Dosimetry Modeling at the Fuel-Water Interface

Presented to the:
International High Level Radioactive Waste Management Conference

Presented by:
William H. Miller, Professor
Amanda Kline, Ph.D. Candidate
University of Missouri-Columbia

Brady Hanson, Staff Scientist
PNNL

May 3, 2006
Las Vegas, NV

This presentation has been funded in whole or in part by the U.S. Department of Energy

Introduction

- **Dissolution of fuel is affected by oxidants and reductants:**
  - **These products are a function of:**
    - **Initial radiolytic products formed**
    - **Spatial distribution of these species**
    - **Resulting chemistry among these products and fuel**
  - **Initial radiolytic products are a function of:**
    - **Type of radiation**
    - **Magnitude and energy of radiation**
    - **Fuel pellet or grain size (surface-to-volume ratio)**
    - **Fuel-to-water ratio**

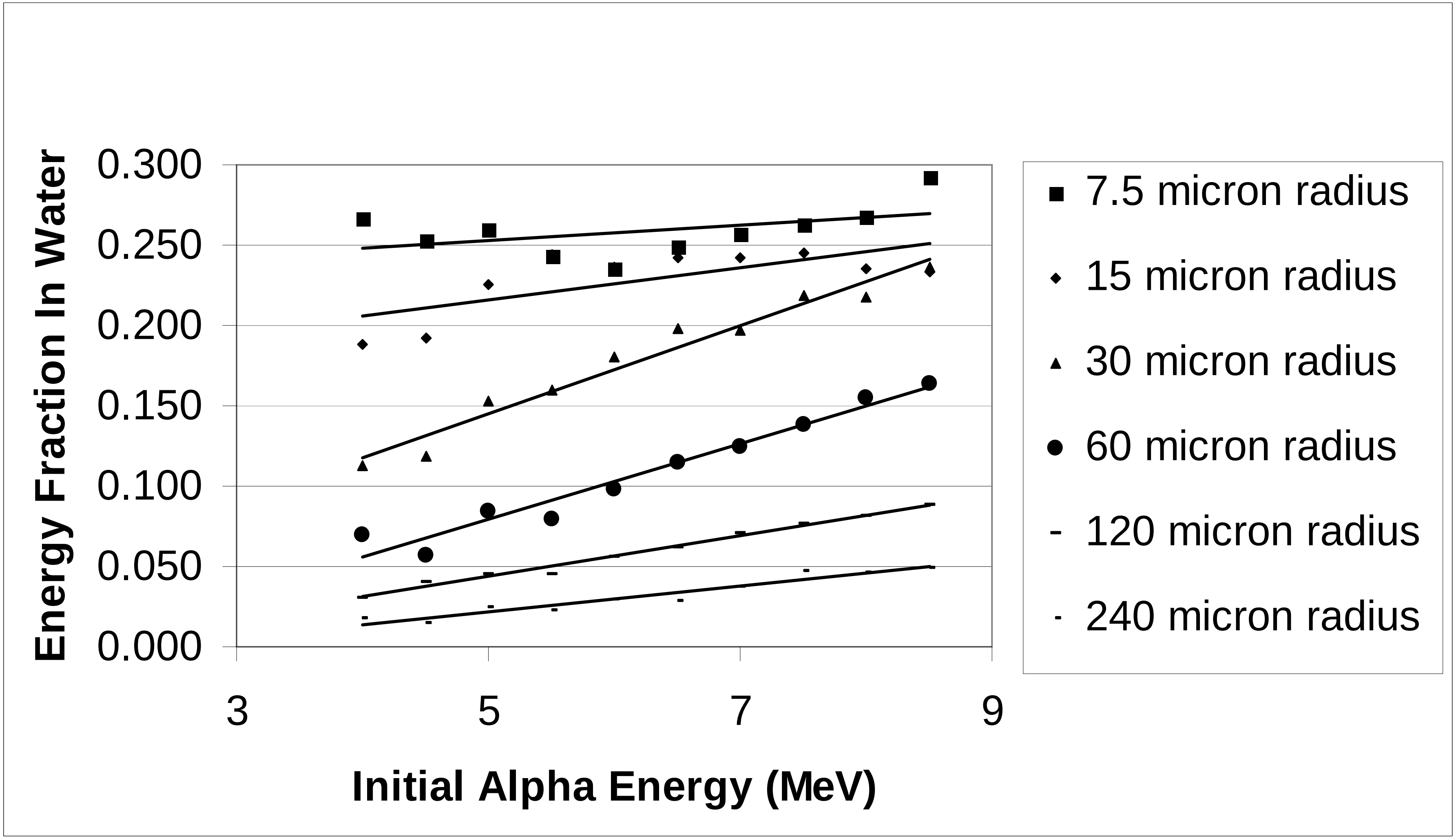
Objective

- **Provide systematic dosimetry model for predicting dose to water from SNF:**
  - **As a function of radiation type**
  - **As a function of radiation energy**
  - **As a function of distance from the fuel**
  - **For fuel dimensions ranging from pellets to grains**
  - **For different fuel-to-water ratios**
  - **For assumed average fuel composition at Yucca Mountain and as a function of decay**
  - **For a variety of simulated, experimental conditions**

