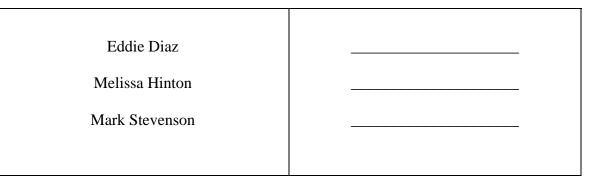


# Examining the Technology for a Sustainable Environment Grant Program

An Interactive Qualifying Project Report Submitted to the Faculty of WORCESTER POLYTECHNIC INSTIUTE In partial fulfillment of the requirements for the Degree of Bachelor of Science

Submitted to: Professor James Demetry Professor Joseph Petruccelli Worcester Polytechnic Institute: Washington, D.C. Project Center

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This report is submitted in partial fulfillment of the degree requirements of Worcester Polytechnic Institute. The views and opinions expressed herein are those of the authors and do not necessarily reflect the positions or opinions of the Environmental Protection Agency or Worcester Polytechnic Institute.

# Abstract

This project was performed with the support of the Environmental Protection Agency and involved the examination of the Technology for a Sustainable Environment (TSE) grants program. We selected ten researchers funded by the TSE program, interviewed them, and reviewed their research in terms of qualitative and quantitative academic, industrial, and potential environmental impacts. For each of the ten researchers, we wove this information together into a story. We also developed overall conclusions and recommendations.

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# **1 Executive Summary**

For the past ten years, the Environmental Protection Agency (EPA) and the National Science Foundation (NSF) have sponsored the Technology for a Sustainable Environment (TSE) grant program. In May 2004, the EPA reviewed the TSE program to determine whether it was a worthwhile program and whether funding of the program should continue. The review panel determined that the TSE program was instrumental in advancing environmental research, and as a result recommended that funding of the program continue. Some questions were left unanswered, however, concerning what happened to the results of the research once the term of the grants had expired.

The goal of our project was to define an array of outcomes to assess the success of the TSE program, and to use our results to develop case studies in order to identify and document in detail the effects of research conducted by ten Principal Investigators (PIs) who were supported by the TSE program. We selected the ten PIs based on the scientific focus of the grant (.e. solvent replacement or green engineering) and the year in which they conducted their research. This provided our study with a variety of topics across the entire lifespan of the TSE program. We organized the impacts made by the results of the research into three main categories: academic, industrial, and environmental.

We collected data on the research conducted by the ten selected PIs through:

- Interviews with each of the PIs as well as graduate students involved in the research.
- Citation searches of articles written as a result of the research in order to show how effectively the information has been disseminated in the academic community.
- Searches of Scorecard and AirData, databases containing the amounts of chemical emissions in the United States, for industries that could be potentially affected by the

research in order to determine an upper-bound for potential reduction in chemical releases.

Academic impacts were the easiest to determine. Out of the ten PIs we interviewed, nine of them had worked with at least one graduate student in the course of their research. Five wrote highly cited articles based on their TSE-supported project, many of which were published in high-impact scientific journals. Two developed college courses based on their work, while a third created labs that allow his students to recreate his experiments.

Even though the TSE-supported research had a number of effects in academia, industrial impacts were less prevalent. Most technology or processes developed from the findings of the TSE-supported research have not yet been adopted by industry. A few different factors contribute to the absence of technology transfer. The most common reasons are that the findings are too recent or that there is too much financial risk involved in the adoption of the technology or process. PIs who have had an impact typically worked with companies both during and after the research period. By involving industry in their research, these PIs got companies to invest in their ideas from the beginning stages. Unfortunately, trade secret sensitivity prevented some of the PIs from informing us of the extent of the impact of their research.

Since the industrial impact of the selected PIs' research has been limited, there also has not been much in the way of environmental impacts. In cases where technology or processes developed as a result of the research have been adopted, it is still difficult to determine how a technology or process would affect the environment. Several years often pass before there are noticeable changes, and the information in databases like the Scorecard and AirData are a few years old due to the lag time in collecting emissions data. In order to have some idea as to the potential pollution prevention of the research if its results were adopted into industry, we

searched the Scorecard and AirData for harmful chemicals that would be reduced or removed by the new process or technology in industries affected by the developments of the PIs' studies. The result was an upper-bound pollution-reduction potential We recommend that the TSE continue to conduct these evaluations in the future, in order to keep up-to-date with the results of the research it funds. To aid the TSE in future evaluations and also increase the impact of the PIs' research once the grant period is complete, we recommend that the TSE:

- Encourage both potential and current PIs to be as specific as possible as to which chemicals would be reduced, removed, or added as a result of their new technology or process.
- Strongly encourage industrial involvement both during and after the research, possibly by providing incentives to companies.
- Implement a method to keep in contact with PIs after the term of the grant expires.
- Help the PIs publicize their work in order to make the general public aware of its benefits.

# **2** Introduction

For over thirty years the Environmental Protection Agency (EPA) has existed to protect human health and the environment. In order to accomplish this goal, Congress has authorized the EPA to create and enforce environmental regulations in fields such as industry, commerce, and transportation. Innovative solutions are needed to help industry meet fulfill the requirements for these regulations, and the EPA helps by sponsoring and supporting research for that purpose.

The Technology for a Sustainable Environment (TSE) program is an academic research grants program created by the EPA and National Science Foundation (NSF). The TSE is geared towards funding research in pollution prevention that will improve industrial processes in order to make them environmentally safer while still ensuring economic competitiveness. In the last ten years over two hundred such grants have been awarded. Many of the researchers have earned awards for their work, published their findings in academic journals, or have accomplished both in part due to the TSE funding. Their research has led to scientific and technological advances and helped support the education and training of a new generation of environmental researchers. However, there are more beneficial outcomes of the TSE program that still need to be measured and documented.

In May 2004, ten years after the TSE program started, the EPA and the NSF jointly sponsored an evaluation meeting to see what outcomes the research had produced. The evaluation panel of external experts discussed whether the goals of the TSE program had been achieved, whether the outcomes have been both measurable and effective, and whether a federally-funded program was still needed for this type of research. The evaluators decided that the TSE program has been very effective and that it plays an important role in furthering

environmental research, but they noted that specific questions still remained as to how the outcomes affect academics, industry, and the environment.

Even though the TSE program was deemed successful in some aspects, further study of the questions produced at the meeting is needed to show the full value of the program. Some of these questions include:

- What patents and licensing have been produced from the research projects?
- What research are the principal investigators (PIs) currently conducting?
- How much funding was awarded in addition to the TSE grants in order to further related research? If so, who provided this funding?
- What impact has the TSE program had on the careers of graduate students who were trained under the program?
- Which technologies developed by the research are being used in industrial practices?
- Has the research resulted in the reduction of toxic materials and pollutants?
- How much economic savings have resulted from sustainable technologies?
   (Schuster, et al., 2004, Background)

To this list we added the following question: Has the research affected any of the curricula at the universities that were awarded the TSE grants? This project seeks to answer those questions in a way that helps the EPA more clearly understand the benefits of the research projects.

Our goal was to define an array of outcomes to assess the success of the TSE program, and to use our results to develop case studies in order to identify and document in detail the effects of research conducted by ten PIs who were supported by the TSE program over the last decade. Our qualitative approach was to interview the PIs, who are professors, and former students involved in the projects concerning their research and its effects on industry, on academic curricula and on stimulating other research. We also asked if their research is being continued and if so what funding has kept it going. We inquired if any patents have been granted as a result of the research. Our quantitative approach used data from the Presidential Green Chemistry Challenge Database, AirData, and the Scorecard to estimate the environmental implications of the research, if it were to be adopted by industry. Our project showed how the research funded by the EPA's TSE program has created better technology and helps to contribute to the EPA's mission of protecting the environment and human health.

In order to successfully complete this project, we needed to have an understanding of the Technology for a Sustainable Environment (TSE) program and all of the tools and methods used to evaluate it. We needed to be familiar with the hazards of specific chemicals in order to see how the results of the research would be an improvement over the traditional process or technology from an environmental standpoint. When either interviewing Principal Investigators (PIs) or reading annual project reports, it was necessary to develop a basic understanding of the process or technology being improved. This was so we could accurately assess where the improvements could be implemented and how the change could affect the industry where it is utilized.

# 3.1 The Technology for a Sustainable Environment Program

When the Environmental Protection Agency (EPA) and National Science Foundation (NSF) formed a partnership in 1995 to create the TSE program, the two agencies had a few common objectives for their combined efforts. The goal of the TSE program is "to research, develop, and promote implementation of scientific and technical advances to reduce water, material, and energy intensity and increase the use of benign material and energy. The program funds research that advances the discovery, development, and use of innovative technologies and approaches to avoid or minimize the generation of pollutants at the source" (Schuster, et al, 2004, Executive Summary). For the EPA and NSF the TSE program is a way to further research in the areas of Green Chemistry, Biochemistry, Industrial Ecology and Non-Reaction-Based Engineering for Pollution Avoidance (NCER, 2003, Introduction). The program is geared towards finding innovative pollution prevention techniques. The TSE program funds research that is focused and adaptable in society, promoting more interaction between industries and researchers. An example of this is a grant where the research conducted on chemical coatings led to the General Motors Research and Development Center teaming up with the TSE-funded researchers to develop new methods in green manufacturing technologies (TSE Survey Results, 2004). In 2003 the TSE program gave out 45 grants worth a total of 9.5 million dollars, with 3.5 million dollars from the EPA. Each grant is funded solely by the EPA or NSF.

## **3.1.1 Current TSE Grant Program Information**

A PI is required to provide the following information when applying for TSE funding and also annually in their report:

- Annual progress on the research
- Student involvement
- Cooperation with industries
- Any proposed pollution reductions
- Published papers that are relevant to the research.

As part of completing a thorough TSE grant application, the PIs have to document the potential environmental effects, such as the minimization of toxics or changes that have been implemented to an industrial process (NCER, 2003, Eligibility Information). Applicants must also provide qualitative data and an estimated timeline of when their results could be adopted by industry, to demonstrate how their outcomes might be implemented. The TSE grant program encourages student and industry involvement in the research project (NCER, 2003, Program Description). Researchers are also encouraged to include the views of professionals from industries when performing the research; they are aware of which processes can be improved and together with

the researchers can help achieve a practical solution. Industries could possibly adopt to create more efficient and possibly environmentally friendly technology. Student involvement in the research helps train the next generation of pollution prevention researchers.

# **3.1.2 Previous Evaluation of TSE Program**

The EPA and NSF cosponsored an evaluation conference, in May 2004, to determine if the TSE was fulfilling its goals as an academic research grant program. A panel of experts evaluated the program after receiving feedback from former PIs and discussing questions determined by the panel chair. Documentation of their findings may be found in Schuster, et al, 2004.

The panel discussed whether the goals of the TSE program had been achieved, whether the outcomes have been both measurable and effective, and whether a federally funded program was still needed for this area of research. Among the evaluators of the TSE program, they felt, "there was a general consensus that the outputs of the program have been of high quality" (Schuster, et al, 2004, Background and Overview). The TSE program was judged to be valuable enough to continue funding since the program is "crucial to environment health and the economic competitiveness of the United States" (Schuster, et al, 2004, Executive Summary).

While there was documentation on some measurable outcomes of the PI's work, through annual reports from the PI, additional outcomes need to be measured so that the TSE program could be assessed more thoroughly. The program needed to be assessed so that the office that maintains the EPA's portion of the TSE program could demonstrate the success of the TSE program to other offices within the EPA. Examples of additional outcomes that were explored include: what impact the research had on the graduate students, by what amounts toxic materials

have been reduced over the years, the economic impact of the research, examples of pollution prevention, etc. In addition, an outcomes assessment is needed at this time because the EPA has not had the chance to fully look at the TSE program and what has occurred with the funding in its ten years of existence.

# **3.2 Academic Impacts**

The research funded by the TSE program is done in academic settings. It is important to know what the goals of the researcher are when trying to determine a project's success. In a discussion with Professor Bergendahl of Worcester Polytechnic Institute, (personal communication, October 4, 2004) who is presently working on a research project funded in part by the National Institutes of Health, we learned what goals he has while conducting such a research project. The biggest goal for him was getting his work published. If the work does not get published to the scientific community it is as if the work has not been done. Secondly, Professor Bergendahl provided two criteria for evaluating the academic impacts of a research project: dissertations of the graduate students working on the projects and published papers written by the PIs about their research results. Some other measures for evaluating academic impacts of the research are: production of other publications (such as books), citations of PI's published writing, textbooks and courses incorporating results of the research.

#### **3.3 Industrial Impacts**

The impact on industry due to the research can occur while the research is being conducted or after it has been completed. For example, these impacts can result from the

involvement of industrial partners or awarding of patents. PIs were encouraged to have industrial partners while they perform their research (NCER, 2003, Program Description). The relationship of industrial partners and the PIs varied for every research project; yet the interaction between the industrial partners and the PIs may be an indication of the industrial impact of the research (NCER, 2003, Background). Patents did not necessarily show a direct connection of a PI's research being used in an industrial process; they were examples of the innovative, original, and inventive ideas that were formulated though completing the research. The existence of patents suggests that the discoveries made through research could potentially be brought into industry. The best way to show if a discovery was brought into industry is by the existence of licenses. A license is filed when a patent holder grants an industry permission to produce a product using the patent holder's discovery. The impact of the research on industry is more fully revealed by figures on the products produced using the license.

# 3.4 Presidential Green Chemistry Challenge Award Program

The EPA is working towards reducing the amount of pollution as part of the Pollution Prevention Act of 1990 (EPA, 2004, Green Chemistry Award Facts). Green chemistry is "the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances" (EPA, 2004, Green Chemistry). The Presidential Green Chemistry Challenge Award Program was founded in 1995 as a means of promoting green chemistry, specifically the economic, environmental and scientific benefits of it (EPA, 2004, Green Chemistry Award Facts). The program distinguishes achievements in green chemistry by giving awards in following categories: small business, academic investigator, and sponsor for a project (i.e. industrial-supported research) (EPA, 2004, Green Chemistry).

The award program has two resources that were beneficial to this project: the applications of the nominees and the internal database of this program. The requirements for the application are extensive, providing information on how the research could impact the environment, human health, and the technological benefits of the nominated work (EPA, 2004, Green Chemistry). The Office of Pollution Prevention and Toxics runs the Presidential Green Chemistry Challenge Award Program and they have a database that contains qualitative and quantitative data taken from the nominees' application. The nominee's entry from the database and their application together couldprovide potential quantitative information on how the proposed research could impact industries and the environment if it were to be adopted. These applications and database entries were of use to this project because seven out of the ten PIs chosen for this project were nominees for the Presidential Green Chemistry Challenge Award.

### **3.5 Toxics Release Inventory**

The Toxics Release Inventory (TRI) of the EPA contains data on amounts of hazardous chemicals released, which are organized by region, industries, facility, or type of chemical. The origin of the database goes back to the Emergency Planning and Community Right-to-Know Act (EPCRA) of 1986. "EPCRA's purpose is to inform communities and citizens of chemical hazards in their areas" (EPA, 2004, Introduction). The EPCRA requires that industry report on certain chemicals. As of 2003, 582 chemicals were to be reported on in three areas: the amount of chemicals stored on site, chemicals released from the facilitity, and transfers of the chemicals from industrial facilities. The chemical information is collected from self-reporting by the industrial facilities and entered into the TRI database. The TRI Explorer is the search engine for

the TRI database, available online at <u>www.epa.gov/triexplorer/</u>. Below is a picture of the TRI Explorer user interface.

Reports: ▹ <u>Chemical</u> ▶ <u>Facility</u>	Geographic Location 🗓 U.S. by State 💙 Chemical Released 🗊
► <u>Federal Facility</u> ► Trends	All chemicals
🕨 Geography 🗓	Industry 🗓
⊩ Industry	All Industries 🛛 👻
Maps:	Year of Data i
► <u>Dynamic</u>	2002 🔽
	Data Set i
	The default is the current data update (as of August 2, 2004)
	Select 2002 Public Data Release data set (frozen April 1, 2004 and released to the public June 25, 2004)
	Generate Report

Figure 1: TRI Explorer (EPA, 2004, TRI)

The search engine has two components. The left side is where the user chooses how the searched data will be organized. The right side shows which characteristics the TRI Explorer would search for. The search can be performed in terms of: chemical, facility, geography, industry or year. For example, a user could search for all chemicals released by the lumber industry in Maine for the year 2002, organized by chemicals. The results would show any chemical releases by Maine's lumber industry, sorted by specific chemicals, during 2002. The TRI Explorer was used to determine if any of the chosen PIs' research could potentially affect any industries that submit information to the TRI. "Reporting Year (RY) 2002 is the most recent TRI data available. The TRI 2002 Data Release page provides an overview of the TRI information. Facilities reporting to TRI were required to submit RY 2002 data to EPA by July 1, 2003" (EPA, 2004b, TRIExplorer).

# 3.6 AirData

The EPA AirData Web site <u>www.epa.gov/air/data/info</u> contains yearly summaries of United States air pollution data that are taken from EPA's air pollution databases. AirData has two types of data: emissions data (taken from EPA's National Emission Inventory (NEI) database) and monitoring data (taken from EPA's Air Quality System (AQS) database). Its emissions data are estimated from amounts of material consumed or product produced, which are given to EPA by state environmental agencies. Most estimates are for individual sources, such as factories. The rest of the estimates are county totals for classes of sources, such as vehicles. The most recent data in AirData are emissions from the year 1999.

# 3.7 Scorecard

Environmental Defense, a leading national nonprofit organization containing over 400,000 members, launched Scorecard on Earth Day 1998. Currently, GetActive Software, a company founded by the technical team that built the Scorecard web site, powers Scorecard. "Scorecard integrates over 400 scientific and governmental databases to generate its customized profiles of local environmental quality and toxic chemicals. Since Scorecard draws all its data from authoritative sources and combines them using state-of-the-art informatics, users can be confident they are receiving credible information that reflects the best available science. All data sources are clearly cited on Scorecard, with hyperlinks back to online references whenever available." (Environmental Defense, 2004, About Scorecard). A major source of Scorecard's information comes from the EPA's TRI database. Part of Scorecard's function is to combine this data along with various other sources to show which industries and facilities in the U.S. are releasing certain chemicals. For more information on Scorecard, please see the official web page, <u>www.scorecard.org</u>.

# 4 Methodology

The goal of this project was to determine the outcomes of research conducted with grant support from the Technology for a Sustainable Environment (TSE) program. In order to do this, we compiled case studies on ten principal investigators (PIs) funded by the TSE program. In developing these case studies, we determined the educational impact of the research: whether it prompted changes in current school curricula, resulted in published articles in academic journals, or stimulated graduates in further related research. We looked for impacts on industry, mainly through the creation of licensable technologies, patents, new industrial processes, and partnerships with corporations. We also determined the environmental impacts that could potentially occur due to these research results. This chapter addresses how we achieved this analysis and also discusses specific tools that were at our disposal, such as AirData and Scorecard, and how they aided in our analysis.

# 4.1 Selecting PIs

Over 200 projects have been awarded funding from the TSE program. Our liaisons narrowed this large population down to a more manageable size by selecting 27 potential PIs. Before selecting the PIs for study, we stratified the potential investigators by the year and field of study of their projects, i.e. alternative synthesis, solvents, and life cycle analysis. The PIs were grouped by the subject matter of their research grants. Within each subject area, the PIs' projects were sorted by the year that the proposal was submitted to the EPA. From these strata we selected our ten PIs so our study spanned a variety of research topics over the entire lifespan of the TSE program. We chose to have a range in subject matters to provide analysis of the different topics supported by the TSE funding.

# 4.2 Cases Studies

Case studies were used in order to learn more about a PI's research and the outcomes of that research so that our liaisons could better understand the outcomes of research that the TSE funded. A case study provides a detailed report in which a systematic method is used to review the information available, collect data and then analyze it (Yin, 1994, p 16). Case studies are used to evaluate a large system or organization with one case study focused on each different component of the system. The case studies in this project were used to write a document outlining the effects of the PI's research; including information such as the environmental problem that the research concerned, a description of the research, and the important impacts of the research. For our project we compiled a case study for each of the chosen PIs, thus ten case studies were compiled. The information collected early on from the TSE application, the PIs' annual reports, published papers, and patents provided the groundwork while the information from phone interviews provided the details for the case studies.

