

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

Narrative:

General:

Coordination meeting of project personnel from NDRL (plus Dr. K.P. Madden of RCDC) held on 9/13/99. Project coordination meeting of NDRL personnel and PNNL co-PI planned for 10/4-6/99 at NDRL.

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

1. Task Status

Bibliographic assistant position for compilation for high temperature water radiolysis data advertised, and compilation begun. Postdoctoral research associate to develop code and to perform simulations hired - start date: 4/1/2000.

2. Issues / Concerns

None

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

1. Task Status

High temperature cell schematics discussed with AECL consultants. Preliminary experiments at room temperature begun.

2. Issues / Concerns

None

Task 3. (Investigator: Dani Meisel, NDRL)

1. Task Status

Preparations for experiments begun. Postdoctoral research associate to perform bibliographic compilation and to perform experiments hired - start date: 10/1/99.

2. Issues / Concerns

None

Task 4: (Investigator: Thom Orlando, PNNL)

1. Task Status

Begun gearing up to address water reactions and photochemistry of iron oxides. Begun calculations on secondary electron interactions with overlayers. Hired postdoctoral research associate - start date: 8/15/99.

2. Issues / Concerns

None

Cost Performance:

NDRL: No expenditure except budgeted (senior personnel) salaries at NDRL in period 8/15/99 to 9/30/99.

PNNL: Funding provided directly as separate grant to PNNL.

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Status Summary of NERI Tasks - Phases 1-3:

Phase 1:

Milestone/Task Description	Planned Completion Data	Actual Completion Date
Task 1. 1. Compilation of information on radiation chemistry of water and aqueous solutions at elevated temperatures. 2. Algorithms for TRACKIN 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	
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	
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	
Task 4. 1. Results from the irradiation of doped zirconia films with water overlayers. 2. Results from adsorption/desorption following pre-irradiation. 3. Results from radiolytic defect production in clean iron oxide.	8/14/2000 8/14/2000 8/14/2000	

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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	
Task 2. 1. Tested protocol for O ₂ measurement from gamma irradiation. 2. Results from the effect of H ₂ 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	
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	

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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 ₂ O 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		Progress		Milestone		Summary		Rolled up task		Rolled up progress		Rolled up milestone