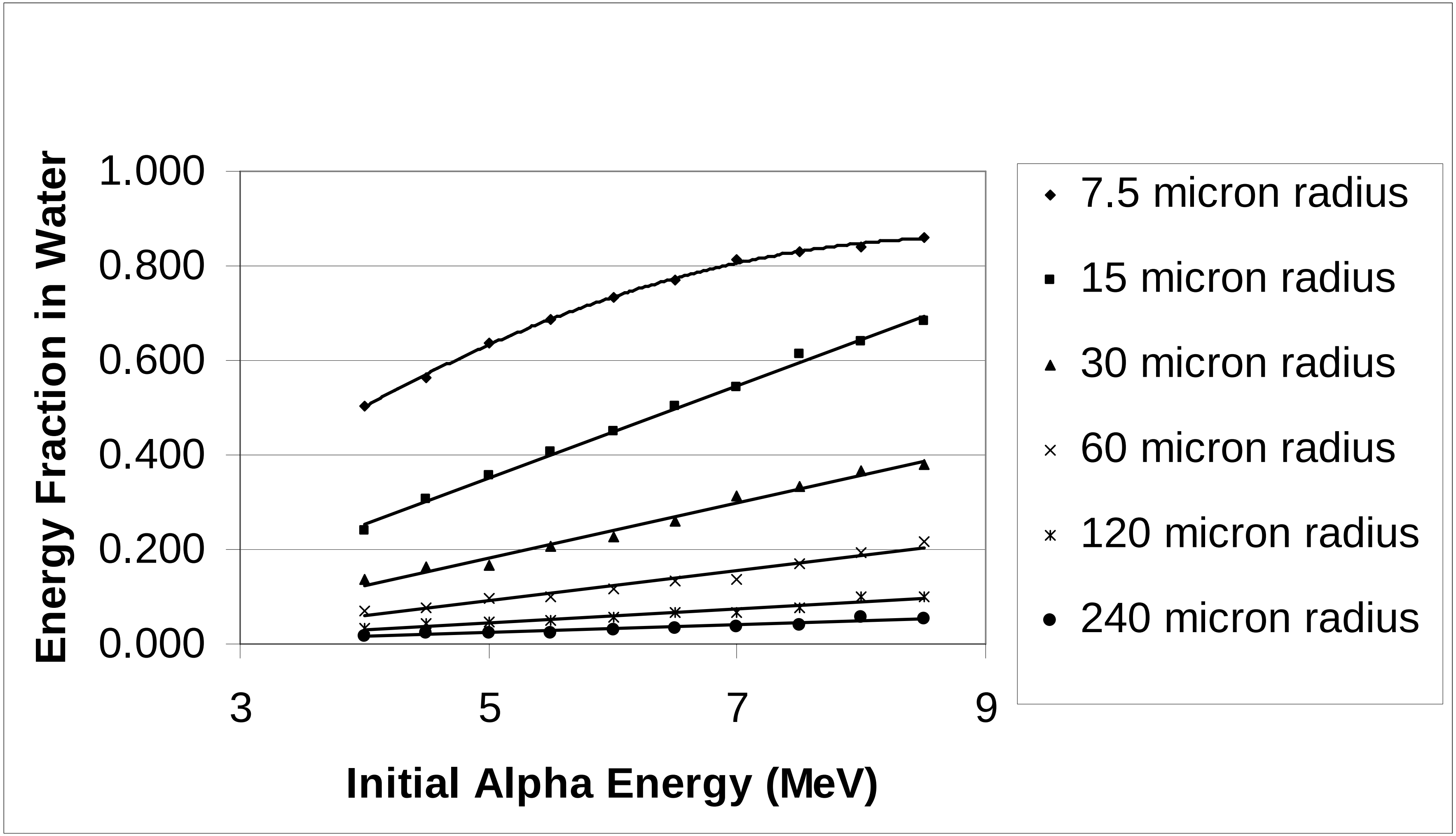
Radiation Transport Modeling

- Alpha Dosimetry
  - Random walk (Monte Carlo) model implemented in Mathematica
- Gamma Dosimetry
  - MCNP5
- Beta Dosimetry
  - MCNP5 – multiple runs to simulate energy spectra
- Geometries
  - 17 x 17 fuel pin, Westinghouse pellets
    (0.392 cm radius x 0.940 cm)
  - Grains from 7.5μ to 240μ in radius