# 4.2.1 Assessing the Academic Impact

The TSE program is an academic grants program; PIs, most of whom are university professors, run the individual research projects. These projects provide an opportunity, if taken, for researchers to work with other members of the academic community. Students, both graduate and undergraduate, also play a vital role in the research. The experience they gain while participating in the research expands their career options and allows them to apply their findings if they pursue a career in industry. They may also choose to further the research themselves either through research for the purpose of industrial use or academic use. After

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completing their research, both the PIs and their students may have published their findings, continued with further research, or both. If the PIs have taught classes, they may have altered the syllabi of their courses in order to pass on their findings to their future students. The results may also have appeared in college or graduate courses taught by others, in professional development courses, and in educational materials. The most efficient and direct way of determining how the research had impacted the academic world was through interviewing the PIs and former students involved in the research. Besides providing us with direct information, their responses directed us towards the outcomes of their research such as published papers, patents, or licenses.

### 4.2.2 Conducting Interviews

Interviews were vitally important to our project; the data we gathered from them were our only first-hand sources of information regarding the individual research projects. The PIs were the most accessible subjects for those interviews, since each investigator's contact information was easily located in the grant files. Any contact information for the graduate students was given to us by the PIs during the phone interview.

In order to maintain consistency in responses, the same set of questions was used for each interviewee. If any of the answers to the questions had been found in the grant files, those questions were omitted during the interview. After calling the PIs, we reviewed the responses with our liaisons. If our liaisons had further questions, or if some information was unclear, we contacted the PIs a second time. When all the information was organized, we emailed the PIs their respective information sets to ensure accuracy. Any final changes the PIs recommended were then made. Questions which were asked during PI interviews can be found in Appendix B, while questions which were asked during student interviews can be found in Appendix C.

After conducting the interviews we put together all the information and created a Word document for each of the PIs. Those documents included answers to the standardized questions, interviews with their graduate students, a listing of published papers, patents, and citations of their research. We also noted on each of the Word documents any other important information that might only pertain to that particular PI. All the collected information was then given to our liaisons.

## **4.2.3 Archival Research Using Published Papers**

One item of interest which we discovered in the grant files was whether the PIs had published, or made a presentation of, their findings, and if so where and when. For example, they could have published their findings in an academic journal, or they could have used their results to contribute to the writing of textbooks. By publishing their findings, or presenting at conferences, the PIs had a chance to stimulate further research outside of their particular campuses, as it would alert other potential investigators to the possible advancement of the field of study. By tracking citations to published works written by the PIs or former students on the TSE-funded research project they conducted, we were able to demonstrate how effective the research has been in stimulating further study. Those citations were found at the EPA Library's Science Citation Search. By inputting a cited article's author, journal, and year published, the citation search returned the titles, authors, and journals of any citing article.

#### **4.3 Assessing Industrial and Environmental Impact**

Through our interviews with PIs, we learned of the possible ways in which their research could ultimately affect industrial processes by way of associated new technologies. We

subsequently chose to estimate the potential industrial and environmental impacts for the grants conducted by a subset of the selected PIs. This analysis looked at the potential impact of the research on industry and the environment

The methods described here yielded the quantitative results for our project. Three resources supported the estimation process: the Presidential Green Chemistry Challenge database, Scorecard, and the Air Quality System.

#### 4.3.1 Referencing the Presidential Green Chemistry Challenge Database

The Presidential Green Chemistry Challenge Database contains qualitative and quantitative data that has been taken from submissions by researchers who have applied for the award. We found that seven of our chosen PIs had entries in this database. Since most of our qualitative information came from the interviews with the PIs, we were interested primarily in the quantitative data held in the database. These data estimate the quantities of chemical substance emissions that would be removed or reduced as well as the emission amounts that would be added if the technology were adopted. It is important, however, to note that these numbers estimate the maximum potential effects for the improved industrial process.

We originally planned on using the data to show the differences between the current and improved industrial processes assuming the technology is implemented. For the seven PIs that we performed this analysis on, there was no quantitative data available. Instead we used the information about which chemicals were reduced, eliminated, or added that was available from the database entries. The information on chemicals was used with the Scorecard and AirData as described below.

#### 4.3.2 Archival Research using the Toxics Release Inventory & Scorecard

As stated in the background chapter of this proposal, the TRI is a database containing information concerning chemical hazards in regions across the country. For a select few of the PIs we determined which specific industries could use technology that could be developed from the PI's research. We also determined which specific chemicals the research worked towards reducing or eliminating. Initially, we searched the TRI for the quantities of chemical emissions that the potentially affected industries released and compared these amounts to the total quantity of chemicals released. These results were used to estimate the possible reduction in chemical emissions that could occur if the technology stemming from the TSE-supported research was adopted by industry. Every time we used the TRI we selected the most recent reporting year given, 2002.

For example one TSE researcher, Dr. DeSimone's second TSE research grant investigated the possibility of replacing solvents in the lithography process with carbon dioxide; he is trying to incorporate carbon dioxide into the process to replace toluene. Before using the TRI database, the industries that use toluene in their lithography process needed to be identified. When using the TRI we selected a very broad industry type because there are only 28 Standard Industry Classification (SIC) codes to choose from. In this example, the closest industry type in the TRI to be affected by Dr. DeSimone's research was "electrical equipment industry (SIC 36)". This industry type was way too broad so we went to Scorecard, because it allows us to go one step further, narrowing down results to a more specific industry type. In Scorecard, after we selected toluene and the industry type "electrical equipment industry (SIC 36)" there were options for additional subsets for the industry type. In this case we looked at the emissions resulting from the subset industry type "Semiconductors and Related Devices (SIC 3674)"

because Desimone's research was related to the semiconductor industry. We now have a number in pounds or tons per year for the amount of toluene being released by the "Semiconductors and Related Devices" industry. The only problem with Scorecard is that since the data is being taking from the TRI and other sources, its information is not as recent as the TRI. So although we have more accurate data, now the emissions we are analyzing come from the year 2001 instead of 2002. These data obtained from the Scorecard were used to estimate how Dr. DeSimone's research, if implemented, could potentially affect the environment and industries by showing an upper bound for potential reduction of specific toxic chemicals.

In performing this research, some issues about the data collected arose. Since TRI contains self-reported data facilities might not have reported their data accurately, most likely there is more of toxics being emitted than they actually state. Data most likely have changed since Scorecard was last updated (2001). In addition, it is uncertain what portion of the industries we select could actually be affected by a PI's research. It is likely that other industries we did not select could still potentially be affected by a PI's work.

Finally, it is also important to keep in mind that although many of the PIs have provided research that could potentially estimate environmentally harmful material, not all possible chemicals, wastes, or toxics were in the TRI database. So our quantitative analysis was only performed on the materials that were in the database, but in most cases the research could potentially remove more chemicals than we were able to show.

# 4.3.3 Archival Research using AirData

Although the Scorecard's database contains much useful information for many harmful chemicals, there are still some hazardous emissions that cannot be searched by any industry type

(e.g. carbon monoxide, sulfur dioxide). However, we can perform this task at the EPA's website, specifically at the AirData page <u>http://www.epa.gov/air/data/</u>. So we used AirData to find the data on industry types that cause these emissions for these few air pollutants simply because it was not possible in Scorecard.

The first thing we did in AirData was look in the reports and maps section. Then, AirData allowed us to obtain information from a targeted geographical location in the U.S. (see Figure 2).

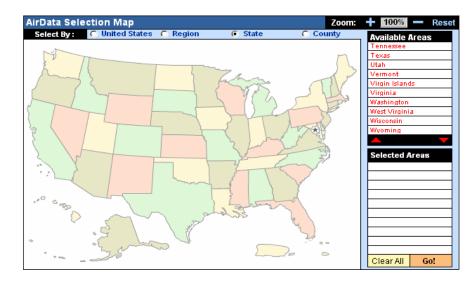


Figure 2: AirData Selection Map

# (AirData, 2004)

Since we were interested in emissions for the whole country, we selected the United States as our target area. Depending on the type of emission, we selected facility emissions for either criteria air pollutants or hazardous air pollutants. Criteria air pollutants are substances for which EPA has set health-based standards and hazardous air pollutants (HAPs) are substances that are known or suspected to cause serious health problems such as cancer. We were only interested in the criteria air pollutants because all the HAPs were already possible to analyze with scorecard. From there we chose the specific chemical and had the database include the following items for

the most recent year given: percent of total emissions, facility name, facility mailing address, county name, Standard Industrial Classification (SIC), and state abbreviation.

For exemplary purposes we will look at carbon monoxide (CO) emissions, which was the focus of Dr. Ramirez's research. There were two ways we searched for these emissions in AirData. The first way we searched CO emission was through the facility SIC report. This gave us an overview of how much CO is being released by every industry type listed in AirData (785 SIC codes). Table 1 shows the first five industry results (out of 785) that were displayed.

Table 1: CO Emissions from the First Five Industry Types in AirData

<u>Row #</u>	<u>Industry Type (SIC)</u>	Industry Type (SIC) Number of Percent of Total Facilities Facilities		<u>Pollutant</u> <u>Emissions</u>	Percent of Total Emissions	
SORT						
1	0111 - Wheat	1	0.0035	19.3	< 0.01	
2	0115 - Corn	2	0.0069	1.87	< 0.01	
3	0174 - Citrus Fruits	1	0.0035	0.06	< 0.01	
4	0181 - Ornamental Nursery Products	3	0.0104	13.2	< 0.01	
5	0182 - Food Crops Grown Under Cover	5	0.0173	23.6	< 0.01	

The "Industry Type" column on the far right was very important because it allowed us to show what specific industry the results of a particular research project might affect. For example, Fred Ramirez's research led to creating a model for a more cost effective electric arc furnace which could reduce CO by at least 90% in some plants. Thus, the quantitative information we were interested in was listed under the industry type, "Blast Furnaces And Steel Mills". Table 2 shows the actual quantitative data we used for our analysis. From this data we can say that the industry "Blast Furnaces and Steel Mills" produces 721,717 tons/year of CO and that this one industry makes up 17.19% of all CO emissions out of a possible 785 industries.

Table 2: CO Emissions from Industry Type "Blast Furnaces and Steel Mills"

<u>Row #</u>	Industry Type (SIC)	<u>Number of</u> <u>Facilities</u>	Percent of Total         Pollutant           Facilities         Emissions		Percent of Total Emissions	
SORT 🗧 🖬						
325	3312 - Blast Furnaces And Steel Mills	155	0.536	721,717	17.19	

To get more detailed information we had to perform a second search, this time using the facility emissions report. The facility emissions report ranks each facility listed in AirData by how much CO they release a year. Table 3 shows the data for the top five facilities that release CO in the U.S. The database allowed us to view 500 facilities at a time if we desired.

<u>Row #</u>	<u>Pollutant</u> <u>Emissions</u>	Percent of Total Emissions	Facility Name	Facility Mailing Address	<u>County</u>	<u>State</u>	Industry Type (SIC)
SORT	<b></b>						
1	165,519	3.94	Bethlehem Steel Corp.	U.S. 12 & S.R. 149, Burns Harbor, In 46304	Porter Co	IN	3312 - Blast Furnaces And Steel Mills
2	89,928	2.14	U S Steel Co Gary Works	One North Broadway, Ms-70, Gary, In 46402- 3199	Lake Co	IN	3312 - Blast Furnaces And Steel Mills
3	73,290	1.75	Bethlehem Steel	5111 North Point Boulevard, Sparrows Point, Md 21219	Baltimore Co	MD	3312 - Blast Furnaces And Steel Mills
4	61,724	1.47	Columbian Chemicals Company	S7-T29s-R35w, Ulysses, Ks 67880	Grant Co	KS	2895 - Carbon Black
5	61,265	1.46	Columbian Chemicals Company	Route 2, Proctor, Wv 26055	Marshall Co	wv	2895 - Carbon Black

Table 3: Top 5 Worst CO Releasing Facilities in the U.S.

Searching in this manner allowed us to see which industry types were in the top facilities releasing the most CO. This information is helpful because if there are only a few facilities releasing large amounts of CO with the targeted industry type for the research, then one can imply that implementing the research in a few facilities could possibly lead to a major reduction of the total amount of CO released by all facilities. In our example, 17 facilities categorized as "Blast Furnaces and Steel Mills" fall into the top 100 worst facilities for producing CO (about 14% of all CO emissions!).

As was with the Scorecard database, there are some issues with this analysis. Once again facilities might not have reported their data accurately, and most likely there is more CO being emitted than they have actually reported. Data most likely have changed since AirData was last updated. Information for this AirData report came from an extract of EPA's National Emission Inventory (NEI) final version 3, February 2004. However, the last reporting year for AirData was 1999 (which we used for all of our PIs that the data could be applied to). In our example, it

is uncertain how much of the steel industry could actually adopt Dr. Ramirez's model because we do not know what exactly falls under the category "Blast Furnaces and Steel Mills". In addition, other industries that we did not analyze could possibly benefit from his electric arc furnace that we did not take into account.

Lastly, it is also important to keep in mind that although many of the PIs have provided research that could potentially remove environmentally harmful material, not all possible chemicals, wastes, or toxics were in AirData. So our quantitative analysis was only performed on the materials that were in the database, but in most cases the research could potentially reduce other chemicals that we were unable to show.

# **5 Results & Discussion**

This chapter contains the stories of each of the ten selected PIs. These stories outline the accomplishments of the PIs while conducting their Technology for a Sustainable Environment (TSE) supported research and also covers what they did once their research was complete. For each PI, we covered several topics:

- The environmental problem their research attempted to alleviate.
- How they planned to solve the problem through their research.
- Articles published in high-impact journals.
- Industrial involvement in research and licensing.
- The creation of new school courses or the alteration of current ones.
- What the PIs are currently doing in their fields of study, and how that correlated with their TSE-supported research, if it did at all.
- Student involvement in the research, including information from interviews with some of the participating students.
- For some of the PIs, estimates on how technology developed by their research projects could potentially affect the environment if it were employed by industry.

# 5.1 The TSE-Funded Research of Dr. Eric Beckman

The TSE grant program funded Dr. Eric Beckman of the University of Pittsburgh on two separate grants focusing on replacing solvents with Carbon Dioxide ( $CO_2$ ) to improve industrial processes and to benefit the environment by using chemicals that are less harmful. Dr. Beckman was funded from October 1995 to September 1998 for the research project "Design and Synthesis of  $CO_2$ -Soluble Affinity Ligands for Use in  $CO_2$  Extraction of Proteins". Dr. Beckman was also funded in December 2003 for the research project "In-situ Generation of  $H_2O_2$  in CO<sub>2</sub>: Platform for Green Oxidations". This project is due to last until November 2006.

In industry, several environmentally harmful materials are used to make many commercial and industrial chemicals. Through new advances in technology, industries have received further opportunity to improve their processes which in some cases could also improve the environment. Both the process of purification of proteins from cell broth and systemization of Hydrogen Peroxide  $(H_2O_2)$  can be improved through the use of  $CO_2$  instead of harmful chemicals. These processes are useful in the production of many chemicals.  $CO_2$  has the benefits of being accessible, easy to release back into the environment, and is not a volatile organic compound (VOC). VOCs are gases that are harmful to both human health and the environment (EPA, 2004d, VOCs). The production of many types of materials such as paints, adhesives, and permanent markers produce VOCs. The threats to human health depend on the type of VOC, the duration of exposure, and the amount to which the person has been exposed. Health effects include facial irritation, headaches, and damage to the liver or the central nervous system. The effects of VOCs on the environment vary depending on the specific compound. Large amounts of VOCs in the atmosphere contribute to the formation of smog, when VOCs react with oxides; ozone and other harmful compounds are created.

Dr. Beckman's first grant was aimed at improving the purification of proteins from cell broth. Previously, the technique of reverse micellar extraction was used as an attempt to improve the protein extraction; however, it only worked in a select few scenarios. Dr. Beckman worked towards making the micellar extraction more possible by using  $CO_2$  in the process. His research goal was to produce  $CO_2$ -soluble surfactants and affinity ligands (molecules that can

attached themselves to other molecules to create larger molecules), and then use those molecules to demonstrate their behavior in  $CO_2$ .

Dr. Beckman was successful in designing a series of surfactants and affinity ligands that exhibit high solubility in liquid CO<sub>2</sub>. However, this work led him to the conclusion that materials used were too expensive to make the processes economical, even though they would be greener. Around 1999, Dr. Beckman learned that the compounds he was using were not only expensive, but also not as environmentally friendly as he had originally hoped.

After working on his first TSE grant, Dr. Beckman's work focused on greener reactions. While reading an article on how to make Propylene Acid, he discussed with one of his students, Dan Hancu, how the process could be simplified. Dr. Beckman came up with an idea of swapping  $CO_2$  for the solvent that was presently used. Lyondell Chemicals had patents on new innovative methods for making  $H_2O_2$ . The two parties talked and Lyondell Chemicals contributed \$250,000 to support Dr. Beckman's future research.

Dr. Beckman is currently working on his second TSE grant, which focuses on generating  $H_2O_2$ . He is working on a bio-functional catalyst that will do two things. The first function of the catalyst is to make  $H_2O_2$ , and the second function is to make an oxidation catalyst. The research is mainly focused on producing Propylene Oxide (used in foam cushioning), Phenol (used in polycarbonate), and Adipic Acid (used in nylons) with limited waste using the bio-functional catalyst. For the past four months Dr. Beckman has focused on Adipic acid, which is the most complicated of the three chemicals. Although he began the research with the TS-1 catalyst, the work has also led him to use different oxidation catalysts.

Both of these grants show that  $CO_2$  is a successful solvent and perhaps can be used in other reactions. Dr. Beckman promotes the thinking of  $CO_2$  as an ideal solvent for research

applications rather than just an environmentally safe solvent. His current research shows that the oxidation process can be cleaner using different types of solvents.

Dr. Beckman's research did not have an extensive impact on the curriculum. The research has not affected Dr. Beckman's teaching, with the exception of bringing green chemistry examples into his elective course. The school's curriculum also has not been affected, mainly due to the fact that he focuses more on chemistry than most other chemical engineers. Dr. Beckman also did not collaborate with any other faculty outside his department or institution. In terms of graduate student involvement there were three students funded with Dr. Beckman's first grant and two are being funded by the second grant. His graduate student, Dan Hancu, was not available to talk to.

Dr. Beckman did have a significant number of industrial partners for both of his TSE grants. For his earlier TSE grant, Dr. Beckman worked as an industrial partner with Genencor International, a biotechnology company that focuses on discovering, developing, and selling biocatalysts and other biochemicals. Genencor helped with supplying materials, giving analysis, and co-writing published papers and patents. In addition to supplies, Genencor provided about \$60,000 to \$70,000 of funding throughout the entirety of his three year grant. For his current TSE grant, Dr. Beckman has two industrial partners: Lyondell Chemicals and SNF. Lyondell Chemicals funded Beckman between his two TSE grants with \$250,000. For Dr. Beckman's current grant they help with catalyst preparation and characterization, and patenting. Also SNF, a French company, makes basic chemicals. They provide pilot testing facilities, knowledge on catalysts, and are giving fifty thousand dollars in funding for his three-year grant.

Along with having strong industrial partners, Dr. Beckman also was successful in producing valuable outcomes. His first TSE grant led him into the research area of  $CO_2$ -soluble

materials. The Chemical and Transport Systems Division, a part of the National Science Foundation's (NSF) Directorate for Engineering, funded more research that Dr. Beckman conducted. This includes attempts to design a non-fluorinated, highly CO<sub>2</sub>-soluble material using a combination of computer simulation and experiment. The basis for this work was started with some TSE money and preliminary results were achieved when Dr. Beckman received the NSF support.

Dr. Beckman has the following completed patents:

- US Patent 6638749, October 28, 2003. "Carbon dioxide soluble surfactant having two fluoroether CO2-philic tail groups and a head group." Inventors: Eric Beckman, Eliador Ghenciu, Nathan Becker, Landon Steele, Alan Russell.
- US Patent 6342196, January 29, 2002. "Synthesis of hydrogen peroxide." Inventors: Eric Beckman and Dan Hancu.
- US Patent 6596884, July 22, 2003. "Synthesis of hydrogen peroxide." Inventors: Eric Beckman and Dan Hancu.
- US Patent 6710192, March 23, 2004. "Dense phase epoxidation." Inventors: Dan Hancu, Eric Beckman, and Tiberiu Danciu.

