

To: Christiane Williams, Associated Colleges of the South

From: Dr. Jimmie M. Purser, Millsaps College

Date: March 21, 2003

Re: 2002 technology fellowship project

Project Rationale:

For the past 20 years, I have served in both the Computer Science and Chemistry Departments at Millsaps College. With my 2002 sabbatical, my plan was to prepare to return to Chemistry full-time. My project was related to exploring applications of visualization in the natural sciences:

“I will be on sabbatical from Millsaps College in the Spring of 2002. My sabbatical will focus on modeling, simulation, and data visualization in the Sciences. In particular, it will focus on the PC Spartan package distributed by WaveFunction, ArcView Software for data visualization, and Environmental simulation software to be specified later. The expected outcome of my sabbatical will be materials to be integrated into the sciences’ curricula at Millsaps College and other ACS institutions.”

I surveyed several molecular modeling packages and settled on three primary ones: HyperChem, PC-Spartan, and CaChe. I worked with the 30-day trial versions of HyperChem and CaChe. I have submitted a faculty development grant at Millsaps to buy CaChe with ZINDO. I have and am using PC-Spartan.

The principal outcomes from my project can be found on my home page:

<http://home.millsaps.edu/~pursejm>

as the links:

[ArcView/GIS Starter Tutorial.](#)

[Research Home Page](#) [password =Millsaps]

This starter tutorial was used at Millsaps as a precursor to the GIS Workshop which was funded by an ACS Information Fluency Grant. It has also been used in my Environmental Chemistry Course. I now have three research students whose work will be presented in March at a National ACS meeting.

Summary of Outcomes:

In addition to creating the starter tutorial, the expertise which I gained during the project allowed me to do the following:

- (1) Be an author on the “ACS Information Fluency Grant for GIS Workshop at Millsaps College” which was funded.
- (2) Be asked to participate as an acknowledged expert on visualization in science for an international broadcast from WLU which was funded by Culpeper Foundation and the

Rockefeller Foundation - "Tech It or Leave It" – where I talked about visualization in science, including molecular modeling and GIS. (02/06/03)

(3) Introduce GIS into my new Environmental Chemistry course during this spring.

(4) Begin a research project in chemistry on molecular modeling and sunscreens and have two papers accepted for presentation at the National ACS Meeting in New Orleans.

Conclusion:

The support from ACS for my sabbatical work is greatly appreciated and I feel has allowed me to accomplish many of my goals. I intend to do further work with the starter tutorial and to continue development of my research website.