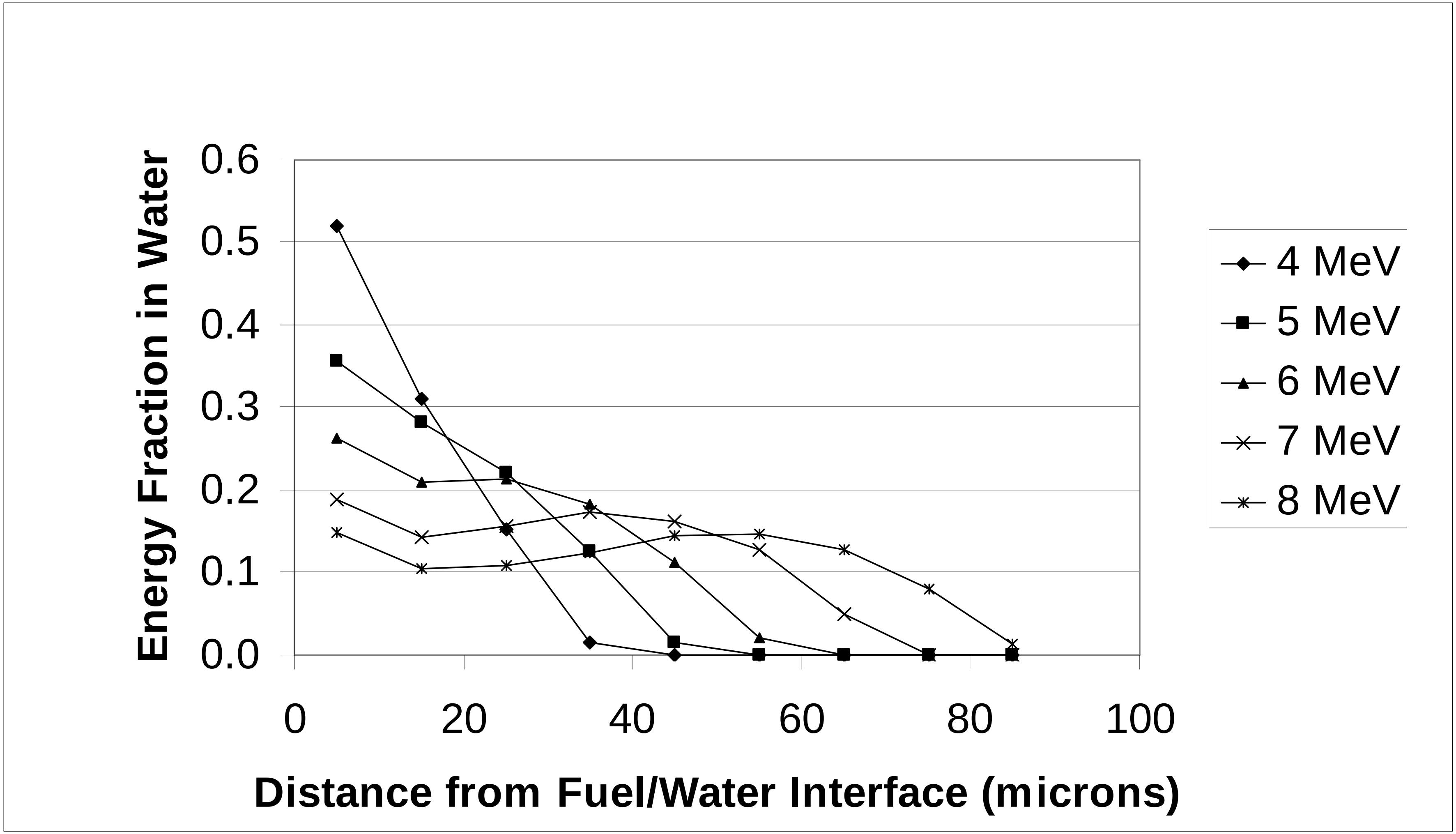
Alpha – Infinite Matrix of Grains



Alpha – Infinite Water



Alpha Spatial Energy Deposition – 7.5μ Grain



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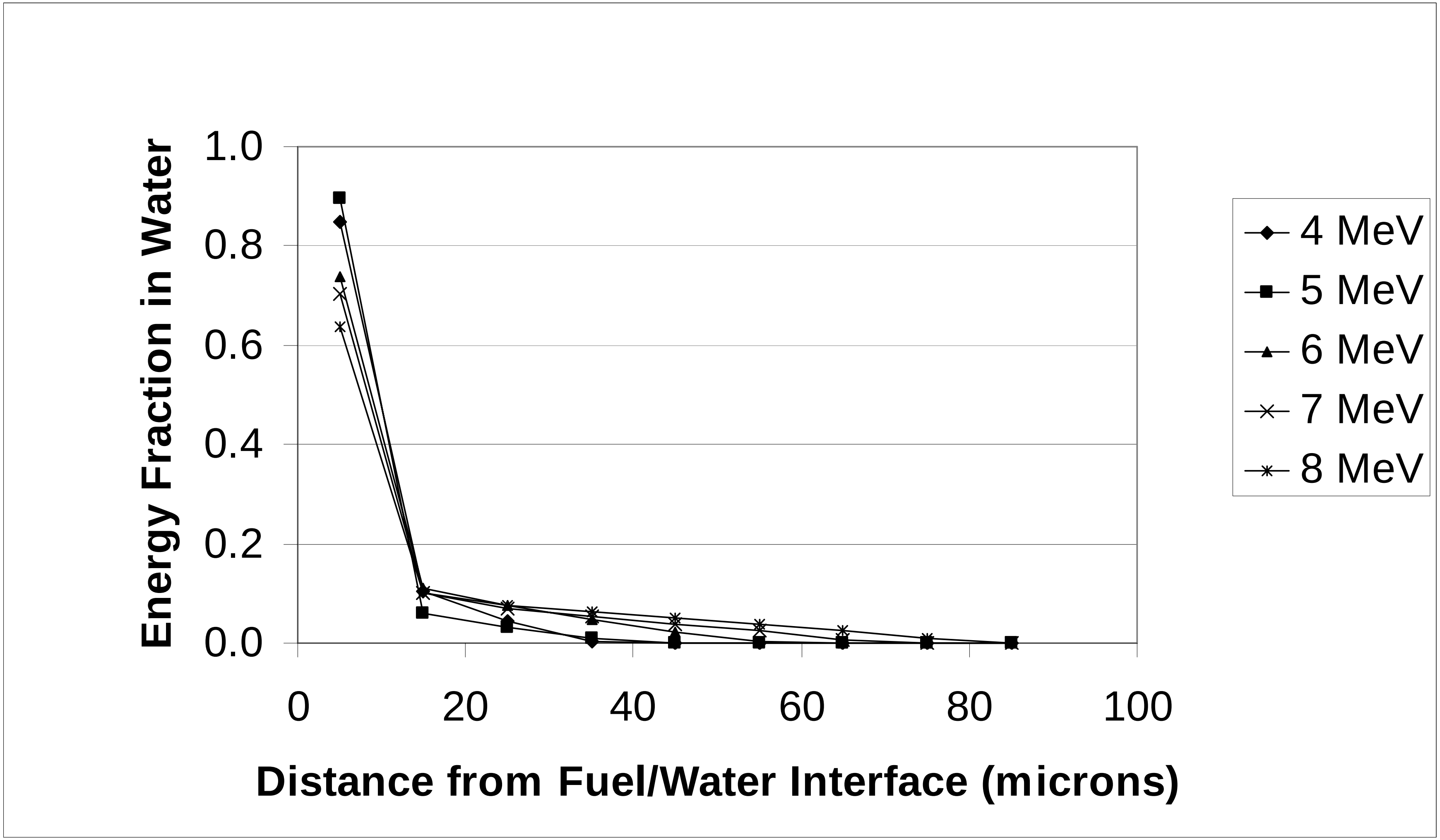
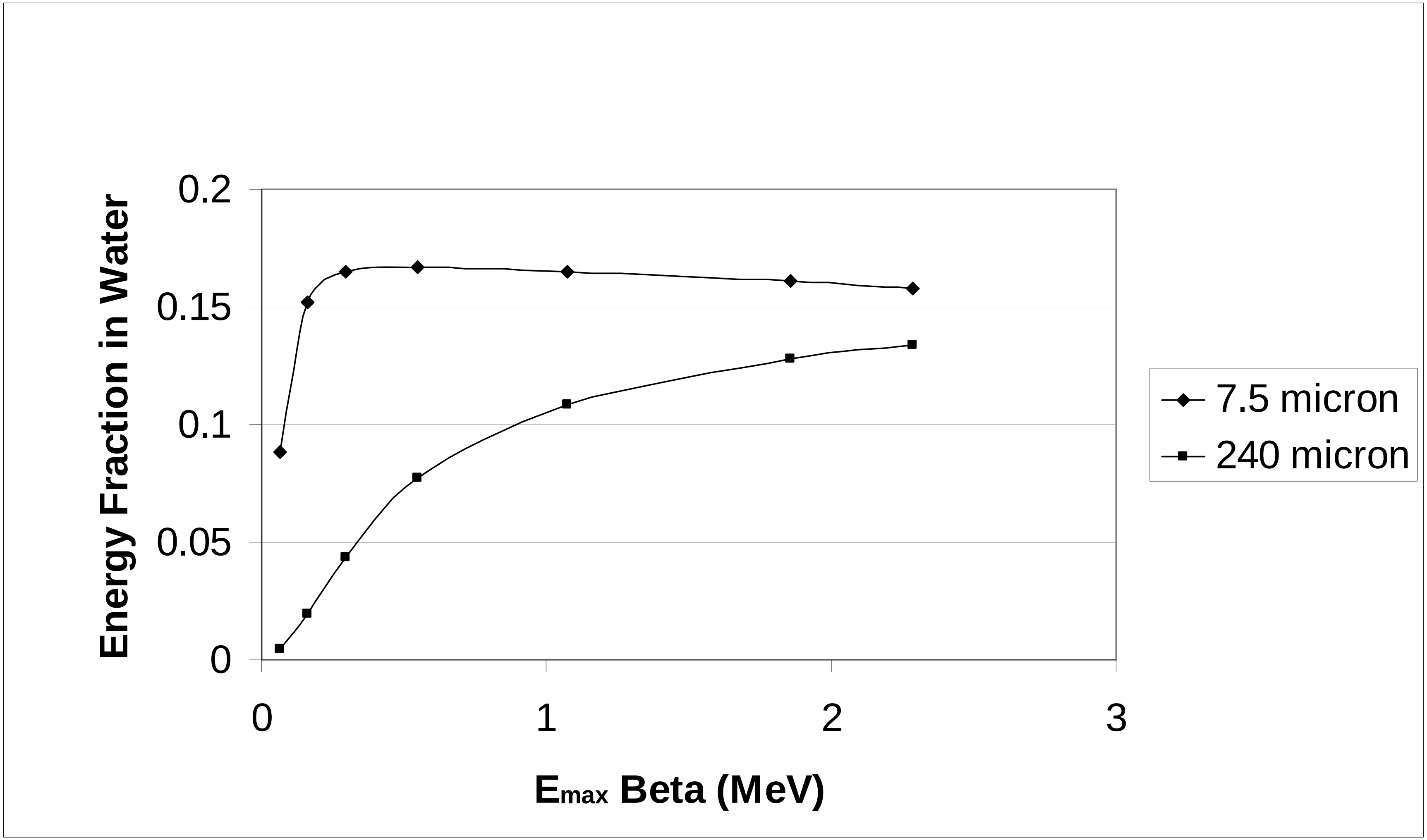
OCRWM Office of Science and Technology and International