Dr. Beckman has the following patent filed; not yet completed:

 US Patent Application 20040186319, September 23, 2004. "Synthesis of N-vinyl formamide." Eric Beckman, Toby Chapman, Cedrick Gilbert Favero, Christopher Capelli, Harold Swift

#### 5.1.1 Potential Quantitative Impact of Dr. Beckman's Research

Dr. Beckman's research proposes to eliminate and reduce a wide variety of chemicals and waste. Table 4 simply shows the other chemicals that were not listed by industry, if at all, in either AirData or Scorecard. The table's information shows whether Dr. Beckman was reducing, replacing, or eliminating that chemical. Table 5 shows emissions of Propylene, Methyl Tertiary Butyl Ether, Chlorine, Ethyl Benzene, and Styrene that were taken from Scorecard (RY2001). This table shows emissions from several chemical industries that were thought to be the closest industries related to Dr. Beckman's research according to their code name. Note that for the five toxins that were in Scorecard, combined they equate to 13,057,024 pounds per year released by these chemical industries.

Toxic/Waste	Proposed Status
organic solvent	replaced
n-alkane	replaced
chlorofluorocarbon	replaced
cyclic propylene carbonate	replaced
aromatic solvent	replaced
hydroxide base	replaced
chlorohydrin	elminated
organic side products	reduced
salt waste	elminated
waste water	elminated
2-alkyl anthraquinone	elminated
2-alkyl hydroquinone	elminated
long chain alcohol	replaced

Industry Type (SIC)	Propylene (pounds)	Methyl Tertiary Butyl Ether (pounds)		Ethyl Benzene (pounds)	Styrene (pounds)	Total (pounds)
2819: Industrial inorganic chemicals, nec	29,106	623	503,489	7,082	4,610	544,910
2821: Plastics materials and resins	2,548,941	0	94,229	159,198	1,451,142	4,253,510
2865: Cyclic crudes and intermediates	216,738	27,451	30,747	1,077,979	410,196	1,763,111
2869: Industrial organic chemicals, nec	5,202,451	171,632	588,925	170,212	331,672	6,464,892
2899: Chemical preparations, nec	11,100	6,638	7,002	5,469	392	30,601
Total (pounds)	8,008,336	206,344	1,224,392	1,419,940	2,198,012	13,057,024

### 5.1.2 Dr. Beckman's Published Articles Citations

Table 6 lists the numbers of citations of articles written by Dr. Beckman on the research he conducted with TSE support. Self-citations were removed because they do not necessarily indicate that other researchers are expanding upon the information in the article. Black cells indicate that the article had not yet been published in that year. The rightmost column contains the total number of citations for a given article, the total number of citations for all articles, and the average number of citations per article. In reading the table there were 17 citations and there was an average of 8.5 citations per each article that Dr. Beckman wrote. For the most part, citations for each article take time to enter into the mainstream. Once the article has been widely introduced, citations rise dramatically. Then, after reaching a peak, the information becomes old, perhaps outdated due to further research, and the number of citations decreases. Dr. Beckman's article: "Solubilization of subtilisin in CO2 using fluoroether-functional amphiphiles" published in 1998 shows the trend of citations. At first it was not cited much, then after being out for a couple years the article had a peak of citations after two and four years of being published. After the peak in citations in 2002 the number of times that the article was cited decreased.

									total # of
	1997	1998	1999	2000	2001	2002	2003	2004	citations
Affinity extraction into carbon dioxide. 1. Extraction of avidin using a biotin-functional									
fluoroether surfactant	0	0	0	0	1	1	2	1	5
Solubilization of subtilisin in CO2 using fluoroether-functional									
amphiphiles	0	0	1	3	2	3	2	1	12
Total # of citations per year	0	0	1	3	3	4	4	2	17
Average # citations per article per year	0	0	0.5	1.5	1.5	2	2	1	8.5

Table 6: Dr. Eric Beckman's Citations

## 5.2 The TSE-Funded Research of Dr. Joseph DeSimone

Another researcher who was funded twice by the TSE grant program was Dr. Joseph DeSimone of the University of North Carolina. His research focuses on replacing solvents with CO<sub>2</sub> to better improve the industrial process and also to benefit the environment by using less harmful chemicals in the process. Dr. DeSimone was funded from November 1997 to October 2000 for the first research project: "Nonionic Surfactants for Dispersion Polymerizations in Carbon Dioxide". Funding for his next project "Environmentally Responsible Processes for High Resolution Pattern Transfer and Elimination of Image Collapse using Positive Tone Resists" came in November 2001 and lasted until October 2004.

Researchers were starting to look into ways to use  $CO_2$  in industrial processes to improve the existing systems. The benefits of  $CO_2$  are that it is: non-toxic, non-flammable, easy to recycle, natural, inexpensive, and widely available. The success of implementing  $CO_2$  depends on the ability to design and synthesize efficient surfactants. When  $CO_2$  is used it can replace chemicals that are harmful to the environment. Here is information on the processes that Dr. DeSimone worked to improve.

Polymers are substances used in the manufacture of items such as plastic bags, vinyl siding, and carpets. Some polymers presently are made with solvents that are considered to be volatile organic compounds (VOCs). VOCs are harmful chemicals that are released as gases as a result of a reaction (EPA, 2004d, VOCs). VOCs are harmful to human health and the environment. The impact on health depends on the type of VOC, the duration of exposure, and the amount a person is exposed to. Health effects range from facial irritation and headaches to liver or central nervous system damage. The effects on the environment vary depending on the specific compound. Large amounts of VOCs in the atmosphere contribute to the formation of smog, when VOCs react with oxides; ozone and other harmful compounds are created.

Dr. DeSimone has worked on making surfactants used in synthesis of materials starting with Tg polymers. These polymers are primarily used in adhesives and coatings. Dr. DeSimone worked towards using CO<sub>2</sub> as a surfactant to produce the following polymers: polyvinyl chloride (PVC), polyvinylidene fluoride (PVF<sub>2</sub>), ethylene-vinyl acetate copolymers (EVA), artificial rubber from styrene, and 1,3-butadiene (SBR).

Additionally Dr. DeSimone worked towards improving lithography, a process in which an image is placed onto a wafer and then the chemicals which make the image are removed (Dr. Joseph DeSimone's Presidential Green Chemistry Application). The research focused on using liquid and supercritical  $CO_2$  so that the process of film deposition and removal can be done without using the solvents that are normally used in the lithography process. The most important benefit of performing the film deposition and removal process in positive tone is the elimination of hazardous solvents. This is because the use of solvents and water leads to large aqueous

waste. Positive tone refers to the level of resistance used in the lithography process. Recent work in lithography has moved towards positive tone rather than negative tone because of the better quality images produced with the positive tone. Additional issues that occur in the lithography process that  $CO_2$  helps to improve upon are reducing image collapses, enabling solvent-

free coatings of large wafers, and eliminating ion contamination. Image collapse is where the image produced in the lithography process collapses due to high surface tension. When water is not used but  $CO_2$  is, there is no source of surface tension and thus no collapse occurs. Since  $CO_2$  is used in place of solvents and water, coatings are made without solvents and there is no ion contamination because there is no water involved.

Dr. DeSimone has brought examples of his work into his polymer chemistry class and his sophomore organic chemistry class. He has also worked towards developing and maintaining the National Science Foundation (NSF) Science and Technology Center. The work from his first grant aided him in obtaining support for the research center. The center is a multi-disciplinary effort with participants from five academic centers and two national laboratories: University of North Carolina at Chapel Hill, North Carolina State University, North Carolina A&T University, University of Texas at Austin and the Georgia Institute of Technology in partnership with Sandia National Laboratory and Oak Ridge National Laboratory. More information on this center can be found at <a href="http://www.nsfstc.unc.edu/">http://www.nsfstc.unc.edu/</a>. Dr. DeSimone collaborated with members of the NSF Science & Technology Center and received supplementary funding for his two research projects funded by the TSE program.

Through the two TSE research projects, seven of Dr. DeSimone's students were funded. One graduate student was Luke Zannoni who worked with Dr. DeSimone on his research project,

"Dry Lithography: Environmentally Responsible Processes for High Resolution Pattern Transfer and Elimination of Image Collapse using Positive Tone Resists". Mr. Zannoni was involved in the research funded by another grant. When the TSE grant was obtained, there was an opportunity for him to apply the knowledge and skills that he had obtained while working on the other grant to the new areas funded by the TSE program (personal communication, November 29, 2004). His work in graduate school influenced him in his motivation to conduct research as a profession, with the preference of doing it outside of academia. The work with Dr. DeSimone has not prompted him to conduct further research in the same or similar area of study. Mr. Zannoni has published the following articles:

- Zannoni, L. A.; Simhan, J.; DeSimone, J. M. "Progress Towards the Development of a 157-nm Photoresist for Carbon-Dioxide-Based Lithography" *Proc. of SPIE*, 2003, 5039, 1327-1332.
- Zannoni, L.A.; DeSimone, J. M. "Synthesis Characterization, and Properties of Copolymers Prepared in Dense Carbon Dioxide Towards the Development of a 157 nm Photoresist" *PMSE*, 2002, 87, 197-198.

Currently Mr. Zannoni is employed at the National Starch and Chemical Company conducting research in the Corporate Research Group.

In addition to his academic activities, Dr. DeSimone has complied a record of collaboration with several industries. The research conducted with his first grant, Nonionic Surfactants for Dispersion Polymerizations in Carbon Dioxide, led to improvements in the dry cleaning industry and the use of  $CO_2$  in the manufacture of Teflon. Dr. DeSimone also collaborated with the following industries: MiCELL Technologies, BOC, and SCF Consortium (which included: Air Products, Bayer, BF Goodrich, DuPont, Eastman, General Electric,

Hoechst-Celanese, Xerox) for the research mentioned above. For the work involving the lithography process, Dr. DeSimone had industrial support in monitoring his research from Dupont, Stockhalven, and MiCELL Technologies.

Dr. DeSimone has been issued the following patent:

 US Patent 6451287, September 17<sup>th</sup>, 2002. "Fluorinated Copolymer Surfactants and Use Thereof in Areosol Compositions." Inventors: Joseph DeSimone, Terri Johnson Carson, John Miller, Sharon Wells Kennedy.

## 5.2.1 Potential Quantitative Impact of Dr. DeSimone

Implementation of Dr. DeSimone's research would reduce the amount of Silicon Dioxide, Methyl Ethyl Ketone (MEK), Ethyl Acetate, and Toluene used in the lithography process in the semiconductors industry. Table 7 shows data taken from Scorecard on the chemicals Methyl Ethyl Ketone and Toluene released by the "Semiconductors and Related Devices (SIC 3674)" industry. According to Scorecard (RY 2001), there are 2,000 pounds per year of Toluene and 8,000 pounds per year of Methyl Ethyl Ketone that were released by the "Semiconductors and Related Devices" industry.

Industry Type (SIC)		Methyl Ethyl Ketone	Total Pounds
3674: Semiconductors &			
related devices industry	2000	8000	10000
Total (pounds)	2000	8000	10000

Table 7: Scorecard data for Methyl Ethyl Ketone & Toluene

### 5.2.2 Dr. DeSimone's Published Articles Citations

	D1. 3	oseph	DCDI	mone	5 Citu	tions			
	1997	1998	1999	2000	2001	2002	2003		total # of citations
Cationic dispersion polymerizations in liquid carbon dioxide	0	3	1	2	0	0		1	8
Critical micellization density; a small-angle scattering structural study of the monomer-aggregate transition of block copolymers in supercritical CO2				0	0	3	2	1	6
Dispersion polymerizations of styrene in carbon dioxide stabilized with poly(styrene-b- dimethylsiloxane)	0	3	4	9	5	9	13	10	53
Interfacial activity of polymeric surfactants at the polystyrene- carbon dioxide interface		0	0	2	2	0	3	1	8
Light scattering study of diblock copolymers in supercritical carbon dioxide CO2 density- induced micellization transition		0	1	4	4	3	0	6	18
Poly(vinyl acetate) and poly(vinyl acetate-co-ethylene) latexes via dispersion polymerizations in carbon dioxide		0	1	4	1	5	8	5	24
Structure of diblock copolymers in supercritical carbon dioxide and critical micellization pressure				0	0	1	1	3	
Total # of citations per year	0	6	7	21	12	21	28	27	12
Average # citations per article per year	0	1.2	1.4	3	1.714	3	4	3.86	17.428

Table 8: Dr. Joseph DeSimone's Citations

Table 8 lists the citation of articles written by Dr. DeSimone on the research he conducted with TSE support. Self-citations were removed because they do not necessarily indicate that other researchers are expanding upon the information in the article. Black cells indicate that the article had not yet been published in that year. The rightmost column contains the total number of citations for a given article, the total number of citations for all articles, and the average number of citations per article. Dr. DeSimone had 122 citations from all the articles

listed and had an average of 17.5 citations per every article published. For the most part, citations for each article take time to enter into the mainstream. Once the article has been widely introduced, citations rise dramatically. Then, after reaching a peak, the information becomes old, perhaps outdated due to further research, and citations get lower. Dr. DeSimone did not have any articles that followed this trend exactly, the article "Cationic dispersion polymerizations in liquid carbon dioxide" shows how the citations taper off after the article has been out for several years. The number of citations reaches its peak within two years of publication but as article gets older in terms of its published year the citations per year decrease

## 5.3 The TSE-Funded Research of Dr. Nancy Ho

Dr. Nancy Ho of Purdue University was funded from October 1997 to October 2000 by the TSE Program for the research grant: "Development of Biotechnology to Sustain the Production of Environmentally Friendly Transportation Fuel Ethanol from Cellulosic Biomass".

Although Dr. Ho's desires seem to be concentrated on replacing gasoline with ethanol, currently her most important research result is in the improvement of methods for producing ethanol from cellulosic biomass. Traditional methods for producing ethanol have used corn as their primary feedstock. In ethanol production, cellulosic biomass is an alternative feedstock for corn. "In particular, ethanol can be produced from cellulosic biomass (corn stover, rice straw, wood, grasses, waste papers, etc.), which is abundantly available throughout the world – especially in our country. These feedstocks are also inexpensive and some of them exist as municipal or industrial wastes" (Ho, 2004).

Since corn is an agricultural product, producing ethanol from cellulosic biomass, which is an agricultural waste, instead of corn could indirectly help the environment. This is because corn farming requires many herbicides, insecticides, and fertilizers. In addition, there is a lot of energy input and land consumption from corn farming. Since approximately 85 percent of fuel ethanol is produced from corn, using cellulosic biomass as a replacement would lower the dependency on corn in the production of ethanol, thus possibly reducing the amount of pesticides, fertilizer and energy required for production.

Producing ethanol from cellulosic biomass used to be inefficient. This was because former yeasts could only ferment the glucose, which makes up about 70% of the sugar. Previous yeasts could not ferment the xylose, the remaining 30% of the sugar. With the support of the TSE Program, Dr. Ho found a way to genetically engineer yeast so that it ferments xylose as well as glucose. This great improvement has made the production of ethanol from cellulosic biomass far more efficient. As a result, cellulosic biomass as a replacement for the corn feedstock has become more realizable. In addition, improved yeasts have the potential of greatly lowering the cost of ethanol.

Dr. Ho's research has not gone unnoticed. In 1998 she received the R&D 100 Award (given to the 100 most technologically significant new products or inventions of that year) for her yeast because it could inexpensively produce ethanol from cellulosic biomass. She was also in 1999 Discover Magazine for technological innovation as one of twenty-seven finalists out of over 4000 applicants. Along with this recognition, the yeast has also already found its way into industry. Archer Daniels Midland (ADM), the leading ethanol producer in the world, tests all the yeasts that Dr. Ho develops. Another company in Ottawa, Iogen Corp., is currently using the yeast and has non-exclusive rights to it through licensing.

Dr. Ho has one completed patent:

• US Patent 5789210, August 4, 1998. "Recombinant yeasts for effective fermentation of glucose and xylose." Inventors: Nancy Ho and George Tsao.

There are several uses for ethanol, but Dr. Ho focuses on its potential use as a transportation fuel. Traditionally, ethanol is used as an additive for gasoline, so a significant decrease in ethanol production costs would help the economy and could put less demand on petroleum. Table 9 shows some of the advantages and disadvantages of using ethanol as a transportation fuel. Regardless of whether ethanol will ever replace gasoline, the research has made ethanol a more possible alternative than it had been in the past. And although the main focus of the research has been ethanol, Dr. Ho says that further genetic manipulation of the yeasts could also have other economic benefits such as in the production of citric and lactic acids, which are used as food additives.

Currently Dr. Ho is still trying to make the yeast yet even more efficient. She is also working on biodesulfurization, to remove sulfur from coal and petroleum to produce cleaner and more cost effective fuel. This is very similar to the research for which Dr. Ho was funded by the TSE program.

Advantages	Disadvantages
Can now be made from cellulosic biomass,	Is not as widely used in industry as
a waste product.	gasoline for transportation fuel. Involving
	industry and society would be expensive.
Less dependence on foreign oil	Synthetic ethanol from petroleum is less
	expensive than ethanol from fermentation
	(Green Chemistry Data).
Lower SOx and CO2 emissions.	Higher NOx and VOC emissions.
(Greenhouse gases)	(related to smog formation)

## 5.4 The TSE-Funded Research of Dr. George Kraus

Dr. George Kraus of Iowa State University was funded by the TSE Program during the period October 1996 to September 1999 for his research: "Photochemical Alternatives for Pollution Prevention".

Friedel-Crafts alkylation and acylation reactions are used to produce many commercial and industrial products such as: tertiary butyl hydroquinone(TBHQ), ibuprofen, valium, and several other drugs. Unfortunately, Friedel-Crafts reactions are harmful to the environment because to work they usually need toxic, air sensitive, or acidic reagents. Dr. Kraus used light to develop environmentally safe photochemical reactions as an alternative to the Friedel-Crafts reactions that can be used to achieve the same products. His methods use safer feedstocks, solvents, reactants, and step processes. This wide variety of chemical changes led to testing many different compounds so there would be a wide range of practical implications to industry. Table 10 shows which hazardous materials could be reduced as a result of this research, and which materials would replace them. It is also important to note that all Dr. Kraus's chemical reactions require fewer steps than the Friedal-Craft Reactions. Dr. Kraus says that he replaces acid chlorides (which are corrosive), with stable solids, such as quinones.

Table 10: Friedal-Crafts vs. Photochemical Reactions

Friedal-Crafts Reactions	Kraus's Photochemical Reactions (Added)
Acid Chlorides (corrosive) – replaced	Aldehydes, ethers, acetals, branched alkanes, benzoquinone, naphthoquinone.
Halocarbon or hydrocarbon organic solvents - replaced	Supercritical CO2 (supplemented w/5% tertiary butanol) or hydrocarbon solvents.
Water sensitive Lewis acid (i.e. Tin (IV) Chloride, aluminum trichloride) - replaced	Sunlight or artificial light.

Dr. Kraus has also been applying the TSE-funded research when working with industrial partner Kemin, a company that creates agriculture products. His main focus with Kemin has been on improving the methods to create TBHQ, an anti-oxidant, which will be used as a food additive. The current method Kemin is using has product yields of about 75%. Dr. Kraus's methods have a product yield of approximately 90%. Presently, however, using Dr. Kraus's method will not be as cost efficient as the traditional approach. Aside from his work with Kemin, Dr. Kraus's research has led to a patent disclosure to Iowa State University for TBHQ synthesis. In addition to the disclosure, there is already a full patent (US Patent No. 5466799) on his synthesis of benzodiazepines, which are related to Valium (muscle relaxant).

The TSE-funded research has also affected Iowa State University. In one of the Green Chemistry courses they have created experiments similar to his photochemical reaction research in their organic chemistry laboratory. Outside of the classroom, the TSE program funded two graduate students, Yanhua Lu and Alex Melekhov, to work with Dr. Kraus. Yanhua Lu was interviewed and made the following comment about the TSE-funded research. "I was very inspired and impressed by the idea that scientists can bless the nature and environment by carefully designing experimental protocols and incorporating innovative methodology and technology".

Ms. Lu was a graduate student from 1996 to 1999 and her first research project was working with Dr. Kraus on the TSE-funded research (photochemical alternatives to Friedal Crafts reactions). Shortly after Ms. Lu obtained her M.S. in chemistry in 1999, she joined the pharmaceutical industry. During the interview with Ms. Lu (personal communication, November 20, 2004), she was said the following about her new career: "Whether in drug discovery research lab or in process, manufacturing facilities, tons of waste is generated every

day. This not only imposes a high cost for company disposal, but also creates a higher cost for the environment to accept it." Ms. Lu also said that she was inspired by green chemistry and uses her knowledge from the TSE-sponsored research in her career. One example of this is when she was working in the drug discovery research lab. With the help of her colleagues, Ms. Lu says, they have replaced a toxic solvent with water to achieve the same chemical yield for one of the products.

Although his TSE grant has expired, Dr. Kraus is still working on the research initially funded by the TSE program. Currently, Dr. Kraus is trying to further improve his production methods for TBHQ. He is also working on a photochemical method used to make isoflavones (important as dietary supplements) and with phenylanthracenes, which are not as practical but more of a scientific curiosity. Dr. Kraus continues to research environmentally safer reactions that potentially could be adopted by industry.

# 5.5 The TSE-Funded Research of Dr. Chao-Jun Li

Presently chemical and pharmaceutical industries use large amounts of organic solvents in their processes. Solvents are liquids that dissolve substances; the term organic solvent refers to petroleum-based liquids that dissolve substances. The use of solvents leads to high operational costs for the industry and large environmental effects. Operational costs are largely due to the fact that a high amount of solvent, compared to the amount of reactants, is needed for each reaction. The products of many of these reactions are volatile organic compounds (VOCs). VOCs are harmful chemicals that are released as gases as a result of a reaction (EPA, 2004d, VOCs). VOCs are produced in the manufacture of such products as paints, adhesives, and permanent markers. VOCs are harmful to human health and the environment. The impact on

health depends on the type of VOC, the duration of exposure, and the amount exposed to. Health effects range from facial irritation and headaches to damage to the liver or the central nervous system. The effects on the environment vary depending on the specific compound. Large amounts of VOCs in the atmosphere contribute to the formation of smog, and when VOCs react with oxides, ozone and other harmful compounds are created. Dr. Chao-Jun Li's research aims to use produce solvents that are not as costly, in terms of operation and industrial impacts, as organic solvents.

Since the beginning of the TSE grants program in 1995, Dr. Li has had three research projects funded by the program. The first grant was aimed at finding ways to conduct carboncarbon bond forming reactions that are normally conducted in anhydrous organic solvents (which are solvents not involving water) in media involving water. By producing alternative methods for synthesis, the use of large amounts of organic solvents can be avoided, and their harmful affects minimized.

Dr. Li's second grant built on his first in terms of dealing with carbon-carbon bonds. He looked at the synthesis applications of metal-mediated reactions through the use of water-based solvents. Dr. Li paid close attention to improving the catalytic process and also introducing Carbon Dioxide (CO<sub>2</sub>) as a possible alternative to organic solvents.

The current grant that Dr. Li is working on builds upon his second TSE grant. The research focuses on innovative carbon-carbon bond formation reactions for chemical syntheses. Incorporating  $CO_2$  and water will have large environmental benefits. This research will improve catalysts and reduce the amount of waste from the reactions.

Dr. Li sees his research in the long term as not to try to improve on a reaction that already exists, but to change the way that the reaction is looked at. He tries to question what is assumed

so that new ideas can be brought into the research. For the most part this research will work towards developing new chemistry methods for chemical synthesis.

Dr. Li's research led to him develop a green chemistry graduate class last year. Other universities, such as the University of Massachusetts (Amherst) and the University of Oregon, have begun similar classes using Dr. Li's research, though during the course of his three grants Dr. Li did not collaborate with other faculty. Dr. Li's work has also been brought into undergraduate classes; his research was used as an example of real life application of the class's subject matter. Presently he holds a research chair position at McGill University and is working towards developing the green chemistry program there. His research helps contribute to the work that McGill University is doing to promote awareness of green chemistry and encourage further research in that field.

Dr. Li conducts more research than just that which is funded by the TSE grants. For that reason Dr. Li works to obtain further funding. He has received funding in addition to the TSE grant funding, but none of it has gone solely to benefit any of his TSE work. He has received further support on various projects related to green chemistry unrelated to his TSE research. For example, NASA supported the development of clean technology for material production. NSF also supports Dr. Li for synthesizing natural products and biologically important compounds using green methods. He had support from the American Chemical Society's Petroleum Research Fund for making certain natural products based on the green reactions that he developed. He also had Louisiana Board of Regents Industrial Tie support for developing environmental technologies related to a private industry.

Dr. Li has had limited involvement with industry, with respect to patents and industrial partners, while completing his research. At Tulane University, there was no interest in

supporting patents for Dr. Li's research. The university felt that the patent process was too expensive and too hard to monitor. He did not have industrial partners when conducting his research. Dr. Li does not know if an industry has used his work unless they contact him on their own accord, as Millikan Chemicals did when they asked him to be a consultant and help them implement his research into their industrial process. Dr. Li has also found out about industry using his work by meeting with their representatives at conferences.

Dr. Li had the opportunity to speak at the Chiral Conference 2004 in Boston, MA. He presented his paper: "Transition Metal Catalyzed Asymmetric A3 Coupling of Aldehyde, Alkyne and Amine". The presentation was based on a paper from 2002 that had won the Hot Paper award from the ISI. The conference gave Dr. Li the chance to show industries the potential of his research. Pharmaceutical industries specifically became interested in his work and what the work could do for their companies.

Through each of the grants Dr. Li funded one graduate and one postgraduate student. Since there were a lot of graduate students he would fund one for a semester and then fund another student for the next semester. He never had the same student funded throughout the entire TSE grant. Dr. Li referred to Charlene Keh as someone to speak to about the research through the graduate students perspective. Ms. Keh became involved in Dr. Li's research because she was involved in his research group (personal communication, November 17, 2004). She is now working with chemistry at Cordis, a Johnson & Johnson company. She chose to work for industry rather than have an academic career. Thus, she is not performing any research of her own. When asked if her work as a student influenced her choice of profession, Ms. Keh had this to say: "That's hard to say because I'm still a scientist but in industry with very little say in terms of my research project. However, my profession is still a chemist." Ms. Keh's work did

not directly impact where she is now but the work with Dr. Li did not deter her from working as a chemist.

It is difficult for Dr. Li to determine if there are any data from industries demonstrating the benefits of technology developed using his research. This is for two reasons: industries keep their processes confidential and Dr. Li does not know what part of his research they are using.

#### 5.5.1 Dr. Li's Published Articles Citations

Table 11 lists the numbers of citations of articles written by Dr. Li on the research he conducted with TSE support. Self-citations were removed because they do not necessarily indicate that other researchers are expanding upon the information in the article. Black cells indicate that the article had not yet been published in that year. The rightmost column contains the total number of citations for a given article, the total number of citations for all articles, and the average number of citations per article. In the case of Dr. Li there are a total of 112 citations from all of his articles relating to his research supported by the TSE and there was an average of seven citations per article. For the most part, citations for each article take time to enter into the mainstream. Once the article has been widely introduced, citations rise dramatically. Then, after reaching a peak, the information becomes old, perhaps outdated due to further research, and citations get lower. An example of this trend is Dr. Li's titled: "The Barbier-Grignard-type carbonyl alkylation using unactivated alkyl halides in water" published in 2003. As the table shows the article was cited twice in 2003 and then six times in 2004. The number of times Dr. Li's paper is cited increases as the time it has been available increases. Since this paper was published so recently we could not determine when the number of citations would start to decrease.

		tations		
	2002	2003	2004	total
A novel chiral gallium lewis acid catalyst with semi-crown	0	1	0	1
ligand in aqueous asymmetric Mukaiyama aldol reactions				
Aldol reaction via in situ olefin migration in water	0	2	2	4
Aldol- and Mannich-type reactions via in situ olefin		2	3	5
migration in ionic liquid				
Cu(I)Br mediated coupling of alkynes with N-acylimine and	0	4	2	6
N-acyliminium ions in water				
Developing metal mediated and catalyzed carbon-carbon	1	0	1	2
bond formations in air and water				
Direct formation of tetrahydropyranols via catalysis in ionic	1	1	3	5
liquid				
Direct formation of tetrahydropyranols via solid acid resin-		1	0	1
catalyzed reactions in water				
Gallium-mediated allylation of carbonyl compounds in water	0	1	7	8
Highly enantioselective catalytic direct addition of alkynes to	1	22	19	42
imines in water				
InCl3-catalyzed reaction of aromatic amines with cyclic		2	1	3
hemiacetals in water: facile synthesis of 1,2,3,4-				
tetrahydroquinoine derivatives				
Indium chloride catalyzed cross-coupling of dihydropyran	1	5	1	7
and dihydrofurans with anilines in water				
Indium-mediated domino reaction of nitroarenes with 2,3-		1	1	2
dihydrofuran in water: an efficient synthesis of 1,2,3,4-				
tetrahydroquinoline derivatives				
Palladium catalyzed coupling of aryl halides with	0	0	2	2
arylhalosilanes in air and water				
Quasi-nature synthesis: catalysis by late-transition metals in		7	6	13
air and water	I		_	-
Ruthenium-catalyzed tandem olefin migration-aldol and		0	3	3
mannich-type reactions in water and protic solvent		Ŭ	Ŭ	Ŭ
The Barbier-Grignard-type carbonyl alkylation using		2	6	8
unactivated alkyl halides in water		-	Ŭ	Ũ
Total # of citations per year	Λ	51	57	112
Average # of citations per article	0.44444	3.1875		7
Average # of citations per article	0.44444	5.1075	0.0020	1

### Table 11: Dr. Chao-Jun Li's Citations

# 5.6 The TSE-Funded Research of Dr. Krzysztof Matyjaszewski

Production of polymers is useful for a wide variety of applications, including plastics, paints, tire manufacturing, and chemical processing. When forming a polymer chain, a process called chain polymerization, volatile organic compounds (VOCs), a major contributor to smog formation, are required in order to avoid what is known as the Trommsdorff effect (Dr. Krzysztof Matyjaszewski's Presidential Green Chemistry Application). The Trommsdorff effect occurs when there is an increase in the viscosity of the solution the reaction is taking place in. This produces an autoacceleration, which is acceleration in the rate of molecular weight increase of the polymer chain being formed.

Dr. Krzysztof Matyjaszewski, professor of chemistry at Carnegie Mellon University, worked on developing atom transfer radical polymerization (ATRP), a method for chain polymerization, which uses less VOCs while still avoiding the Trommsdorff effect. Dr. Matyjaszewski was awarded two TSE grants to pursue this line of research, using the second grant to build upon the findings of the first.

In order to replace VOCs used in polymerization, and by doing so reduce the process' contribution to smog formation, Dr. Matyjaszewski needed to develop new catalysts that would prevent autoacceleration without the negative environmental effects of VOCs. He developed a few hybrid catalysts, US Patent Nos. 5,763,548 and 5,807,837, the most effective of which used copper(I) bromide and 2,2'-bipyridine with copper(II) bromide and hexamethyltriethylenetetramine (Me6TREN). These catalysts produced no Trommsdorff effect and allowed reduction in the amounts of VOCs used in the polymerization. During his second grant, Dr. Matyjaszewski developed an ATRP that used silicon dioxide with metal ligands as a feedstock to produce more new catalysts. The new catalysts developed by this method could potentially reduce the amounts of VOCs used even more, to the point where they may eventually be eliminated from the process entirely.

Dr. Matyjaszewski worked with a couple of graduate students on each grant. One of the students, Nick Tsarevsky, began working with Dr. Matyjaszewski at the beginning of his Ph.D. candidacy. In 2004, their work was recognized when the American Chemical Society's (ACS) Division of Environmental Chemistry awarded Mr. Tsarevsky a scholarship in green chemistry.

He is currently working on a method for producing biodegradable polymers, which will be presented to the ACS in 2005. In an interview with Mr. Tsarevsky (personal communication, November 17, 2004), he stated that the work he conducted with Dr. Matyjaszewski would definitely have an effect on his choice of career, adding that he planned to be involved in research or teaching once he obtained his Ph.D.

Due to the many possible uses for polymers, Dr. Matyjaszewski's improved ATRP process has attracted a great deal of interest from industry. Dr. Matyjaszewski himself helped form two industrial consortia at Carnegie Mellon University, which involved more than 20 companies. Trade secrets kept him from disclosing the names of the companies involved. These consortia resulted in the licensing of his process to companies like PPG, Ciba, Kaneka, Rohmax, Dionex, and Mitsubish.

#### 5.6.1 Potential Quantitative Data of Dr. Matyjaszewski's Research

According to AirData, a database of the EPA monitoring air quality, 43,364 facilities in the United States released VOCs into the air in 1999. Table 12 shows five industry types that could potentially be affected by Dr. Matyjaszewski's ATRP. These five industries account for 8.8% of the total VOC emissions in the United States. It is not known how much of the VOC emissions from these facilities is due to polymerization. If, however, Dr. Matyjaszewski's ATRP is adopted by these facilities, the table indicates that it could reduce VOC emissions anywhere up to 147,044 tons per year.

Industry Type (SIC)	Number of Facilities Emitting VOCs	Percent of <u>Total</u> <u>Facilities</u>	<u>VOC</u> Emissions (tons)	Percent of Total VOC Emissions
2821 - Plastics				
Materials And			01.050	1.05
Resins	314	0.724	31,270	1.87
2869 - Industrial Organic Chemicals, Nec	370	0.853	77,845	4.66
2899 - Chemical	570	0.055	77,045	00
Preparations, Nec	137	0.316	3,867	0.23
3089 - Plastics Products, Nec	608	1.4	24,398	1.46
2851 - Paints And Allied Products	361	0.832	9,664	0.58
TOTAL	1790	4.125	147,044	8.8

Table 12: Industries types could be affected by reduction of VOCs using Dr. Matyjaszewski's research from AirData

#### 5.6.2 Dr. Matyjaszewski's Published Articles Citations

Table 13 lists the numbers of citations of articles written by Dr. Krzysztof Matyjaszewski on the research he conducted with TSE support. Self-citations were removed because they do not necessarily indicate that other researchers are expanding upon the information in the article. Black cells indicate that the article had not yet been published in that year. The second-to-last row is the total number of citations for a given year. The bottom row is the average number of citations per article in a given year. The rightmost column contains the total number of citations for a given article, the total number of citations for all articles, and the average number of citations per article. For the most part, the information from articles takes time to reach those who would continue the research. Once the article has been widely introduced, citations rise dramatically. Then, after reaching a peak, the information becomes old, perhaps outdated due to further research, and citations get lower.

	1999	2000	2001	2002	2003	2004	total
Copper(I)-catalyzed atom transfer radical polymerizations	0	14	28	27	21	10	100
Electrospray ionization mass spectrometry study of copper(I) and copper(II) bipyridine complexes employed in ATRP		0	1	0	1	1	3
Gradient copolymers by atom transfer radical copolymerization		0	3	0	3	5	11
Immobilization of the copper catalyst in atom transfer radical polymerization	1	9	10	5	5	9	39
Mechanistic aspect of reverse atom transfer radical polymerization of n-butyl methacrylate in aqueous dispersed system		1	4	6	11	3	25
Removal of copper-based catalyst in atom transfer radical polymerization using ion exchange resins		3	7	5	1	7	23
Water-borne block and statistical copolymers synthesized using atom transfer radical polymerization		1	2	10	2	2	17

Table 13: Krzysztof Matyjaszewski's Citations

Preparation of segmented copolymers in the presence of immobilized/soluble hybrid ATRP catalyst system					0	5	5
Use of an immobilized/soluble hybrid ATRP catalyst system for the preparation of block copolymers, random copolymers and polymers with high chain end functionality					0	4	4
Total	1	28	55	53	44	46	227
Average	0.5	4	7.857	7.57	4.89	5.111	25.222

## 5.7 The TSE-Funded Research of Dr. Fred Ramirez

Many traditional processes used for manufacturing lead to harmful or toxic gases, wastewater, and other emissions. Old processes need to be replaced so that these emissions are removed or reduced. The environment and human health are suffering as consequence of stagnant manufacturing methods. This is why it is essential that there is constant research for greener alternatives to current methods. A major problem with industry is that once a process has been started up, it can be very difficult to get a company to change its methods. Even if a new production method shows great potential for environmental and financial improvements, many companies are reluctant to change because the initial replacement costs will be expensive.

Dr. Fred Ramirez has targeted the steel manufacturing industry with his TSE grant funding for his research "Optimal Operation of Electric Arc Furnaces to Minimize the Generation of Air Pollutants at the Source". With this grant he has designed a model for a more cost-efficient and environmentally friendly electric arc furnace (EAF). An EAF is used to recycle scrap steel to create new steel products. When creating his EAF model, Dr. Ramirez concentrated on reducing the amount of carbon monoxide (CO) that traditional furnaces produce while at the same time increasing overall performance of the system. Major problems with CO include its toxicity when there are high levels in the air. The gas affects the central nervous system, contributes to smog formation, and can seriously harm people suffering from heart disease.

During a traditional furnace's operation, a lot of carbon is needed in order for it to operate effectively. Carbon is needed because it reduces the iron oxide levels, which in turn increases yield. The furnace produces carbon from several sources. These include: the scrap metal being put into the furnace, the carbon electrodes at the top of the furnace, and a large amount from the coke that the furnace operator adds. Oxygen needs to be present so that the carbon can release its combustion energy in the furnace. CO is a colorless, odorless and poisonous gas produced by incomplete burning of carbon in fuels. Dr. Ramirez's model uses excess burner oxygen throughout the heating process to reduce CO levels. This excess burner oxygen helps to prevent chemical energy waste by reacting with the combustible gases. The excess oxygen would lead to the production of carbon dioxide, where previously CO would result.

Dr. Ramirez worked with Goodfellow Consultants Inc., a company whose role is to give advice about the mineral industry. With the help of Goodfellow Consultants, Dr. Ramirez was able to receive plant data from two facilities, Keystone Steel & Wire and Chaparral Steel. The steel producing methods for the two companies were very different. The first plant used 88 megawatts of power, a total carbon addition of 8,000 pounds, and a total lancing oxygen of 113,000 Standard Cubic Feet (SCF). Lancing oxygen is the oxygen that is added at the liquid molten steel phase. The second plant only used 60 megawatts of power, a total carbon addition of 3,000 pounds, and a total lancing oxygen amount of 125,000 SCF. Dr. Ramirez used the plant data to find the optimal amount and addition policy of carbon, lancing, and oxygen to use for his model; these are the three major controls of a furnace's performance. The following data are

approximations that have come from the researcher's extensive study on applying his model to predict its effects on the two steel plants. Table 14 shows the improved optimal performance using Dr. Ramirez's proposed model (bold = improvement from the plant's furnace, italicized = worse than plant's furnace) and Table 15 shows the controls that affect performance, comparing traditional furnaces to Dr. Ramirez's model.

Table 14: Dr. Ra	amirez's model's	predicted	effects on	two steel plants

	Plant 1	Plant 2
Carbon Monoxide (Percent Removed)	99.4%	92.0%
Iron Oxide (Percent Removed)	99.8%	61.0%
Yield Improvement (Percent increased)	99.8%	61.0%
Processing Time (Percent increased)	9.7%	- 0.3%
Overall Improved Performance (Percent increased)	52.0%	32.0%

Table 15: Current plant's reactants versus Dr. Ramirez's proposed model

		Plant 1		Plant 2	
		Current Proposed		Current	Proposed
		Furnace	Model	Furnace	Model
Controls	Lancing	113,770	14,140	150,221	117,500
		SCF	SCF	SCF	SCF
	Carbon Injection	9560 lb.	3201 lb.	4149 lb.	6075 lb.
	Oxygen Injection	None	23,294 SCF	None	55,000 SCF

The model has been created and Dr. Ramirez has analyzed it thoroughly but he still needs to test his work in the industrial field. His analysis shows that overall performance and yields for both plants would improve significantly if the technology were adopted. In both plants almost all CO effluent would be replaced by carbon dioxide, a less environmentally harmful gas. Another benefit from the research would be the increase in yields, which is caused by the reduction of iron oxide. This reduction is beneficial because iron oxide has an affect on the workers at the facility. Exposure to iron oxide, fumes, or dust can cause metal fume fever. This fever is very similar to the flu; additional effects include discoloring of the eyes, chest-tightness, and aches.

The only problem with the adoption of Dr. Ramirez's model is that companies are reluctant to try it because the initial change to the EAF would be expensive. Dr. Ramirez has stated "to get the optimal (performance) you need to add carbon, lancing oxygen and gas phase oxygen at a prescribed time profile to get the improvement. This is a new and somewhat expensive control system. The most expensive part is adding solid carbon at a prescribed rate profile".

Dr. Ramirez found the TSE program to be very effective in helping him produce good research. However, he needs help with implementing his research. Since industries are reluctant to try it out, because initially it will be expensive, he suggests creating a federally funded incentives program.

Currently Dr. Ramirez is working on modeling and optimizing certain biotechnological processes. This research is separate from the TSE-funded research and is being funded by the NSF. There was one graduate student, Sam Matson who worked with Dr. Ramirez on the project. Mr. Matson is now employed by Goodfellow Consultants and part of his current work is improving the model that he developed with Dr. Ramirez.

#### 5.7.1 Potential Quantitative Data of Dr. Ramirez's Research

Dr. Ramirez's research is a model for an improved Electric Arc Furnace in the steel industry. The results of this research would have the most influence on the AirData category

"3312 – Blast Furnaces And Steel Mills". Facilities categorized as "3312 – Blast Furnaces And Steel Mills" only make up 0.536% of all the facilities listed in AirData, yet these few facilities account for very large amount (17.19%) of all the CO emissions from all 28,912 AirData listed facilities (see Table 16).

Industry Type (SIC)	Number of Facilities	Percent of Total Facilities	Pollutant Emissions	Percent of Total Emissions
3312 - Blast Furnaces And Steel Mills	155	0.536	721,717	17.19
All Facilities (including SIC 3312)	28,912	100	4,197,827	100

Table 16: AirData facilities that release CO emissions

Of the one hundred facilities with largest CO emissions in AirData one finds that the "3312 – Blast Furnaces And Steel Mills" industry type accounts for seventeen, Table 17A shows that the total CO emissions from these seventeen facilities alone are 626,203 tons per year (14.92% of all CO emissions tracked by AirData).

Table 17: Major Carbon Monoxide Releasing U.S. Steel Mill Facilities (taken from top 100
worst CO releasing U.S. facilities)

Rank	Emissions (tone)	Percent of Total Emissions	Facility Name	Facility Mailing Address	State	Industry Type (SIC)
	165,519	3.94	Bethlehem Steel Corp.	U.S. 12 & S.R. 149, Burns Harbor, In 46304	IN	3312 - Blast Furnaces And Steel Mills
	2 89,928		U S Steel Co Gary Works	One North Broadway, Ms-70, Gary, In 46402-3199	IN	3312 - Blast Furnaces And Steel Mills
	3 73,290	1.75	Bethlehem Steel	5111 North Point Boulevard, Sparrows Point, Md 21219	MD	3312 - Blast Furnaces And Steel Mills
	5 54,305	1.29	Wci Steel, Inc.	1040 Pine Ave., S.E., Howland/Weathersfield/Warren, Oh 44883-6528	ОН	3312 - Blast Furnaces And Steel Mills
10	) 47,389		Ispat Inland Steel Inc.	3210 Watling Street, East Chicago, In 46312	IN	3312 - Blast Furnaces And Steel Mills
1:	5 34,643	0.83	Acme Steel Company	13500 S. Perry Avenue, Riverdale, Il 60627-1182	IL	3312 - Blast Furnaces And Steel Mills
1	3 33,010	0.79	Wheeling- Pittsburgh Steel Corporation -	South 3rd Street Extension, Steubenville, Oh 43952-2729	ОН	3312 - Blast Furnaces And Steel Mills

			Steubenvil			
29	24,208		Ak Steel Corporation	1801 Crawford Street, Middletown, Oh 45043-0001	он	3312 - Blast Furnaces And Steel Mills
38	19,316		Ltv Steel Company	3001 Dickey Rd, East Chicago, In 46312-1610	IN	3312 - Blast Furnaces And Steel Mills
42	16,137		Drummond Company, Inc.	P.O.Box 10246, Birmingham,Al., Al 35202	AL	3312 - Blast Furnaces And Steel Mills
49	13,664	0.33	Youngstown Sinter Company	251 Division Street, Youngstown, Oh 44510-0010	он	3312 - Blast Furnaces And Steel Mills
50	13,491			20th And State Streets, Granite City, II 62040	IL	3312 - Blast Furnaces And Steel Mills
60	11,254		Ltv Steel Company, Inc Cleveland Works	3100 East 45th Street, Cleveland, Oh 44127	ОН	3312 - Blast Furnaces And Steel Mills
77	8,157		Cf&I Steel L P Dba Rocky Mtn Steel Mills	2100 S. Freeway, Pueblo, Co 81004	со	3312 - Blast Furnaces And Steel Mills
85	7,668		Bethlehem Steel Corp/Coatesville	139 Modena Rd, Coatesville, Pa 19320	PA	3312 - Blast Furnaces And Steel Mills
91	7,229	0.17	Rouge Steel Company	3001 Miller Road Rouge Office, Dearborn, Mi 48121-1699	MI	3312 - Blast Furnaces And Steel Mills
95	6,995		Steel Manufacturing Facility	10 South Geneva Road, Vineyard, Ut 84058	UT	3312 - Blast Furnaces And Steel Mills

Regardless of any speculation these charts assume (*see methodology section*), according to AirData, there is still at least an upper bound potential target of 721,717 tons (1,443,434,000 pounds) of carbon monoxide being released by 155 "3312 – Blast Furnaces And Steel Mills" facilities alone for Dr. Ramirez's research. Since this makes up a significant 17.19% of all CO emissions out of 28,912 facilities that are listed in AirData, the possible environmental benefits from adopting the research could be very substantial.

In addition, because the top 17 "3312 – Blast Furnaces And Steel Mills" facilities alone release 14.92% of all CO emissions out of 28,912 facilities that are listed in AirData, the research would only have to be applied to very few facilities to make a significant CO facility emission reduction in the U.S.

Finally Table 18 shows CO emissions data obtained from AirData on the two specific facilities, Chaparral Steel and Keystone Steel & Wire Co, that Ramirez referred to in his report.

There is a large difference in the amount of CO emissions from the two facilities; the cause of this is unknown. Also it is important to note that for Keystone Steel & Wire Co, the facility fell into the industry "Steel wire and related products SIC-3315". Tables 16 and 17 focused on the "Blast Furnaces and Steel Mills" industry, but Keystone Steel and Wire Co falls into a separate industry that wasn't accounted for.

#### Table 18 CO Emissions from Chaparral Steel and Keystone Steel & Wire Co (AirData

<u>Facility</u> <u>Name</u>	<u>Facility</u> <u>Mailing</u> <u>Address</u>		Pollutant Emissions (Tons)	Percent of <u>Total</u> Emissions
	U.S. Hwy.	3312 - Blast		
Chaparral	67 @ Ward			
Steel	Rd., In Mi,	And		
Midlothian	Midlothian,	Steel		
Lp	Tx 76065	Mills	1,602	0.04
	7000 SW	3315 -		
	ADAMS	Steel		
Keystone	ST,	wire and		
Steel and	PEORIA,	related		
Wire Co.	IL 61641	products	5.47	< 0.01

# 5.8 The TSE-Funded Research of Dr. Valerie Thomas

In the United States, there is no method for tracking where trash goes once it enters the waste management system. As a result, most people do not know what happens to their trash after it is taken from their garbage can or recycling bin. This lack of information makes it difficult at best to determine whether trash goes to the proper location and, if it doesn't, how much is being routed improperly.

Valerie Thomas, currently a Congressional science fellow working on energy policies for New Jersey Congressman Robert Andrews, worked on getting information technology (IT) introduced into American waste management procedures with her TSE grant funding. The TSE program Dr. Thomas for her research entitled "Electronic Tags for Produce Lifecycle Management." Since IT is being increasingly used at the beginning of life for a product, Dr. Thomas thought the next logical step would be to use IT at the end of a product's life, in order to make the collection and disposal of such products more efficient. Her work, which she conducted while a research scientist at Princeton University, was primarily focused on the use of radio frequency identification (RFID) tags and global positioning system (GPS) transmitters. Using this technology, IT in waste management could eventually, for example, determine what kinds of waste a person disposes of and use that information to more efficiently route the collection trucks. It could also be used to track where the garbage goes once it is collected, in order to make sure every piece of refuse is disposed of properly. Once she has completed her Congressional fellowship, Dr. Thomas plans to continue this line of research at Georgia Tech in order to develop a practical method for US cities and towns.

Using IT in order to make waste management processes more efficient is not a new idea. In Europe, particularly in Dresden, where Dr. Thomas researched possible current methods that could be implemented in the US, RFID tags are used in order to allow the waste management

facilities to charge households for trash pickup based on the amount they throw away. Originally, Dresden was planning on charging customers by the weight of the trash thrown away. However, adding a scale to each of the trucks proved to be expensive, and there wasn't a large enough difference between households in the weight of trash being thrown away to make the expense worthwhile.

Since the scale plan did not work out, Mobile Automation (MOBA), the company that handles trash pickup for the city of Dresden, fitted trashcans with RFID tags, and equipped each garbage truck with a radio receiver. The tag on the can contains the necessary information on the household owning it, which the receiver on the truck reads in order to determine who is getting charged for the trash pickup. The amount the pickup costs depends on how full the trashcan is when the garbage is collected. While working with Dr. Thomas in her research, MOBA expressed an interest in developing a similar waste management system in the US. However, today there is currently no US town or city that uses electronic systems like the kind used by MOBA in its garbage collection.

Besides using IT to determine how much trash a person is throwing away, Dr. Thomas also wants to use electronics to determine what happens to the garbage after it is taken out of the can. As stated earlier, there is no system for tracking the movement of garbage in the US. Because of this, large numbers of people are left completely in the dark as to what happens once the truck pulls away, having no idea where their garbage goes, how far it must go to get there, and whether it is disposed of properly. Without this information, it becomes difficult to spot problems that may exist, which prevents any correction of these problems.

Dr. Thomas, in an effort to correct this lack of information, has attempted to set up possible methods of using RFID tags or GPS transmitters for this purpose. Problems have arisen

in experimentation, however. Sometimes, the metal from the garbage trucks blocked the signals in both the RFID tags and GPS transmitters. Other times, the compactors in the truck crushed the signal devices. Moreover, GPS transmitters, though more effective, are also very expensive. Recent improvements have been made in GPS technology, though, and Dr. Thomas plans to work with Oxford Location (OxLoc), an England-based company that produces GPS transmitters, when she continues her research at Georgia Tech.

Audrey Lee, an electrical engineering graduate student at Princeton, became involved with the research when she met with Dr. Thomas in September 2003. She wanted to find a directly applicable area of study in electrical engineering that considered topics that were important to her, like environmental issues. Ms. Lee approached Dr. Thomas through Professor Sigurd Wagner, a professor in electrical engineering at Princeton who had been working with Dr. Thomas on Electronic Tags for Product Lifecycle Management. Professor Wagner had specifically been working to help Dr. Thomas use currently available technology to its fullest potential and also allow her to consider other options in pursuit of the goals of the project.

Ms. Lee is currently working on using x-ray fluorescence to detect the presence of heavy metals, such as mercury or lead, in plastics (personal communication, November 18, 2004). By detecting these metals, they can be properly disposed of before the plastic is either incinerated or sent to a landfill, which in turn could lead to pollution of air, water, or soil. She says that Dr. Thomas has been a major influence on both her current research interests and her future career plans. Ms. Lee considers Dr. Thomas to be her mentor, since Dr. Thomas enabled her to apply her engineering background to both the environment and public policy. In May 2004, Ms. Lee won a Student Paper Award from the Institute for Electronic and Electrical Engineers for "GPS

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and Radio Tracking of End-of-Life Products," a paper she wrote with Dr. Thomas using the findings from their TSE-supported grant.

Dr. Thomas, along with Ms. Lee managed to successfully track a disposed phone book using a radio transmitter similar to the kind used to track animals. Though the test was successful, the transmitter's range, one mile, was far too limited for practical purposes. Both Ms. Thomas and Ms. Lee had to physically follow the garbage truck in order to continue to pick up the signal.

IT can be used in this sector for more than logistics in garbage collection, however. It can also be used to contain the necessary disposal or disassembly instructions on the product. For this purpose, Dr. Thomas has already developed a workable system based on barcodes using barcodes printed on cell phones. With a growing number of countries, particularly European countries, requiring that a cell phone be recycled once its usefulness has ended, a system was needed to handle the necessary disassembly instructions for the wide variety of cell phones that exist.

There are barcodes printed on cell phones behind the battery, the barcode on each phone is linked to the phone number of the cell phone. Thus the barcodes identify the phone in the worldwide network of cell phones, making it possible to know who's calling whom, whether for purposes of billing or caller ID. Working with cell phone giant Motorola and Princeton undergraduate student Steven Saar, who today works at Intel Corporation, Dr. Thomas developed web-based software for the purpose of cell phone recycling. When the barcode on the cell phone is scanned, the software identifies the type of phone it is and brings up the necessary instructions for disassembly.

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After demonstrating this new software to Motorola, the question of intellectual property was brought up. Dr. Thomas met with the Princeton University patent office to discuss this issue, and it was decided that it would be best if Motorola handled patent issues for the new technology. Motorola investigated the possibility of patenting, and decided that it was not clear whether or not the work was patentable. They did, however, want to lay some kind of claim to the software, and so they wrote up an intellectual property disclosure, naming Dr. Thomas, Steven Saar, and Markus Stutz, a collaborator at Motorola, as the developers of this technology. In an interview, Dr. Thomas stated that in the end, they wanted people to be able to use systems like the one she developed as freely as possible. Ecotronics, an electronics recycling company based in Vienna, Austria, now uses a process similar to the one developed by Dr. Thomas and Steven Saar when recycling cell phones.

#### 5.9 The TSE-Funded Research of Dr. Richard Wool

Many composite and plastic materials are abundantly used throughout the world for various purposes (i.e. automotive parts, ceilings, roofing, etc.). Most of these materials are being made from scarce resources, some of which are harmful to the environment. For example, conventional methods require raw materials derived from petroleum to create plastics. There has been a strong effort to find a way to use alternate materials in place of environmentally unfavorable traditional resources. The TSE program is currently funding Dr. Richard Wool, a professor at the University of Delaware; he researches green materials, specifically making high performance materials from composite resins. In the plastics example, Dr. Wool researched using soybean oil as an environmentally friendly and cheaper replacement to the petroleumbased feedstocks. The idea of plastics made from soybean oil is used today, yet this is only a small sample of Dr. Wool's many uses for substitute materials.

Dr. Wool's history and involvement with composite materials is very extensive. John Deere has already successfully used and implemented the idea of using soybean oil, instead of petroleum-based feedstocks for plastic manufacturing. Today John Deere makes the parts for some of their tractors using the soybean oil in their plastic molding process. Dr. Wool says the new plastic material is just as strong as the tractor parts that were previously made from petroleum. Dr. Wool is also working on making circuit board material from a chicken feather composite material to replace the current boards on which silicon chips and other electronic components are placed. Currently Intel is researching the chicken feather material to see whether Dr. Wool's product will work. If the idea holds up, chicken feathers would be a good replacement for the circuit board because feathers are a massive environmental waste product. In addition to those companies, Dr. Wool is also currently working with Dow Chemical Corp. and Dupont. These companies are trying to determine if they will be able to implement his allnatural composite material (made from recycled newspaper, cardboard, etc.), combined with a soybean oil-based plastic resin, to make hurricane-resistant roofing. The University of Delaware is currently developing a prototype of the hurricane-resistant roof.

Dr. Wool has also had several other industrial partners, including Avery Denison, 3M, Nike, Diab, Doc Resins, Cytek Corp (formerly UCB Radcure Corp), West Vaco, Georgia Pacific, and Rome & Haas. Wool's wide range of involvement in industry shows how one area of successful research can have many practical uses and benefit several areas of industry. Listed below are Dr. Wool's intellectual properties that some of these other companies are investigating

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under secrecy agreements. Ashland and John Deere have already negotiated with Dr. Wool for further funding.

- Pressure Sensitive Adhesives from Plant Oils, US Patent No. 6,646,033.
   November 11, 2003. Inventors, S. P. Bunker and R. P. Wool
- Sheet Molding Compound from Plant Oils, US Patent Application Serial Number, 10/166,849: Inventors, R.P. Wool, Jue Lu and S.N. Khot
- Low Dielectric Constant Materials from Plant Oils and Chicken Feathers, US Patent Serial Number, 60,396,319: Inventors, R. P. Wool and C.K. Hong
- Rigid Thermosetting Liquid Molding Resins from Plant Oils, US Patent Application UD02-21: Inventors, Erde Can and R. P. Wool.
- A Monolithic Hurricane Resistant Roof made from Low Density Composites, UD04-17, filed October 17, 2003: Inventors, R. P. Wool, M. A Dweib, H.S. Shenton III and R. Chapas

During Dr. Wool's research there were four graduate students funded by the TSE program. John LaScala worked with Dr. Wool at the University of Delaware from 1997-2002. As a graduate student, LaScala continued to work on composite resins from plant oils as his dissertation. After graduating and earning his PhD, he continued further research in this area. Currently, LaScala is developing low VOC composite resins that use plant oil monomers as replacements for styrene (Funded through Strategic Environmental Research and Development Program PP-1271). In addition, he is looking to get involved in doing research on other environmentally friendly and biodegradable polymers. LaScala says he is also trying to obtain a faculty position doing this research as well. LaScala's publications include:

• J.J. La Scala and R.P. Wool, "Property Analysis of Triglyceride-Based Thermosets," *Polymer*, Accepted.

- **J.J. La Scala** and R. P. Wool, "The Rheology of Chemically Modified Triglycerides," *JAPS*, accepted.
- J.J. La Scala and R. P. Wool, "The Effect of Fatty Acid Composition on the Acrylation Kinetics of Epoxidized Triacylglycerols", J. Am Oil Chem. Soc., **79**, 59-63 (2002)
- J.J. La Scala and R.P. Wool, "The Effect of Fatty Acid Composition on the Epoxidation Kinetics of TAG", J. Am. Oil Chem. Soc,, 79, 373-378, 2002.
- R.P. Wool, S.N. Khot, J.J. La Scala, S.P. Bunker, J. Lu, W. Thielemans, E. Can, S.S. Morye, G.I. Williams, "Affordable Composites and Plastics from Renewable Resources," *Advancing Sustainability through Green Chemistry and Engineering*, R.L. Lankey, P.T. Anastas, Eds. ACS: DC, 2002, pp. 177-224.
- S.N. Khot, **J.J. La Scala**, E. Can, S.S. Morye, G.I. Williams, G.R. Palmese, S.H. Kusefoglu, R.P. Wool, "Development and Application of Triglyceride Based Polymers and Composites," *J. Applied Polym. Sci.*, **82**, 703-723 (2001).
- La Scala, J.J., J.M. Sands, J.A. Orlicki, E.J. Robinette, G.R. Palmese, "Fatty Acid-Based Monomers as Styrene Replacements for Liquid Molding Resins," *Polymer*, 45, 7729-7737 (2004).
- La Scala, J.J., J.M. Sands, G.R. Palmese, "Environmentally Friendly Composites," *AMPTIAC*, (Submitted).
- Palmese, G.R., J.J. La Scala, J.M. Sands, "Vinyl Ester Monomers to Reduce Emissions and Toughen Polymers," U.S. Patent Disclosure, April 2004.
- L Scala, J.J., E.J. Robinette, G.R. Palmese, J.M. Sands, J.A. Orlicki, and M.S. Bratcher, "Successful Initial Development of Styrene Substitutes and Suppressants for Vinyl Ester Resin Formulations," *Army Research Laboratory Technical Report*, ARL-TR-3023, August 2003.

Aside from LaScala, there were two other of graduate students, Ian McAninch and Lin Zhu,

who are currently working with Dr. Wool on his research. Wim Thielemans, like LaScala, also worked with Dr. Wool during the research and has earned his PhD as well (For more information on these graduate students see appendices S, T, U, V).

The TSE-funded research has also inspired Dr. Wool to create new academic approaches.

At the University of Delaware he is now teaching a course in green engineering as a result of the research. He also teaches a second class called Polymer Science, which he says is very related to his work with green materials. Dr. Wool has also collaborated with other professors from the University of Delaware, Georgia Tech, Howard University, Michigan State University, Colorado State, and others to explore the creation of a national research center for green materials.

#### 5.10 The TSE-Funded Research of Dr. Yushan Yan

In order to combat corrosion of certain metals, particularly aluminum and aluminum alloys, inorganic coatings, which are more resistant to wear and tear, are applied to the metal. Two widely used coating methods are chromate conversion and anodization. In chromate conversion, acidic chromate solutions produce a thin film that protects certain metals from corrosion and provides a base coating for paints and resins (Environmental Defense, 2004). Anodization uses chromic acid, which reacts with metal on the surface and converts it to metal oxides. Like chromate conversion, anodization protects the coated metal from corrosion and allows for the application of paints that can be used for added protection. Another similarity between chromate conversion and anodization is that both processes use hexavalent chromium (Cr VI), one of chromium's two prevalent naturally occurring valence states, and subsequently release excesses of the metal into the environment. Prolonged exposure to Cr VI is known to be carcinogenic and can also irritate the nose, throat, and lungs, to the point of damaging the septum in severe cases.

A major part of alleviating these potential health risks to the public is the development of metal coatings that do not employ chromium in their manufacture. In order to be a viable alternative, a chromium-free coating needs to be at least as effective, if not more effective, than chromium coatings in its ability to resist corrosion and abrasion as well as its ability to adhere to metal surfaces and support the application of paints. Dr. Yushan Yan, an associate professor of chemical engineering at the University of California, Riverside, was funded by the TSE grant program. He was research was aim at developing such a coating, using zeolite minerals instead of chromium-based acids.

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The coating Dr. Yan developed during the TSE funded research has been tested on small pieces of metal and shows that it could potentially be a viable alternative. If his coating proves to be an effective replacement, the use of hexavalent chromium would no longer be necessary in corrosion protection. This would eliminate a large portion of chromium releases into the environment.

Dr. Yan is currently collaborating with the University of Massachusetts and the US Army and Navy in a four-year, \$1.65 million grant with the Strategic Environmental Research and Development Program (SERDP). During this grant period, he will be applying the coating he developed to larger sheets of metal in order to verify its potential as a replacement. During the latter half of the four years, Dr. Yan may look into licensing the coating he developed, but for the moment he is not considering it.

Dr. Yan had one graduate student supported by the TSE grant funding, Derek Beving. He became involved with Dr. Yan because he was reading up on different research areas to pursue and came across an article on Dr. Yan's work. The two met and became interested in working together. Mr. Beving is still working on completing his PhD in environmental toxicology. He is not sure what he will do after completing his PhD; he will probably not pursue research as a career. Mr. Beving is presently helping Dr. Yan with his Department of Defense grant.

Dr. Yan has the following completed patent:

US Patent 6521198. February 18, 2003. "Metal surfaces coated with molecular sieve for corrosion resistance." Inventors: Yushan Yan, Xiaoliang Cheng, Zhengbao Wang

### **6** Conclusions

#### **6.1 Conclusions on Academic Impacts**

The principal investigators (PIs) have had a wide variety of impacts on the academic world as a result of their research. Almost all of the PIs that we studied sponsored at least one graduate student in their Technology for a Sustainable Environment (TSE)-supported project(s). Several sponsored multiple students. It was also not uncommon for the PIs to collaborate with other faculty members. Some of these collaborators were from a different department than the PI, and some were from different institutions. Dr. George Kraus from Iowa State University, for example, collaborated with Dr. James Tanko from Virginia Polytechnic Institute in his grant research.

The research has also sometimes resulted in the formation of school courses or new information being presented in current ones. Dr. Chao-Jun Li, who currently works at McGill University, formed a green chemistry class at Tulane University after completing the second of his three TSE grants, while Dr. Richard Wool from the University of Delaware also formed a green engineering class. Dr. George Kraus has also used the research he conducted during labs in courses he teaches at Iowa State University.

The most common academic impact, however, is that PIs and students are publishing their findings. Others in the academic research community can find out about the work through publications, and perhaps decide to expand on the research themselves. One of the easiest ways to determine how much of an impact a PI's publications have on the academic community is through citations. Dr. Krzysztof Matyjaszewski from Carnegie Mellon University, easily the most cited PI in our project, had one of his articles, concerning the Atom Transfer Radical Polymerization method he developed with TSE funding, cited in one hundred other publications between 1999 and 2004.

#### **6.2** Conclusions on Industrial Impact

Most of the research has not yet had any direct impact on industrial technology or processes. A number of factors may contribute to this absence of industrial effects. For several PIs, their research is simply too recent. They are either still conducting their experiments or they finished recently. In other cases, the technology carries a financial risk that companies are unwilling or unable to take. For example, Dr. Fred Ramirez's design for an environmentally friendlier electric arc furnace would reduce costs to steel foundries over time, but the initial costs incurred in implementing this technology makes many steel companies reluctant to adopt this new design.

There were some similarities between projects that have made an impact in industry. Many of the PIs who had more success in this area worked in conjunction with multiple companies. Dr. Valerie Thomas developed a method to access the necessary information for recycling cell phones through the bar codes on the phones as part of a project aimed at introducing information technology into waste management practices. She and the students with whom she was working enlisted the help of Motorola and several waste management companies in Europe. Today, a similar practice for storing recycling information for cell phones is being used by Ecotronics in Vienna, Austria. Many PIs also patented their work, granting licenses to companies in certain cases. Dr. Krzysztof Matyjaszewski, for example, has been awarded a couple of patents for his work in greener methods for developing polymers, and currently has awarded licenses to six different corporations.

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Another sign of potential industrial impact is the extent of follow-on funding to continue the research. This funding could be received from a number of different sources, including companies and other government organizations. Professor Yushan Yan, who worked on developing chromium-free aluminum coatings, received a \$1.65 million grant from the Department of Defense after completing his TSE-supported research in order to develop and apply his coatings for larger sheets of metal.

Unfortunately, in areas where there has been an impact, it has been difficult to determine the extent and nature of it. Many of the PIs themselves do not know how their research is being used, and do not find out unless approached and informed by companies who adopted their technology or process. Some of the PIs who did know the effects of their research were not at liberty to go into detail because of trade secrets sensitivity.

#### **6.3 Conclusions on Environmental Impact**

At this time of this study, actual environmental effects could not be determined. All numbers provided are estimates derived from information concerning the potential impact of the research's results. It sometimes takes years for an adopted technology or process to produce a measurable effect. The most recent quantities of emissions in the databases we used were two years old, making it difficult to tell how a technology or process could effect current emissions.

When data concerning hazardous emissions were obtained, the most specific category in which they could be organized was by facility. Since not all of these toxic releases are necessarily due to the traditional process, the estimates provided are an upper-bound potential for the new technology. The resources used to obtain these estimates also focused on emissions due to the production of a product as opposed to its use. While the Toxics Release Inventory

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database or AirData will quantify chemical releases due to the production of a car, they will not do the same for emissions arising from the use of that car.

Sometimes, though, the problem of identifying environmental impacts was not a result of the databases. Grant proposals and reports do not necessarily mention the specific chemicals that could be reduced or removed. The PIs in proposals and reports will often use umbrella terms, like volatile organic compounds, to describe the potential benefits of their research. This is often an intelligent move when it is not obvious which chemicals would be eliminated from a process, but it does not help provide more concrete estimates when trying to measure the potential effects on the environment.

#### **7** Recommendations

In producing our cases studies on the ten principal investigators (PIs) we came up with several recommendations to the Technology for a Sustainable Environment (TSE) grant program. We have made recommendations on the TSE grant application and follow-up procedures after the grant period expires. Additionally we recommend that those maintaining the TSE program perform an examination similar to ours in the future.

#### 7.1 Strengthening TSE Grant Applications

The requirements in the application for the TSE grant program can be made more comprehensive. If a proposal is more detailed due to very specific requirements, those reading it are provided with a better understanding of the proposed research. More details on the application will help determine exactly where the research would be used in an industrial process. If the traditional process and the chemicals used in it are known then it will be easier to determine if any technology developed by the PI will have an effect.

• Recommendation 1: The TSE should have both potential and current PIs be as specific as possible as to which chemicals could be reduced, removed, or added by their new technology or process.

The TSE program does ask that its applicants be specific in stating the potential environmental impacts of their research. However, not all applications name specific chemicals that could be reduced, removed, or added. We suggest that the TSE program encourage the potential PIs to be as explicit as possible in this area when applying. Sometimes such specifics are not known during the application process, so we also suggest that the PIs be encouraged to specify the affected chemicals once the research identifies them. A list of toxics or chemicals that the PI's research is planning to influence would be very helpful. Items on the list could be removed or added in the annual reports from the PIs or from updated data received by the project officers.

# • Recommendation 2: The TSE grant application should strongly encourage potential PIs to have industrial involvement in their research.

We found that most of the PIs we studied who had strong industrial involvement while conducting their research were able to get companies more involved with technology developed from the completed research. For this reason we suggest that potential PIs seek out industrial partners before starting their work. If the PIs were successful in their research, they would not have to spend extra time finding someone to implement the result of their research, because they would already be working with an industrial partner. Additionally, industrial partners can provide support in terms of facilities in which to conduct research, supplies, materials or supplementary funding. Much of the research seemed to have great potential for environmental and industrial benefits. In most cases, however, initial changes to current methods seem very risky and expensive to companies. To support our recommendation an incentives program for companies to implement research is suggested.

#### 7.2 Follow-up Procedures

Each PI is assigned to a Project Officer (PO), a person who primarily communicates with the PI during the time of the research. The TSE program requires that the PI complete an annual progress report and a final report during the time that the PI is funded. These reports provide the

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PO insight into how the research is going, what has been accomplished, what will be tried in the research, and if the work has been publicized. Although we found that reading the grant files was important, talking with the PIs gave us more specific and relevant information about their projects. Information on what developments arise from the research after the funding ends should be organized and published so that general public could learn of the improvements to industrial processes and its benefits to the environment.

# • Recommendation 3: The TSE should implement a publication to publicize the work of the PIs.

Presently the TSE has no set system for informing the general public of the work of their PIs. For the most part the only way that people outside the academic community learn of PIs' work is because the PIs are out there publicizing their own work. In some cases news organizations, publicity departments of universities and scientific offices (such as the EPA) will The work being done by the PI is of value and other people who do not read academic journals should be aware of the progress being made. We propose that the TSE program implement a monthly or quarterly publication that highlights the work being done by some of its funded researchers. The publication should be sent to past and current PIs of the TSE program, all identified industrial partners of the PIs, and the publicity department of the EPA; the publication should be posted on the web so that a greater number of people could see it. For each PI there should be the following information included in the article: background of the PI, what the research is, recent developments, and any involvement with industries. • Recommendation 4: The TSE should implement a method to keep connected to the PIs once the term of the grant expires.

There is strong communication between PIs and their POs during the grant period and we believe this should continue at some level after the grant expires. We recommend that the TSE program establish a method to communicate with the PI on a regular basis such as once or twice a year. The purpose of the communication is so the TSE can be aware of what the PI is working on since the time that the grant ended. This will help with our preceding recommendation that the TSE implement a publication to publicize the work of the PIs. In the long run keeping communication between the TSE and PIs active will allow the TSE to stay informed concerning the developments from their PIs' research. If this communication can be maintained for long enough period of time, the potential environmental changes due to the PI's research will become actual data.

#### **7.3 Future Evaluations of the TSE Grant Program**

• Recommendation 5: The TSE should develop a method to evaluate its program and continue to do so in the future.

We recommend that future evaluations be made of the TSE grant program. An evaluation such as this should be performed every few years so that those running the TSE program can stay aware of what type of research they are funding and how the research is involved with the academic and industrial communities. Other PIs funded by the program should also be examined in the manner in which we examined the 10 PIs in this project. We established a method for choosing PIs, researching background information, conducting interviews, and presenting the information obtained through our work. The methods developed can be used as examples to follow when performing evaluations of the PIs funded by the TSE program.

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#### **Appendix A:** Environmental Protection Agency

The Environmental Protection Agency (EPA), a government agency, has been an integral part of environmental protection for over three decades. "The mission of the Environmental Protection Agency is to protect human health and the environment. Since 1970, EPA has been working for a cleaner healthier environment for the American people" (EPA a, 2004, About EPA). The contributions that the EPA makes cover a large spectrum of activities which are: creating & maintaining regulations, performing research, assisting in state environmental programs, working with industries to promote environmental protection and continuing environmental education. The EPA covers all aspects of environmental protection from the research that leads to regulations, to the partnerships on state and business levels, to sparking interest in the environmental by promoting environmental education. To ensure that the EPA accomplishes their missions, a strategic plan is used. The strategic plan comprises of goals for the long term (three years) and objectives that will facilitate the EPA achieving their goals (EPA, 2004a, Strategic Plan). Additional planning is used with the budget of the EPA. The agency's budget is a part of the Executive Branch (EPA a, 2004, Budget). The budget is prepared by the EPA and then brought in front of the Congress for approval.

The EPA is broken down into many branches to help organize the different activities it performs. Within the branches are additional offices that work with their branch. Here is the organizational chart off the EPA's website:

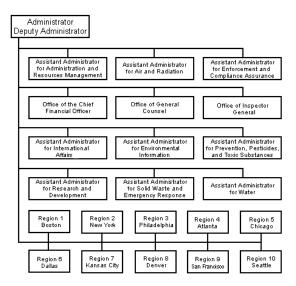


Figure 3: Organization of the EPA (EPA a, 2004, Organization)

Figure one shows the structure of the different departments within the EPA. Each of the offices has specific duties towards continuing the EPA's mission. Each office has its own website with descriptions of the activities the staff perform, along with information, and additional resources. The group will not be working with the entire EPA but only with a couple of offices within it.

We will be working with the Office of Research and Development (ORD). ORD is the office in charge of the scientific research component of the EPA (ORD, 2004, About ORD). This office focuses on eight types of research: air, drinking water, ecosystem assessment and restoration, global change, human health protection, water quality, pollution prevention and new technologies, and endocrine disrupting chemicals. The ORD has five goals that help them accomplish their strategic plan. The goals are to: support the agency, be a high performing organization, be a leader in environmental research, bring together environmental science and technology, and prepare for future environmental issues (ORD, 2004, Strategic Plan).

### Appendix B: Principal Investigator Interview Questionnaire

Name: Date Interviewed: College: Name of TSE Grant

• What research are you currently conducting?

- Has your research created any change in:
  - o your course syllabus?
  - the school curricula?

• Did you collaborate with any faculty outside your department or institution?

• How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

• What is the potential for the project or research?

• What has happened as a result of this research at this point?

• Did your research prompt follow up research or patents?

- Did you have any industrial partners while completing your research?
  - If so what is the extent of their involvement in your research?
  - If not have any industries learned of your work? Have they implemented it or at least looked into using it?
     (if the researchers know: how are they going to begin to incorporate the research into their process)

• How many students were funded by the TSE grant(s)?

• Are there any graduate students that you would recommend talking to about how this research has affected their careers?

• Has there been any quantitative data as a result of your research? Where did it come from?

• Any comments?

Can we call again? Thanks for your time

### **Appendix C:** Graduate Students Interview Questionnaire

Date Interviewed: Name of graduate students Name of PI whom they worked with: College: Name of TSE Grant:

How did you get involved in the TSE funded research?

Did the TSE-funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

- If so what was the new research?
- Has any of your research been published?

If not involved in research, what are you currently conducting working on?

Did your work as a student influence your choice of profession?

### Appendix D: Dr. Eric Beckman Interview

Name: Eric Beckman
Phone: 412-624-4828
Email: Beckman@pitt.edu
Date Interviewed: November 4, 2004
College: University of Pittsburgh, Main Campus
Name of TSE Grant: "Design and Synthesis of CO2-Soluble Affinity Ligands for Use in CO2 Extraction of Proteins" and "In-Situ Generation of H2O2 in CO2: Platform for Green Oxidations" (currently conducting)

#### What research are you currently conducting?

Working on his second TSE grant, generating H2O2. Beckman is working on a bio-functional catalyst that will do two things. First make H2O2 and secondly make an oxidation catalyst. The research is mainly focus on producing propylene oxide (used in foam chusing), phenol (used in polycarbonate), and adipic acid (used in nylons) with limited waste using the bio-functional catalyst. For the past four months Beckman has focused on adipic acid, which is the most complicated. The work has also led him to use different oxidation catalysts other than the TS-1, which he began the research with.

After working on his first TSE grant, Beckman's work focused on greener reactions. While reading an article on how to make propylene acid, he dicussed with a student Dan Hancu how the process could be simplified. The idea of swapping CO2 in for the solvent that was presently used came to Beckman. There were some patents out for new methods of making H2O2 under the Lyondell Chemicals. The two parties talked and Lyondell fund Beckman's research between the times of his two TSE grants.

#### Has your research created any change in your course syllabus or school curricula?

The research has not affected Beckman's teaching, with the expectation of bring a green chemistry examples into his elective course. The school curricula also has not been affected, mainly do to the fact that he does more chemistry than most other chemical engineers.

### Did you collaborate with any faculty outside your department or institution?

He did not collaborate with any other faculty outside his department or institution.

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

For his early TSE grant, Beckman had funding from the Genecor International. They gave about 60 to 70 thousand dollars throughout his three year grant.

For his current TSE grant, Beckman has funding from two sources. Lyondell Chemicals funded Beckman between his two TSE grants with 250 thousand dollars. Also a French company, SNF, has given about 50 thousand dollars for this three year grant.

#### What is the potential for the project or research?

Both of Beckman's TSE grant research show that Carbon Dioxide is a more practical solvent. Promote the thinking of Carbon Dioxide as an ideal solvent for research applications rather than just an environmentally safe solvent. His current research shows that oxidation process can be cleaner using different types of solvents.

#### What has happened as a result of this research at this point?

Beckman's first TSE grant was successful in designing a series of surfactants and affinity ligands that exhibit high solubility in liquid CO<sub>2</sub>. The surfactants were too expensive to be implemented by Genecor International, even though Genecor did work with Beckman in getting patents on the research.

#### Did your research prompt follow up research or patents?

Work on Beckman's first TSE grant led him into the research area of Carbon Dioxide souble materials. The first TSE grant led him into the research area of  $CO_2$  soluble materials. The Chemical and Transport Systems Division that is a part of the National Science Foundation's Directorate for Engineering funded the more research that Dr. Beckman conducted. The research tries to design a non-fluorinated, highly  $CO_2$  souble material using a combination of computer simulation and experiment. The work was started with some TSE money, preliminary results were achieved and with them Beckman received the National Science Foundation support.

Dr. Beckman has the following completed patents:

- US Patent 6638749, October 28, 2003. "Carbon dixoxide soluble surfactant having two fluoroether CO2-philic tail groups and a head group." Inventors: Eric Beckman, Eliador Ghenciu, Nathan Becker, Landon Steele, Alan Russell.
- US Patent 6342196, January 29, 2002. "Synthesis of hydrogen peroxide." Inventors: Eric Beckman and Dan Hancu.
- US Patent 6596884, July 22, 2003. "Synthesis of hydrogen peroxide." Inventors: Eric Beckman and Dan Hancu.
- US Patent 6710192, March 23, 2004. "Dense phase epoxidation." Inventors: Dan Hancu, Eric Beckman, and Tiberiu Danciu.

Dr. Beckman has the following patent filed; not yet completed:

• US Patent Application 20040186319, September 23, 2004. "Synthesis of N-vinyl formamide." Eric Beckman, Toby Chapman, Cedrick Gilbert Favero, Christopher Capelli, Harold Swift.

#### Did you have any industrial partners while completing your research?

With his first TSE grant, Genecor International was the only industrial partner. They helped with suppling materials, giving anaylsis, co-writing published papers and patents.

Beckman's current TSE grant has two industrial partners. Lyondell Chemicals was a partner before applying for this TSE grant. But throughout the research Lyondell has helped with the patents, papers, and providing testing. SNF, the other industrial partner, is a company that makes basic chemicals. They are also interested in Beckman's work and provide pilot testing facilities and knowledge on catalysts.

#### How many students were funded by the TSE grant(s)?

There were three graduates students funded with Beckman's first grant and two are funded by his current grant.

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Dan Hancu (now at GE, 518-387-5011), unavailable over the phone.

# Has there been any quantitative data as a result of your research? Where did it come from?

Hmm, not really -- our first TSE started with the premise that we could design highly CO2soluble materials (fluorinated) that would allow us to create greener analogs to current processes (H2O2, protein extraction, etc.). However, our TSE work led us to the conclusion that fluorinated materials were too expensive to make the processes economical, even though they would be greener. This led us to try to design non-fluorinated analogs (our NSF funding). Then, in ~ 1999, we learned that the fluorinated compounds we were using were not only expensive, but not as green as we thought, so it was fortunate that we started the non-fluorous design work in 1998 -- made us look clairvoyant.

### Appendix E: Dr. Joseph DeSimone Interview

Name: Joseph DeSimone
Phone: 919-962-2166
Email: desimone@email.unc.edu
Date Interviewed: November 2<sup>nd</sup>, 2004
College: University of North Carolina
Name of TSE Grant: "Nonionic Surfactants for Dispersion Polymerizations in Carbon Dioxide" and" Dry Lithography: Environmentally Responsible Processes for High Resolution Pattern
Transfer and Elimination of Image Collapse using Positive Tone Resists"

#### What research are you currently conducting?

DeSimone is working on his current TSE grant involving lithography. He became involved with semiconductors for environmental reasons, Carbon Dioxide has excellent wetting properties (water can be damaging to nano devices), and also new materials work better with Carbon Dioxide.

#### Has your research created any change in your course syllabus?

DeSimone has brought in examples of his work into his polymer chemistry class and his sophomore organic chemistry class.

#### Has your research created any change in the school curricula?

The TSE grants compliment the NSF Science & Technology Center. The center is a multidisciplinary effort with participants from five academic centers and two national laboratories: University of North Carolina at Chapel Hill, North Carolina State University, North Carolina A&T University, University of Texas at Austin and the Georgia Institute of Technology in partnership with Sandia National Laboratory and Oak Ridge National Laboratory. More information on this center can be found at <u>http://www.nsfstc.unc.edu/</u>

#### Did you collaborate with any faculty outside your department or institution?

DeSimone worked with members of the NSF Science & Technology Center.

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

DeSimone received four million from the NSF Science & Technology Center.

#### What is the potential for the project or research?

Did not say.

What has happened as a result of this research at this point?

DeSimone's research done with his first TSE grant led to obtaining support for the NSF Science & Technology Center. Also his research is used in the dry cleaning industries. His work is also used in bringing in CO2 into the manufacturing of Teflon

#### Did your research prompt follow up research or patents?

US Patent 6451287, September 17<sup>th</sup> 2002 Fluorinated Copolymer Surfactants and Use Thereof in Areosol Compositions Inventors DeSimone, Terri Johnson Carson, John Miller, Sharon Wells Kennedy

### Did you have any industrial partners while completing your research?

Yes, he had support from Dupont, Stockhalven, and Micell Technologies. They provided monitoring of his current TSE research grant.

### How many students were funded by the TSE grant(s)?

Seven students.

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Luke Zannoni

# Has there been any quantitative data as a result of your research? Where did it come from?

Does not have any information.

## Appendix F: Luke Zannoni Interview

#### How did you get involved in the TSE funded research?

I was involved in the research funded by another grant. When the TSE grant was obtained, there was an opportunity for me to apply the knowledge and skills that I had obtained while working on the other grant to the new areas funded by the TSE program.

## Did the TSE-funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

The work with Dr. DeSimone has not prompted him to conduct further research in the same or similar area of study.

#### Has any of your research been published?

- Zannoni, L. A.; Simhan, J.; DeSimone, J. M. "Progress Towards the Development of a 157-nm Photoresist for Carbon-Dioxide-Based Lithography" *Proc. of SPIE*, **2003**, 5039, 1327-1332.
- Zannoni, L.A.; DeSimone, J. M. "Synthesis Characterization, and Properties of Copolymers Prepared in Dense Carbon Dioxide Towards the Development of a 157 nm Photoresist" *PMSE*, **2002**, *87*, 197-198.

#### If not involved in research, what are you currently conducting working on?

Currently Mr. Zannoni is employed at the National Starch and Chemical Company conducting research in the Corporate Research Group.

#### Did your work as a student influence your choice of profession?

His work in graduate school influenced him in his motivation to conduct research as a profession, with the preference of doing it outside of academia. Currently Mr. Zannoni is employed at the National Starch and Chemical Company conducting research in the Corporate Research Group.

#### Appendix G: Dr. Nancy Ho Interview

Name: Nancy Ho Phone: 765-494-7046 Email: nwyho@purdue.edu Date Interviewed: October 29<sup>th</sup>, 2004 College: Purdue University Name of TSE Grant: "Development of Biotechnology to Sustain the Production of Environmentally Friendly Transportation Fuel Ethanol from Cellulosic Biomass"

#### What research are you currently conducting?

Currently she is working on biodesulfurization, particularly she is trying to remove sulfur from coal and petroleum to produce cleaner and more cost effect fuel. This is similar to the research Mrs. Ho was funded for by the TSE program where she is researching yeast that could produce a high quality ethanol that could be used as gasoline or even possibly replace it.

#### Has your research created any change in:

This project was not academic related.

#### Did you collaborate with any faculty outside your department or institution?

Yes. She wouldn't give names, but she did say there were a lot?

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

Approximately 400,000 from DOE She is currently receiving approximately 250,000 from USDA grants.

#### What is the potential for the project or research?

The genetically engineered *Saccharomyces* yeast would ferment xylose, which could produce a high quality ethanol that could be used as gasoline or even possibly, replace it. The best part about the research is that this yeast comes from waste products and also the ethanol produced from it would be healthier for the environment than what is currently being used in the industry.

"In particular, ethanol can be produced from cellulosic biomass (corn stover, rice straw, wood, grasses, waste papers, etc.), which is abundantly available throughout the world – especially in our country. These feedstocks are also inexpensive and some of them exist as municipal or industrial wastes. Converting such wastes to ethanol also helps to solve waste disposal problems" (http://www.nancyho.info/).

### What has happened as a result of this research at this point?

Ms. Ho says the research is ready to be used in the industry but also says she can make it even better with more funding. However, no changes in industry have been currently made.

#### Did your research prompt follow up research or patents?

She says that others in Europe are trying to use her yeast research and are catching up to her, would not give the names.

2 patents. 1<sup>st</sup> patent is for her yeast and the second is for her integration methods of genes.

### Did you have any industrial partners while completing your research?

SWAN Biomass (Owned in part by Amaco), Iogen Corp. (Ottawa), ADM

### If so what is the extent of their involvement in your research?

SWAN Biomass was looking into the implementing the yeast. However, it went out of business for other reasons. Iogen Corp. is using her yeast and has non-exclusive rights to the yeast through licensing. ADM is a big ethanol producing company and they test all her yeast.

#### How many students were funded by the TSE grant(s)?

2 students w/their Masters Degrees.

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

No

# Has there been any quantitative data as a result of your research? Where did it come from?

Ethanol is made when yeast ferments the glucose in food crops, such as corn and other starch rich grains. Her yeast produces about 30% more ethanol from the same amount of plant material that previous methods had used.

#### Any comments?

Ms. Ho is angry because she's not getting enough funding from big agencies despite the potential for her work. Says that no other lab in the U.S. can do her work. She is getting frustrated when applying for money.

### Appendix H: Dr. George Kraus Interview

Name: George Kraus Phone: 515-294-7794 Email: gakraus@iastate.edu Date Interviewed: November 3, 2004 College: Iowa State University Name of TSE Grant: "Photochemical Alternatives for Pollution Prevention"

#### What research are you currently conducting?

Although his TSE grant is no longer in progress, Mr. Kraus is still working on the research initially funded by the TSE program. This includes:

Improving TBHQ (tertiary butyl hydroquinone), an antioxidant, to be used as an additive in industry. Working on a photochemical method used to make isoflavones (important as dietary supplements). Working on phenylanthracenes. (not as practical, more of a scientific curiosity)

#### Has your research created any change in:

In one of the Green Chemistry courses at Iowa State University, they have created experiments in their organic chemistry laboratory as a result of the research funded by the TSE grants.

#### Did you collaborate with any faculty outside your department or institution?

Professor Dr. James Tanko at Virginia Polytechnic Institute (VPI).

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

No other government funding. However, there was some funding from Iowa State University.

#### What has happened as a result of this research at this point?

This detailed information is in his final report. (this expands on the following Objectives)

- 1.) "To extend the photochemically mediated acylation and alklation reactions.
- 2.) To use photochemistry to produce acyl radicals which will decarbonylate to alkyl radicals.
- 3.) To evaluate supercritical solvents for our photochemically mediated additions of aldehydes to quinones (with Dr. James Tanko, VPI).
- 4.) To understand the factors that influence the scale-up of the reaction."

#### Did your research prompt follow up research or patents?

Iowa State has submitted a disclosure for TBHQ.

Also there is a full patent on a type of benzodiazepines, which is similar to Valium (muscle relaxant).

#### Did you have any industrial partners while completing your research?

Mr. Kraus is working with Kemin, an agriculture products group.

#### If so what is the extent of their involvement in your research?

Mr. Kraus created anti-oxidant TBHQ that will be used as an additive a solvent Kemin uses. Although the TBHQ is more effective, Kemin is still using their previous solvent because it is less expensive than it would be to use the TBHQ additive.

#### How many students were funded by the TSE grant(s)?

About eight students.

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Yanhua Lu - sunfloweryhlu@hotmail.com Alex Melekhov - azepine99@yahoo.com

# Has there been any quantitative data as a result of your research? Where did it come from?

The current solvent Kemin is using can only give them about 75% of the product that they want.Using Kraus's TBHQ additive with the solvent gives about 90% of the product. However currently using the additive still will not be as cost efficient as current methods.

#### Any comments?

Kraus found the TSE program to be very effective.

## **Appendix I:** Yanhua Lu Interview

#### How did you get involved in the TSE funded research?

From 1996 to 1999, I was a graduate student in Iowa State University. Dr. George A. Kraus was my major professor. My first research project involved investigation of an environmental friendly photochemical alternative to certain Friedel-Crafts reactions. This project was funded by TSE.

# Did the TSE-funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

#### If so what was the new research?

I was very inspired and impressed by the idea that how scientists can bless the nature and environment by carefully designing experimental protocols and incorporating innovative methodology and technology.

I joined pharmaceutical industry after I obtained my M.S. in chemistry in 1999. No matter in drug discovery research lab or in process, manufacturing facilities, tons of waste is generated every day. This not only imposes a high cost for company disposal, but also creates a higher cost for the environment to accept it. Inspired by the "green chemistry" idea and experience, my colleagues and I developed a special protocol for iodination on 2-indole carboxylic acid. We replaced toxic solvent of DMF with water to achieve the same chemical yield. And the reaction can be easily scaled up in large quantities.

#### Has any of your research been published?

The above research was published in a poster presentation at 222<sup>nd</sup> ACS national meeting:

 <u>Lu, Yanhua;</u> Cai, Jianping; Goodnow, Robert, Jr.. Novel solvent system for iodination of 2-indole carboxylic acid. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, United States, August 26-30, 2001 (2001).

#### Did your work as a student influence your choice of profession?

My graduate work under Dr. George Kraus' guidance focused on the syntheses of potentially pharmaceutical active natural products. Both my graduate study experience and my mentor's inspiration and encouragement led me to become a pharmaceutical scientist and choose medicine and health care as my career.

### Appendix J: Dr. Chao-Jun Li Interview

Name: Chao-Jun Li
Phone: 514-398-8457
Email: cj.li@mcgill.edu
Date Interviewed: November 1, 2004
College: Tulane University (Located in McGill University at present time)
Name of TSE Grants:
"Water as Solvent for Metal-Mediated Carbon-Carbon Bond Formations"
"Forming Carbon-Carbon Bonds in Water and Other Alternative Media"
"Carbon-Carbon Bond Formations in Water and Other Alternative Media"

### What research are you currently conducting?

Li current grant builds on Li's second TSE grant. His research focuses on innovative carboncarbon bond formation reactions for chemical syntheses. Incorporating CO2 and water will have large environmental benefits. This research will improve catalysts and reduce the amount of waste from the reactions.

### Has your research created any change in your course syllabus or the school curricula?

Li's research has led to him develop a Green Chemistry graduate class last year. Other universities have begun similar classes at their institutions using Li's research in their courses. Such universities include University of Massachusetts (Amherst) and University of Oregon. Li's work has also been brought into the undergraduate classes; his research was used as an example of real life application of the class's subject matter. Presently Li is at McGill University; he has a research chair position and is working towards developing the green chemistry program there. Li's research helps contribute to the work that the university is doing to promote awareness of green chemistry. McGill is working with other universities to promote and encourage green chemistry research.

### Did you collaborate with any faculty outside your department or institution?

No. For all three TSE grants Li did not collaborate with any other faculty.

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

Li does more research than just the research that is funded by the TSE grants. For that reason Li works to obtain funding for his research. He has received funding in addition to the funding through the TSE grants; just none of it has gone solely to benefit any of his TSE grants.

### What is the potential for the project or research?

Li sees his research in the long term as not to try to improve on a reaction that already exists, but change the way that the reaction is looked at. Question what is assumed so that new ideas can be brought into the research. For the most part this research will work towards developing new chemistry methods for chemical synthesis.

### What has happened as a result of this research at this point?

Li had the opportunity to speak at the Chiral Conference 2004 in Boston, MA. He presented his paper: "Transition Metal Catalyzed Asymmetric A3 Coupling of Aldehyde, Alkyne and Amine". The presentation was based on a paper from 2002 that had won the Hot Paper award form the ISI. The conference gave Li the chance to show industries the potential of his research, if used by industries. Pharmaceutical industries specifically became interested in his work and what the work could do for their companies.

### Did you have any industrial partners while completing your research?

Li had limited involvement with industry, with respect to patents and industrial partners, while completing his research. At Tulane University, there was no interest in supporting patents for Li's research. The university felt that the patent process was too expensive and too hard to monitor. Li did not have industrial partners when conducting his research. Industries find out about the work through published papers and take the information and bring it into their company. Li does not know if an industry has used his work unless they contact him, on their own accord. The Millikan Chemicals asked for Li to be a consultant and help them implement his research into their industrial process. Another way companies inform Li of using his work is if they run into him at a conference and inform Li.

### How many students were funded by the TSE grant(s)?

Through each of the grants Li funded one graduate and one postgraduate student. Since there were a lot of graduate students he would fund on for a semester and then fund another student for the next semester. He never had the same student funded throughout the entire TSE grant

## Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Professor Li referred Charlene Keh (ckeh@optonline.net)

# Has there been any quantitative data as a result of your research? Where did it come from?

It is difficult for Li to determine if there is any data from industries. This is for two reasons: industries keep their processes confidential and Li does not know what part of his research they are using.

### Appendix K: Charlene Keh Interview

### How did you get involved in the TSE funded research?

I was involved with the TSE funded research with Professor Li because I was a graduate student in his research group.

# Did the TSE-funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

No, I do not have an academic career and so I do not do independent research.

### If not involved in research, what are you currently conducting working on?

I am currently working in industry, working at Cordis, a Johnson & Johnson company, still doing chemistry.

### Did your work as a student influence your choice of profession?

That's hard to say because I'm still a scientist but in industry with very little say in terms of my research project. However, my profession is still a chemist.

### Appendix L: Dr. Krzysztof Matyjaszewski Interview

Name: Kzysztof Matyjaszeski
Phone: 412-268-3209
Email: km3b@andrew.cmu.edu
Date Interviewed: November 10, 2004
College: Carnegie Mellon University
Name of TSE Grant: "Elimination of VOC's in the Synthesis and Application of Polymeric Materials Using Atom Transfer Radical Polymerization" and "Towards Elimination of Transition Metals and VOCs from the Environmentally Benign Materials Made by Atom Transfer Radical Polymerization (ATRP)"

### What research are you currently conducting?

Currently wrapping up second grant. Very successful in grants. Will be moving onto a different type of research unless they obtain additional funding.

### Has your research created any change in your course syllabus?

Have not had the chance, teach basic courses.

### Has your research created any change in the school curricula?

The university has a strong green chemistry environmental program. There is a lot of interaction between the environmental and chemistry departments.

### Did you collaborate with any faculty outside your department or institution?

No

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

None.

### What is the potential for the project or research?

Every research wishes that his research is important. That the research can be commerliazied and improve the environment and industry.

### What has happened as a result of this research at this point?

There has been a lot of industry interaction. The first TSE grant was foundation research where the second (current) TSE grant built on the research where the first one left off. Kris will not be trying to get additional funding through the EPA to further his research.

### Did your research prompt follow up research or patents?

Look in reports

Did you have any industrial partners while completing your research?

Look in reports

### How many students were funded by the TSE grant(s)?

A couple for each of the grants

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Nick Tsarevsky nvt@andrews.cmu.edu

# Has there been any quantitative data as a result of your research? Where did it come from?

Not available. Industries don't report to him.

### Appendix M: Nick Tsarevsky Interview

### How did you get involved in the TSE funded research with Prof. Matyjaszewski?

At the beginning of my PhD studies I started working on a project related to the application of ATRP to heterogeneous aqueous systems such as miniemulsions. The purpose was to find a way to decrease the amount of organic volatile reagents in the polymerization. Later, we moved on a project related to catalyst development for homogeneous (solution) ATRP in water.

# Did the TSE funded research you worked on as a student prompt you to conduct further research in the same or similar area of study? a) If so what was the new research? b) Has any of your research been published?

The importance of our research was recognized by the ACS Division of Environmental chemistry last year. I was awarded the Kenneth G. Hancock scholarship in Green Chemistry. Recently I started working in another "green chemistry" related field: the synthesis of biodegradable polymers. This will be published shortly (the very first results were published in 2002) and will also be presented at the ACS Spring 2005 meeting.

### If not involved in research, what are you currently working on?

Still involved in research - finishing my PhD thesis

### Did you work as a student influence your choice of profession?

I am still a student but what i learnt with Prof. Matyjaszewski will definitely influence my choice. I intend to be involved in academic (research/teaching) job.

### **Appendix N: Dr. Fred Ramirez Interview**

Name: Fred Ramirez Phone: 303-492-8660 Email: Fred.Ramirez@colorado.edu Date Interviewed: 11-10-04 College: University of Colorado, Boulder Name of TSE Grant: "Optimal Operation of Electric Arc Furnaces (EAF) to Minimize the Generation of Air Pollutants at the Source"

### What research are you currently conducting?

Ramirez is working on modeling and optimizing biotechnological processes. The NSF is funding this research. This research is separate from the TSE-funded research.

### Has your research created any change in your course syllabus or the school curricula?

No, but the research does come up during some of his lectures.

### Did you collaborate with any faculty outside your department or institution?

No

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

Goodfellow Consults - approximately 15,000 dollars

### What is the potential for the project or research?

Replacing Carbon Monoxide with Carbon Dioxide in Steel Manufacturing Plants by using his model for a new electric air furnace (EAF). At the same time the overall performance for the process would increase significantly.

### What has happened as a result of this research at this point?

The model has been created and has been analyzed. However industry is reluctant to adopt it because changing the current methods would be expensive.

### Did your research prompt follow up research or patents?

No

### Did you have any industrial partners while completing your research?

Goodfellow Consultants provided Mr. Ramirez with the operating data from too steel companies, Keystone Steel & Wire and also Chaparral Steel

### If so what is the extent of their involvement in your research?

The two steel companies allowed Ramirez to use their plant data on their current steel producing methods

### How many students were funded by the TSE grant(s)?

1 student (Sam Matson) who is now currently works for Goodfellow Consultants.

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Yes. Sam Matson. matsons@yahoo.com

# Has there been any quantitative data as a result of your research? Where did it come from?

The following data are approximations that have come from the researcher's extensive study on applying his model to the 2 steel plants:

Plant 1 – 99% of carbon monoxide could be removed. Yields improved by 100%. However, processing time increased a little. Overall Performance increase of 52%.

Plant 2 – 92% of carbon monoxide could be removed. Yields improved by 61%. Processing time deceased. Overall performance increase of 32%.

### Any comments?

Ramirez found the TSE program to be very effective in helping him produce good research. However, he needs help implementing his research. Industries are reluctant to try it out because initially it will be expensive. He suggests creating a federally funded incentives program.

### **Appendix O: Sam Matson Interview**

### How did you get involved in the TSE funded research?

I help Fred Ramirez write the proposal and performed research on the project for my Master's and PhD degree in chemical engineering

Did the TSE-funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

### If so what was the new research?

I have continued in developing the model that I started during the research

### Has any of your research been published?

No

### If not involved in research, what are you currently working on?

I am a process engineer at an engineering consulting firm. Part of my work is improving the model I developed in school.

### Did your work as a student influence your choice of profession? If so, how?

I worked as a Coop student as an undergrad as an engineering consultant and continued contact with my employer throughout college. Writing the TSE proposal was intended to keep me in the steel-making field and prepare me for future work.

### Appendix P: Dr. Valerie Thomas Interview

Name: Valerie Thomas Phone: 202-225-5801 Email: <u>Valerie.Thomas@WAP.org</u> Date Interviewed: November 5, 2004 College: Princeton University (currently Congressional fellow, going to Georgia Tech next year) Name of TSE Grant: "Electronic Tags for Produce Lifecycle Management"

### What research are you currently conducting?

Getting information technology into waste management practices RFID tags (read information from further away than bar codes) Used in East Germany (radio receiver on truck, ID on trashcan)

Currently working on energy policies for NJ Congressman (Robert Andrews?)

### Has your research created any change in your course syllabus or the school curricula?

No

### Did you collaborate with any faculty outside your department or institution?

Sigurd Wagner (Electrical Engineer @ Princeton)

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

No funding flow, though there were contributions made by Motorola. Will be receiving starting funds from Georgia Tech once there next year

### What is the potential for the project or research?

Read barcode on cell phone or other recycled electronic, which will contact web-based software (see students section) for dismantling/recycling instructions

GPS could possibly track where the product goes when it is disposed of, though currently metal in the trash or the garbage truck could interfere with the signal. GPS locators also very expensive

Tracking can also be done with a radio transmitter, like the kind used to track animals, but the range is currently much too short to be of any practical use.

Improvements have been made to GPS locators, working with Oxloc (see industrial partners) on testing improved GPS locators for this purpose

### What has happened as a result of this research at this point?

Little has happened in the United States up to this point, even though the concept is used in several European countries (i.e. Germany, Scandinavia)

Worked with East Germany (Dresden) on developing a similar system in the US (MOBA, in particular, would be interested in a US market in these systems)

No town in the US has electronic systems in garbage trucks for the purpose of waste logistics, even though it is relatively common in Europe.

No quantitative data concerning where recycled products in the US end up, how far they travel to get there, whether they are going to the correct location, etc.

### Did your research prompt follow up research or patents?

Follow-up research was done with GPS locators. No patents, but Motorola did make an intellectual property disclosure. Austrian company (Ecotronics) using cell phone recycling methods

Plans to continue research at Georgia Tech

# Did you have any industrial partners while completing your research? If so what is the extent of their involvement in your research?

Motorola – Contributed to research, particularly in the area of cell phone recycling. MOBA (Mobile Automation) – German company involved in waste disposal logistics. Oxloc (Oxford Location) – Oxford, England company making GPS locators.

### How many students were funded by the TSE grant(s)?

Steven Saar: undergraduate student, helped develop the web-based software that brings up recycling info. Graduated and currently works at Intel

Audrey Lee: Ph.D. candidate in Electrical Engineering

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Audrey Lee: <u>jalee@princeton.edu</u> Steven Saar: Try <u>ssaar@alumni.princeton.edu</u>

# How does electronic tagging have the potential to make product recycling and life cycle management cheaper?

By knowing what kinds of products a household is disposing of, waste management can more efficiently route trucks for pickup

Some cities/towns have attempted to charge trash pickup by weight; however putting a scale on the truck is very expensive. Much cheaper and more efficient to put a radio tag that reads which trashcan is being dumped, and how full it is, and charging households that way.

### Appendix Q: Audrey Lee Interview

### How did you get involved in Electronic Tags for Product Lifecycle Management?

I first became involved with the Electronic Tags for Product Lifecycle Management project last September when I was considering taking a leave from graduate school. I had begun to question my interest in my Electrical Engineering research on Quantum Computing because I did not see a direct application for it and why it was important to me. Talking to Dr. Thomas helped me realize that there was a way for me to use my Electrical Engineering background and apply it to environmental problems that I felt strongly about. By working on the Electronic Tags project, I was able to find a research area that I was passionate about and where I could enthusiastically apply myself.

### Has any of your work related to this project been published?

At the Institute for Electronic and Electrical Engineers (IEEE), International Symposium on Electronics and the Environment (ISEE) in Phoenix, Arizona in May 2004, I won a Student Paper Award for and presented "GPS and Radio Tracking of End-of-Life Products," which I wrote with V. M. Thomas.

### What are you currently working on?

I am currently working on using Field-Portable X-Ray Fluorescence to detect heavy metals in plastics. This research has important environmental implications as it will facilitate the detection of heavy metals before they are incinerated or landfilled and cause pollution.

# Has your work with Dr. Thomas had any influence on either what you are currently doing or what you plan to do once you obtain your Ph.D.?

My work with Dr. Valerie Thomas has had a profound influence on my current research interests and my future career. I became interested in my current research on heavy metals in consumer plastics because she introduced me to the challenges in pollution prevention and product management at end-of-life. I think of Dr. Thomas as my mentor, especially at this juncture in my career where I am exploring my interests and future career after graduate school. She has encouraged me to apply my scientific background to a career in environmental and public policy.

### Appendix R: Dr. Richard Wool Interview

Name: Richard Wool Phone: 302-831-3312 Email: wool@ccm.udel.edu Date Interviewed: November 2, 2004 College: University of Delaware Name of TSE Grant: "Composite Resins and Adhesives from Plants"

### What research are you currently conducting?

Wool researches green materials, specifically making high performance materials from composite resins. Examples include computer chips made from chicken feathers instead of silicon (lower dielectric constant), an all natural composite material (recycled newspaper, cardboard, etc...) used with a soybean oil-based plastic resin to be used for hurricane resistant roofing, and also tractor parts made from soybean oil.

### Has your research created any change in the school curricula?

Yes- He's teaching a course in Green Engineering at the University of Delaware. He also teaches a class called Polymer Science, which is closely related to the green materials he researches.

### Did you collaborate with any faculty outside your department or institution?

Delaware University, Georgia Tech, Howard University, Michigan State University, Colorado State, etc... are working on creating a national research center for green materials.

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

NSF – About 200,000 for the hurricane resistant roof

DOE – About 11 million until bush came into office. The funding was then withdrawn and used elsewhere. Wool's research got to use about 3 million of the initial 11 million.

### What is the potential for the project or research?

Creating safer houses with the new roofing to prevent hurricane damage, creating computer chips from chicken feathers (waste product, low cost, good for environment). The soybean oil will replace petroleum or other more expensive products.

### What has happened as a result of this research at this point?

John Deere tractor parts have already been made from his soybean oil. They are working on a prototype for the hurricane resistance roofing at the Univ. of Delaware.

### Did your research prompt follow up research or patents?

Chicken feather patent Sheet molding patent Hurricane resistance roof patent Pressure sensitive adhesive patent

### Did you have any industrial partners while completing your research?

John Deere, Tyson, Intel, Dupont, DOW, Avery Denison, 3M, Nike, Diab, Doc Resins, USCB Radcure, West Vaco, Georgia Pacific, Rome & Haas.

### If so what is the extent of their involvement in your research?

John Deere makes the parts for their tractors using his soybean oil research. Intel is researching the chicken feathers to see whether they can use them in their computer chips, DOW and Dupont are studying the roofs to see whether they can use his composite material, and he has some confidential project with Nike.

### How many students were funded by the TSE grant(s)?

3 or 4. Wool is planning to email us the names.

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

John LaScala = <u>jlascala@arl.army.mil</u> Wim Thielemans = <u>wim.thielemans@efpg.inpg.fr</u>

# Has there been any quantitative data as a result of your research? Where did it come from?

Yes, it is in his TSE grant file with the section on roofing (DOE information).

### Any comments?

He would like more TSE money. Wool says his best research came from the TSE grants. Wool noted a couple of his publications. Rigidity percolation theory of Polymer Fracture (Journal of Polymer Science). He was also in Newsweek. He noted that 3 of his projects were brought to congress by the head of the EPA.

### Appendix S: John LaScala Interview

### How did you get involved in the TSE funded research?

I worked with Prof. Richard P. Wool as a graduate student at U. Delaware from 1997-2002. He obtained the grant to partially fund my research as well as a few other grad students.

# Did the TSE-funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

As a grad student, I continued to work on composite resins from plant oils as my entire dissertation. After graduating, I did further research in this area (see below).

### If so what was the new research?

I am developing low VOC composite resins that use plant oil monomers as replacements for styrene (Funded through SERDP PP-1271).

In addition, I am looking to get involved in doing research on other environmentally friendly and biodegradable polymers (will apply for grant soon).

I do polymers research, in general. The TSE research I did helped make me a polymers expert.

### Has any of your research been published?

- J.J. La Scala and R.P. Wool, "Property Analysis of Triglyceride-Based Thermosets," *Polymer*, Accepted.
- **J.J. La Scala** and R. P. Wool, "The Rheology of Chemically Modified Triglycerides," *JAPS*, accepted.
- J.J. La Scala and R. P. Wool, "The Effect of Fatty Acid Composition on the Acrylation Kinetics of Epoxidized Triacylglycerols", *J. Am Oil Chem. Soc.*, **79**, 59-63 (2002)
- J.J. La Scala and R.P. Wool, "The Effect of Fatty Acid Composition on the Epoxidation Kinetics of TAG", *J. Am. Oil Chem. Soc.*, **79**, 373-378, 2002.
- R.P. Wool, S.N. Khot, **J.J. La Scala**, S.P. Bunker, J. Lu, W. Thielemans, E. Can, S.S. Morye, G.I. Williams, "Affordable Composites and Plastics from Renewable Resources," *Advancing Sustainability through Green Chemistry and Engineering*, R.L. Lankey, P.T. Anastas, Eds. ACS: DC, 2002, pp. 177-224.
- S.N. Khot, **J.J. La Scala**, E. Can, S.S. Morye, G.I. Williams, G.R. Palmese, S.H. Kusefoglu, R.P. Wool, "Development and Application of Triglyceride Based Polymers and Composites," *J. Applied Polym. Sci.*, **82**, 703-723 (2001).

- La Scala, J.J., J.M. Sands, J.A. Orlicki, E.J. Robinette, G.R. Palmese, "Fatty Acid-Based Monomers as Styrene Replacements for Liquid Molding Resins," *Polymer*, **45**, 7729-7737 (2004).
- La Scala, J.J., J.M. Sands, G.R. Palmese, "Environmentally Friendly Composites," *AMPTIAC*, (Submitted).
- Palmese, G.R., J.J. La Scala, J.M. Sands, "Vinyl Ester Monomers to Reduce Emissions and Toughen Polymers," U.S. Patent Disclosure, April 2004.
- La Scala, J.J., E.J. Robinette, G.R. Palmese, J.M. Sands, J.A. Orlicki, and M.S. Bratcher, "Successful Initial Development of Styrene Substitutes and Suppressants for Vinyl Ester Resin Formulations," *Army Research Laboratory Technical Report*, ARL-TR-3023, August 2003.
- Plus many presentations at national meetings (AIChE, ACS, SAMPE, ACMA, SERDP, among others)

### Did your work as a student influence your choice of profession? If so, how?

Yes. I am still working with environmentally friendly polymers and I am trying to obtain a faculty position doing this research as well.

### Appendix T: Ian McAninch Interview

### How did you get involved in the TSE funded research?

When I arrived at the University of Delaware in the fall of 2002, Dr. Wool was offering a project focusing on the use of bio-based resins and carbon nanotubes to create high performance composites. Of the research being offered to us, this was one of the more interesting, and I had some experience working with carbon nanotubes during a summer internship with NASA. It was one of my top choices, and this project was the one I received.

# Professor Wool research is very extensive, specifically which area of research are you working with professor Wool on?

My research focuses on creating high performance composites using bio-based resins and carbon nanotubes.

# Do you think that your involvement with Prof. Wool's research might influence your career path or your own future research? If so, how?

My involvement with Dr. Wool's research will probably influence my career path to some extent. Already, due to my involvement, I had the opportunity to participate in the Pan-American Advanced Studies Institute on Green Chemistry (2003). I'm currently thinking about a career in industry, and my involvement with the research will surely open some doors, but it is difficult to say at this point how much influence it'll have on my career path.

### Have/Are you being funded by the TSE program?

Yes, I am.

### **Appendix U:** Wim Thielemans Interview

### How did you get involved in the TSE funded research?

TSE funding started during my tenure as graduate student with Richard Wool. As my research focused on the use of lignin in renewable polymers, it was part of the grant proposal and thus fell under the accepted grant.

Did the TSE-funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

### If so what was the new research?

Yes. I am currently performing research in France at the Ecole Francaise de Papeterie et des Industries Chimiques, a department of the Institut Polytechnique de Grenoble in Grenoble, France on the use of starch, and starch and cellulose nanocrystals in polymers. Even though it shift slightly away from lignin and natural oils, on which I worked with Richard Wool, it perfectly adds on to the expertise I gained at the University of Delaware. The combination of these two research experiences give me an unsurpassed broad knowledge of the most abundantly available natural resources and their potential applications in polymers. This is also the field I envision myself to continue in.

### Has any of your research been published?

I have currently 3 publications from my work at the University of Delaware shown below. There are two publications in the review process at the Journal of Applied Polymer Science and at Polymer Composites respectively. Another 3 publications are being prepared for submission to Biomacromolecules and will finish the dissipation of results from my work with Richard Wool at the University of Delaware.

- W. Thielemans, E. Can, S.S. Morye and R.P. Wool, *Novel Applications of Lignin in Composite Materials*, J. Appl. Polym. Sci., 83, 323-331 (2002)
- M. in het Panhuis, **W. Thielemans,** A.I. Minett, R. Leahy, W.J. Blau, B. Le Foulgoc, and R.P. Wool, *A Composite from Soy Oil and Carbon Nanotubes*, International Journal of Nanoscience, 2(3), 185-194 (2003)
- W. Thielemans and R.P. Wool, *Butyrated kraft lignin as compatibilizing agent for natural fiber reinforced thermoset composites*, Composites Part A: Applied Science and Manufacturing, 35, 327-338 (2004)

### Did your work as a student influence your choice of profession? If so, how?

It actually happened the way around. I wanted to perform research to have some positive impact on today's society and the possibility to work on renewable polymers was a perfect match with my philosophy. So the chance to do this research has certainly helped me to go this route, but I would somehow have found a way to do this. I am currently applying for faculty positions so that I can continue to contribute in my own personal way.

### Appendix V: Lin Zhu Interview

### How did you get involved in the TSE funded research?

I am interested in the project involved and chose it as the project for my Ph.D thesis.

# Professor Wool research is very extensive, specifically which area of research are you working with professor Wool on?

I am working on developing elastomers from renewable resources. Speaking in details, I start with the design of molecular structure, synthesize a monomer from plant oil which is suitable for elastomer synthesis and optimize the properties. Nanoclay is also introduced to the system as a filler to further improve the property by forming nanocomposites.

# Do you think that your involvement with Prof. Wool's research might influence your career path or your own future research? If so, how?

Absolutely. During the research, I got more interested in the material design and the application of the biobased materials. The most important is during the research, I learned how to solve problems, how to make the design possible, and how to optimize the system. From the project, I learned a lot about polymers and composites, all the theories, synthesis and characterization methods. These will be definitely very useful for my future career and research.

### Have/Are you being funded by the TSE program?

Yes.

### Appendix W: Dr. Yushan Yan Interview

Name: Yushan Yan Phone: 951-827-2068 Email: <u>Yushan\_yan@ucr.edu</u> Date Interviewed: November 4<sup>th</sup>, 2004 College: University of California, Riverside Name of TSE Grant: "Zeolite Coatings by In-Situ Crystallization as an Environmentally Benign Alternative to Chromate Conversion and Anodization Coatings"

### What research are you currently conducting?

Just completed the work done with the TSE grant money in August. He is continuing the same work do to a new source of funding. He is working on applying the same coatings develop in his TSE research to larger sections of metal.

### Has your research created any change in your course syllabus?

This research did not have an impact on Yan's courses.

### Has your research created any change in the school curricula?

The research did not have an impact on school curricula.

### Did you collaborate with any faculty outside your department or institution?

Yan did not work with any outside faculty for the TSE research. With his new funding he has the opportunity to work with researchers from the Navy, Army, and University of Massachusetts.

# How much funding did you receive in addition to the TSE grants in order to further your research? If so, from whom?

Yan did not receive any outside funding during his TSE research grant period.

### What is the potential for the project or research?

The work has moved from small pieces of metal to pieces that are three by five feet. Recently the coating was tested in a salt fog test, and it went very well.

### What has happened as a result of this research at this point?

Yan is now in collaboration with the U.S. Navy, U.S. Army, and the University of Massachusetts. The four groups made a proposal to the Strategic Environmental Research and Development Program (SERDP) program. The funding will last four years and is for 1.65 million dollars.

### Did your research prompt follow up research or patents?

Yan Y.; Cheng X.; Wang Z. 2003. Metal surfaces coated with molecular sieves for corrosion resistance. U.S. Patent No. 6,521,198, February 18, 2003

Yan may look into licensing in the latter half of his four-year grant with the Department of Defense.

### Did you have any industrial partners while completing your research?

Yan did not have any industrial partners. Yan's work has been published but that and his patent are the only ways industries will know of his work. The industries might learn of his work done with his current funding, but Yan can not predict how they will learn of it.

### How many students were funded by the TSE grant(s)?

One student

# Are there any graduate students that you would recommend talking to about how this research has affected their careers?

Derek Beving dbeving@engr.ucr.edu

# Has there been any quantitative data as a result of your research? Where did it come from?

With Yan's coating there would be no need for hexavalent chromium. Thus the amount of hexavalent due to chromate conversion and chromic acid Anodization would be zero. Yan knows that Ch conversion and Anodization are the major sources of Cr+6 but he does not know by what percent they contribute to the release of Cr to the environment.

### **Appendix X:** Derek Beving Interview

### How did you get involved in the TSE funded research with Prof. Yan?

I have my Masters in Environmental Toxicology, a broad degree. I was reading up on different things to pursue and came across an article on Yushan Yan's work. We met and became interested in working together. Dr. Yan alreadly had the idea for the TSE grant before meeting me.

# Did the TSE funded research you worked on as a student prompt you to conduct further research in the same or similar area of study?

Still working on completeing his PhD in environmetal toxiclogy. Is not sure what I will do after completing my PhD. Probably will not pursue research as a career. Until I decided what to do, I will stay on as a Post Doc. I am presently helping Yushan Yan with his Department of Defense grant.

### If not involved in research, what are you currently working on?

Still completing PhD.

Did you work as a student influence your choice of profession?

Absolutely.

### Potential Students funded Principal Year of Effect on Environmental Industrial Implemented Investigator Grant Curriculum **Benefits** Involvement Research by TSE program No - Method not cost-effective. Low-Used later discovered research as Low- research not to be as examples in successful but not able Low- Genecor environmentally Eric J. Beckman 1995 class to implement it International beneficial Low- Used High- Uses CO2 to research as make H2O2 which then examples in is used to make several Medium- Lyondell 2003 class acids Chemicals and SNF Yes Medium -Medium - Replaces Changed one harmful chemicals with No - Method not George A. Kraus 1996 class lab low - Kemin cost-effective Light Medium - Replaces Medium - Iogen in Canada, SWAN corn feedstock with Nancy W. Y. Ho 1997 None waste product Biomass Yes High- MiCELL Low- Used Fechnologies, BOC, research as Medium-Used CO2 as SCF Consortium Joseph M. examples in surfacant to produced including 8 DeSimone 1997 class polymers companies) Yes Medium-Use CO2 in Low-Used research as lithography film Medium- Dupont, Not Yet - Project Stockhalven, MiCELL was just recently examples in deposition and removal 2001 class **Fechnologies** completed process Medium - Reduces Very High - Helped VOCs and replaces create 2 consortia them with more nvolving 20+ environmentally benign companies. Licensed Krzysztof catalysts when his method to 6 Matyjaszewski 1998 None producing polymers corporations Yes Medium - Continuation Very High - See above 2001 None of previous grant row Yes Very Low -Very High - Replaces No - Model has a Research is discussed class, almost all CO with very high Very Low - