Name	Duration	Start date	Finish date	1999		2000				2001				2001		
					Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3
1	Radiation chemistry model development	3 years	8/15/99	8/14/02													
2	High temperature and high LET effects	3 years	8/15/99	8/14/02													
3	Interfacial effects of radiation	3 years	8/15/99	8/14/02													
4	Low energy electrons at surfaces and interfaces	3 years	8/15/99	8/14/02													
	Progress	3 years															

Key	Task	Summary	Rolled up progress
	Progress	Rolled up task	
	Milestone	Rolled up milestone	