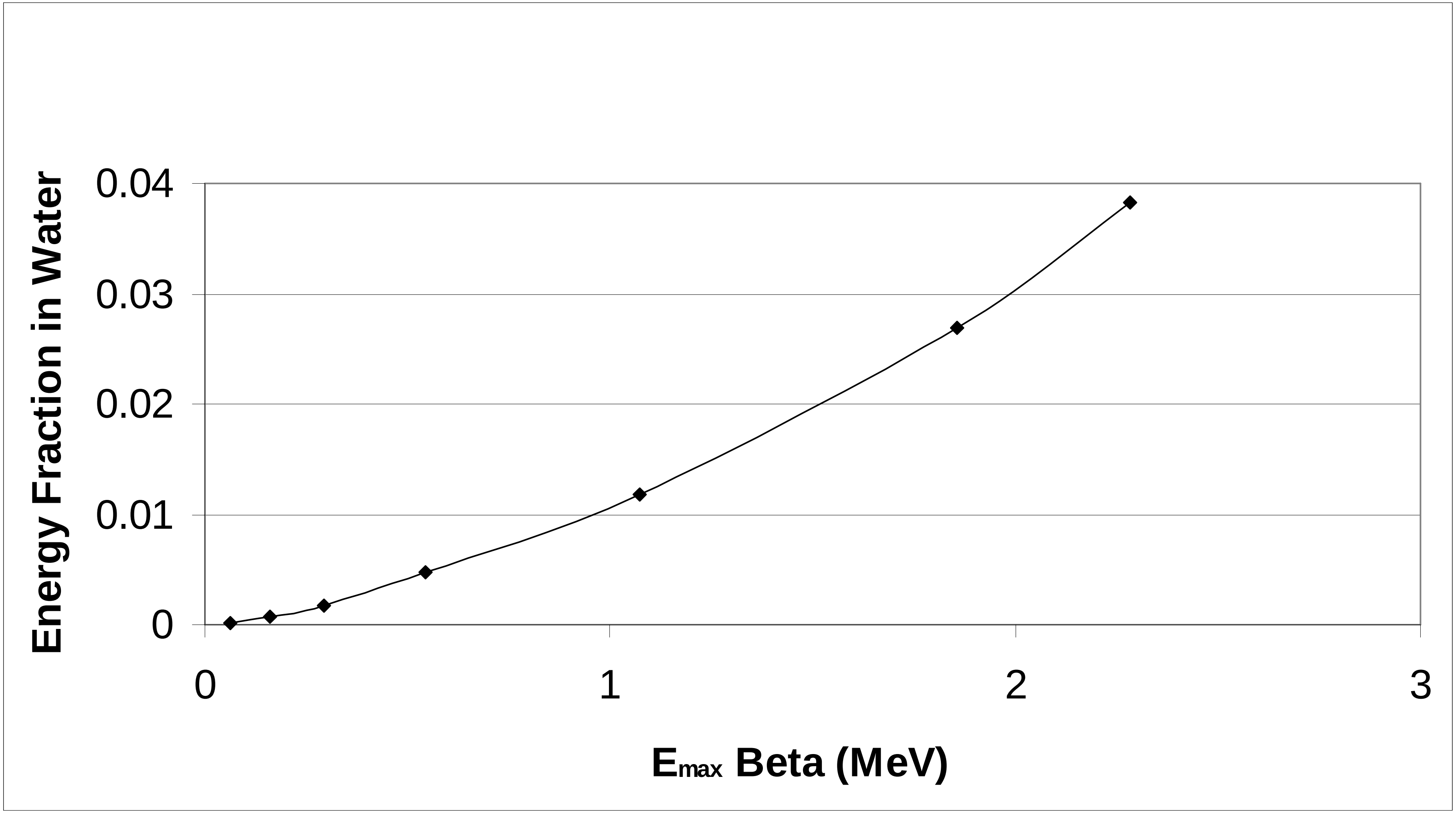
Alpha Spatial Energy Deposition – 30µ Grain



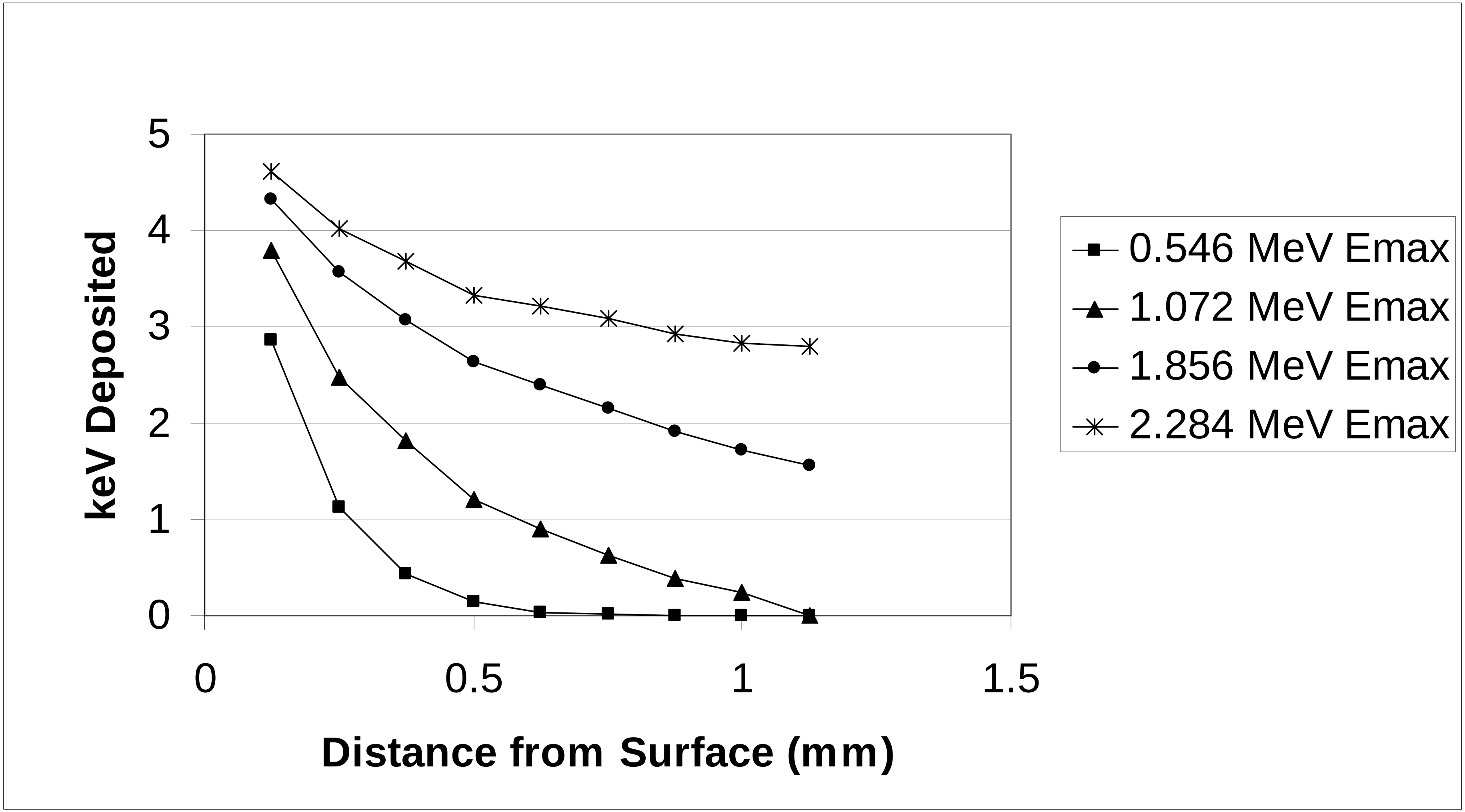
Beta – Infinite Matrix of Grains



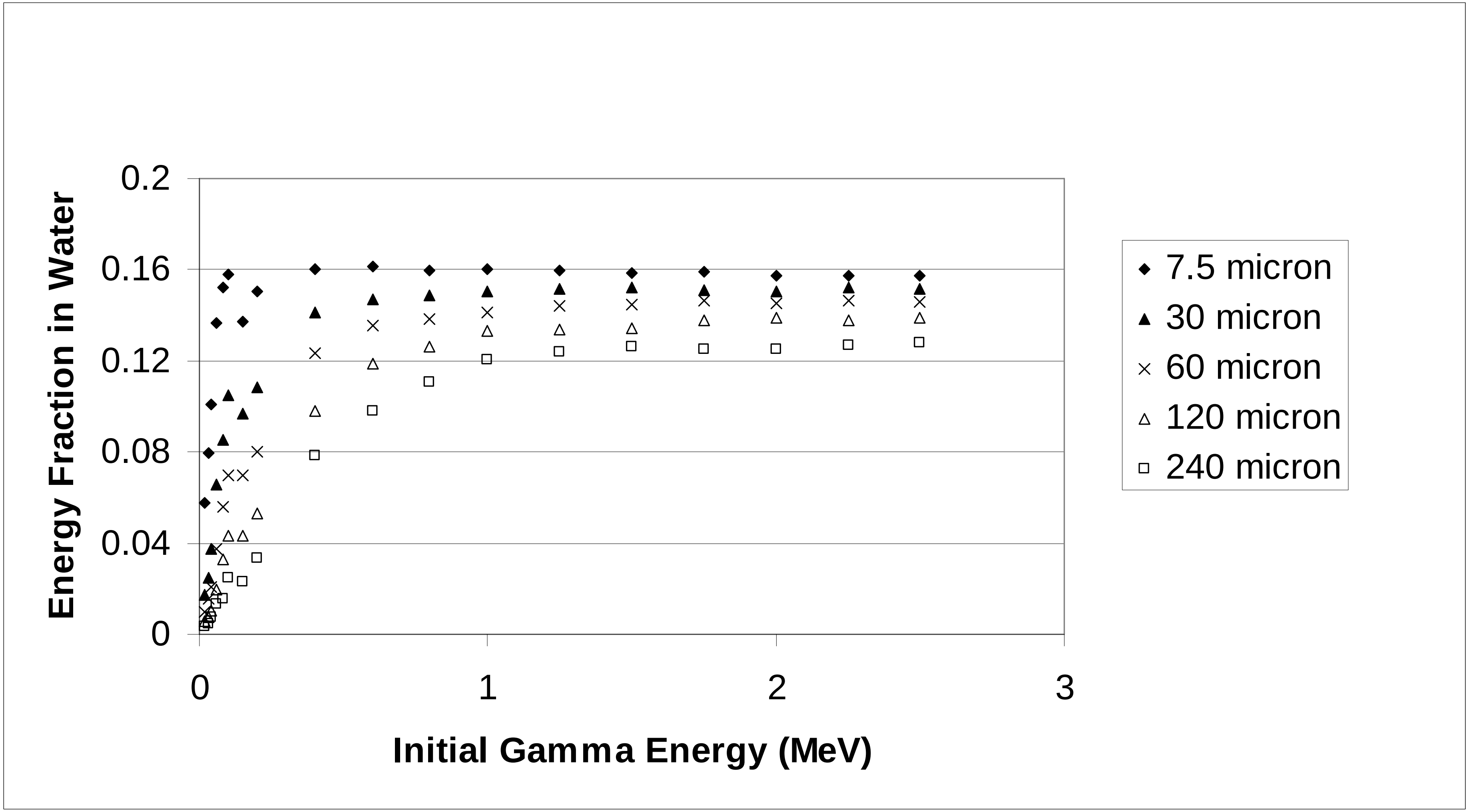
Beta Results – Fuel Pellet



Beta Spatial Energy Deposition



Gamma – Infinite Matrix of Grains



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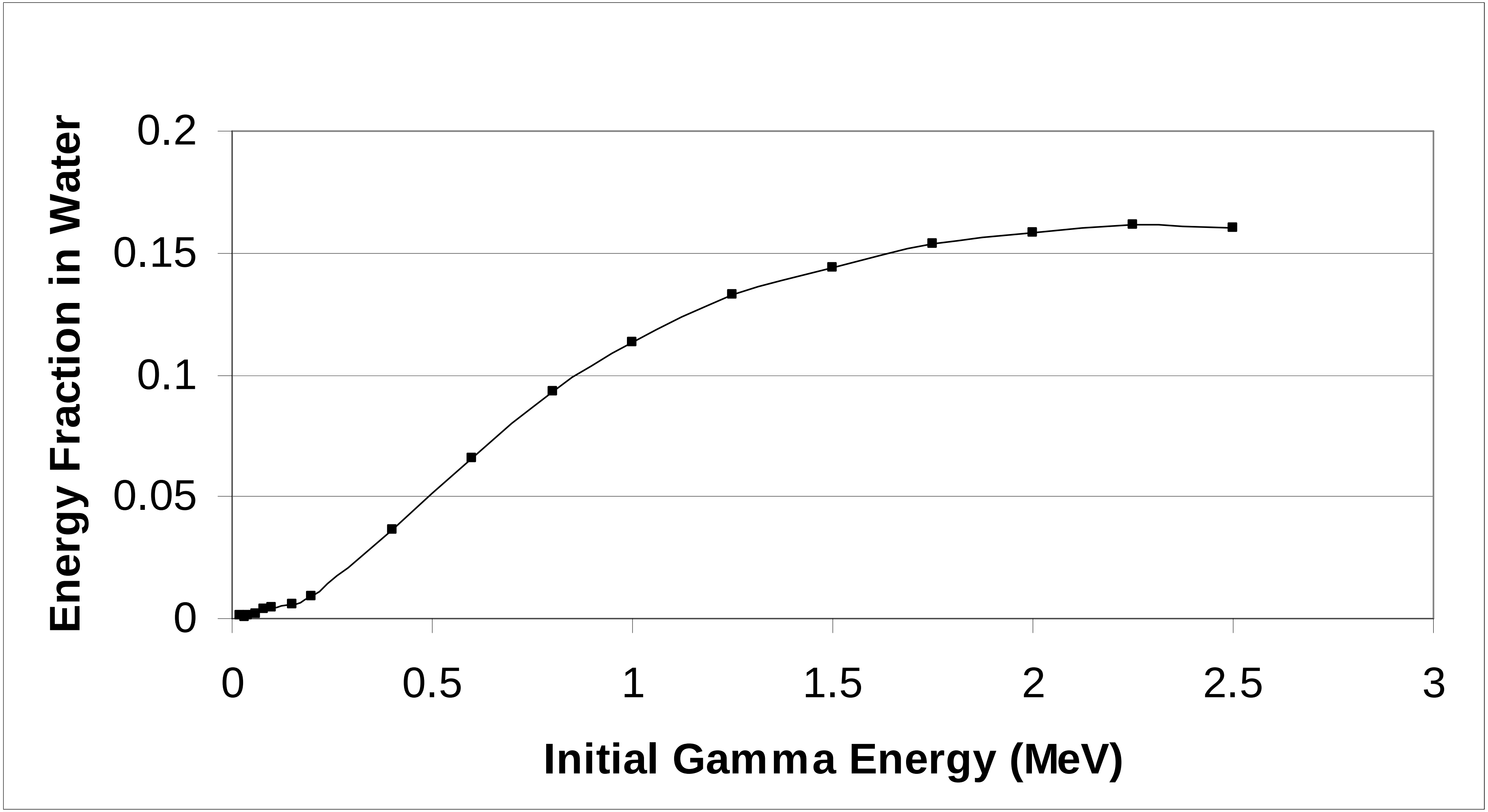
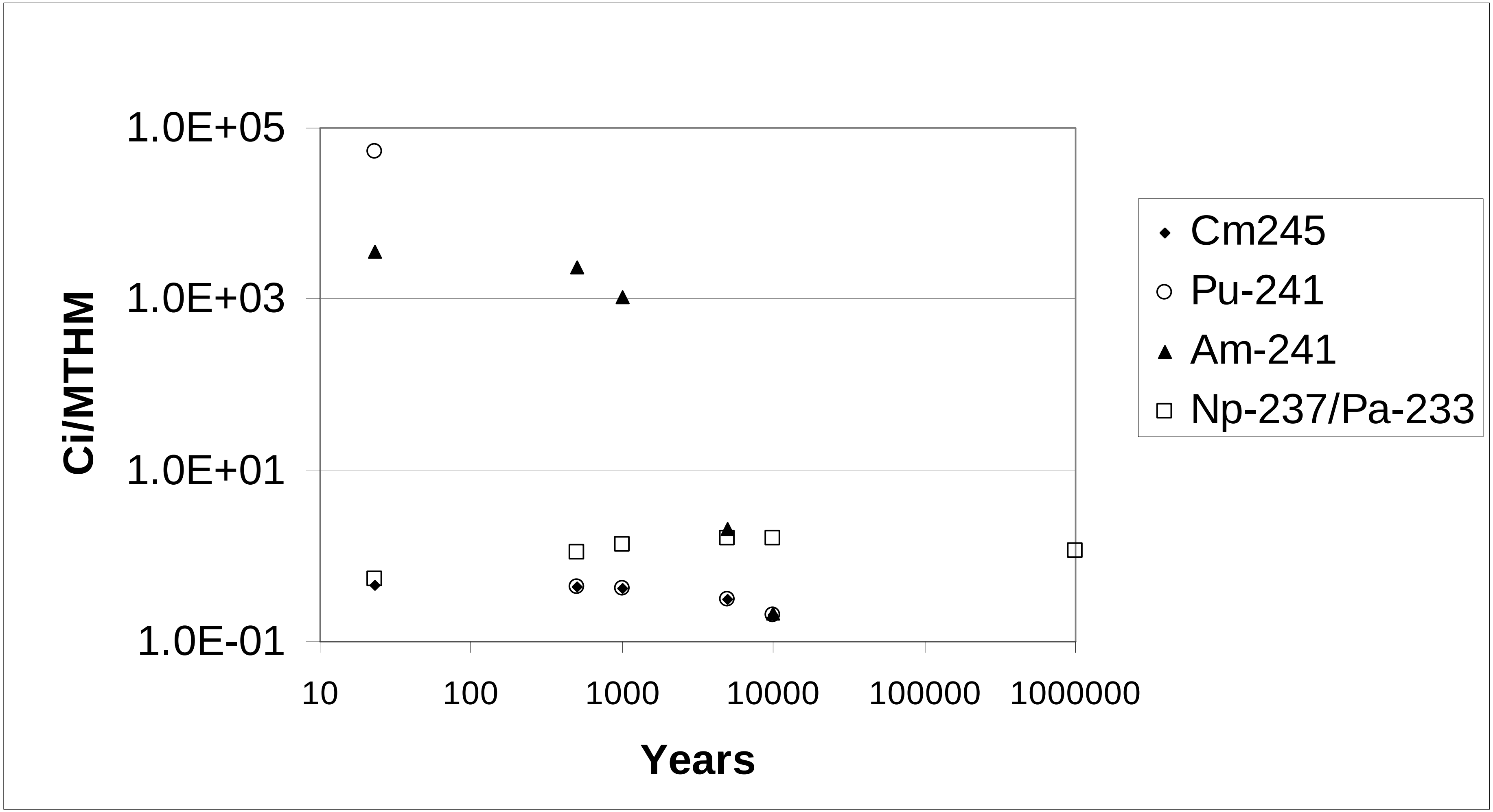
Gamma – Fuel Pellet



SNF Dose to Water Assumptions

- Used Yucca Mountain EIS Fuel for Initial Activities
  - PWR fuel
  - 3.75% enriched
  - Burned to 41,200 MWD/MT
  - Assumes initial 23 years of decay
- Solved coupled, first-order differential equations for transuranic activity vs decay using Polymath 6.0
- Modeled simple decay for fission products

Typical Decay Results



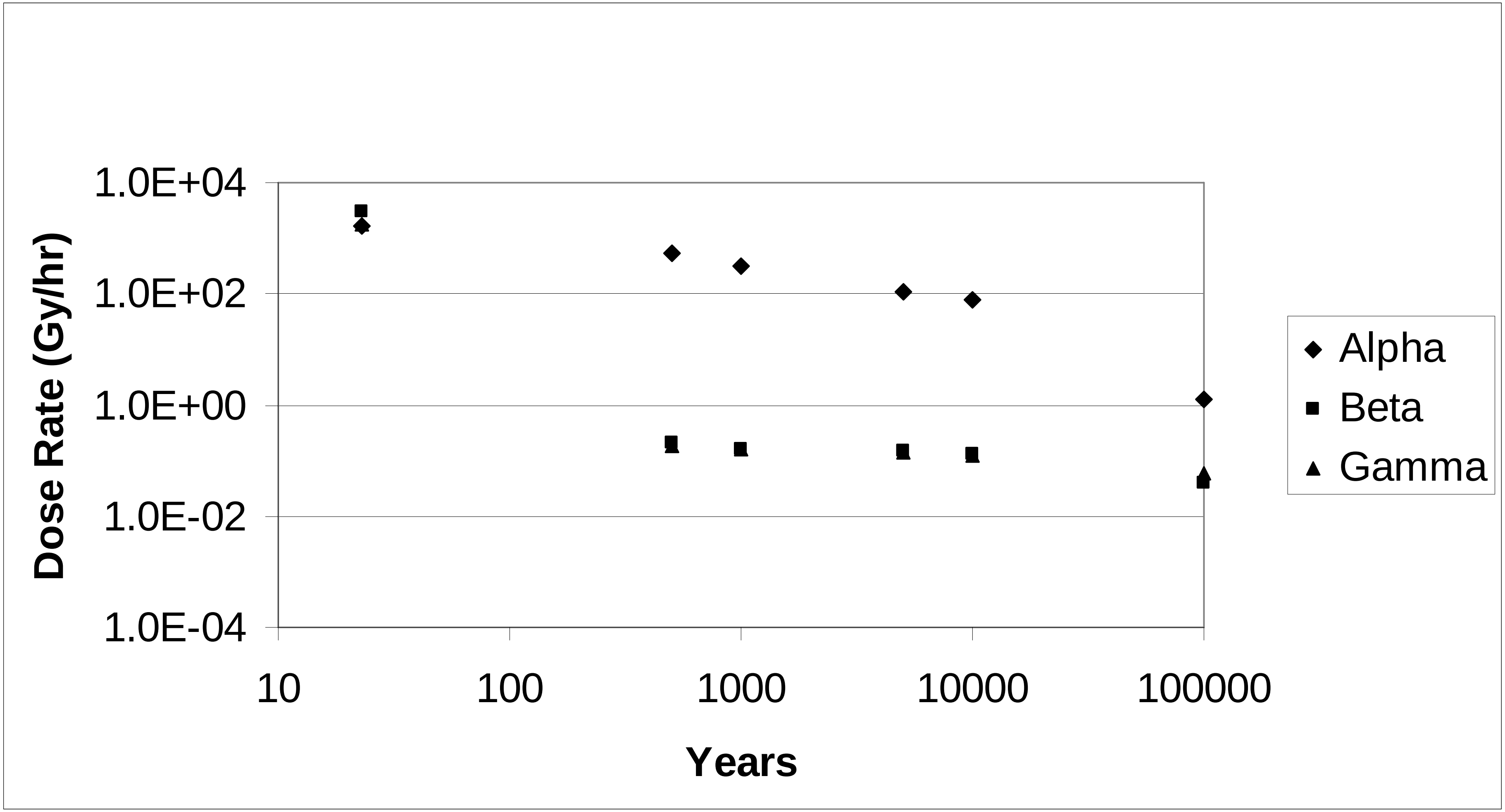
Spreadsheet of Emissions and Yields

Isotope **Cm-245 Chain**	Half Life	Q	Yield Alpha	Energy
Cm-245	8500	5.624	0.050	5.304
			0.932	5.362
Pu-241	14.35	0.022		
Am-241	432.2	5.638	0.016	5.388
			0.130	5.443
			0.845	5.485
Np-237	2.14E+06	4.959	0.062	4.639
			0.033	4.664
			0.080	4.766
			0.250	4.771
			0.470	4.788
			0.016	4.803
			0.025	4.817

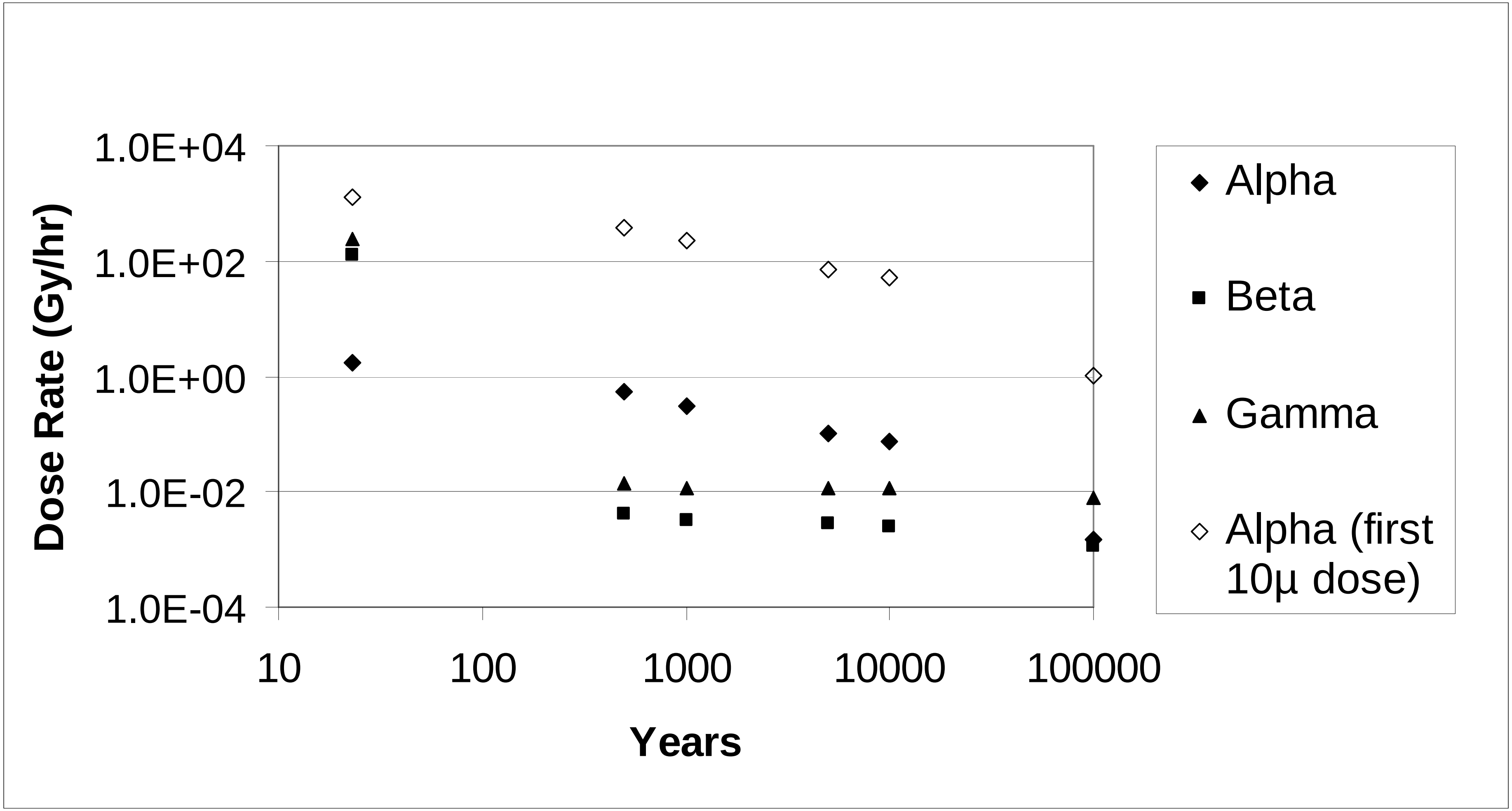
Dose Calculation

- Combine
  - Types of emissions for all major isotopes in SNF
  - Yields and energy of emissions
  - Fraction of energy deposited in water for each emission and energy from transport calculations
  - vs. time
- Results in dose to water

Dose to Water for Infinite Array of 7.5µ Grains



Dose to Water for Infinite Array of Pellets



Verification – Gamma Dose

	This Work*	BSC 2002**
~25 yrs decay	230 Gy/hr	400 Gy/hr
10,000 yrs decay	0.01 Gy/hr	0.03 Gy/hr

* 17x17 array fuel pellets, 3.75% enriched, burned to 41,200 MWD/MT.

** 15x15 array fuel pellets, 4% enriched, burned to 48,000 MWD/MT ("Gamma and Neutron Radiolysis in the 21-PWR Waste Package from Ten to One Million Years," OOO-OOC-DSU0-00700-00-00A. Las Vegas, Nevada: Bechtel SAIC Company, AC: MOL.20021004.0000, 2002).

Verification – Alpha Dose

This Work*	C. Jegou, et. al.**
1300 Gy/hr	**2500 Gy/hr**

* 17x17 array fuel pellets, 3.75% enriched, burned to 41,200 MWD/MT, 23 years of decay.

** Simulated Fessenheim 2 reactor fuel pellets, 3.1% enriched, burned to 47,000 MWD/MT, 15 years of decay. Dose estimated from alpha flux and assuming 10 microns of range. (Jegou, C., B. Muzeau, V. Broudic, A. Poulesquen , D. Roudil, F. Jorion and C. Corbel, "Effect of alpha irradiation on UO_2 surface reactivity in aqueous media," Radiochim. Acta., **93**, 35–42, 2005).

Conclusions

- Comprehensive model has been developed
- Dose to water as a function of radiation type, energy, and fuel size has been calculated
- Model applied to Yucca Mountain SNF
- Model can easily predict dose to water for other experimental conditions
- These dose results, combined with radiolysis yields, can predict initial radiolytic products
- Combined with appropriate chemistry, the production of oxidants and reductants at the fuel/water interface can be predicted

Acknowledgement

- This work was sponsored in part through the Source Term Strategic Thrust Area of the Office of Science and Technology and International within the U.S. Department of Energy Office of Civilian Radioactive Waste Management. This work was performed as non-quality affecting.
- The research of Amanda Kline was performed under appointment of the Office of Civilian Radioactive Waste Management Graduate Fellowship Program administered by Oak Ridge Institute for Science and Education under a contract between the U.S. Department of Energy and the Oak Ridge Associated Universities.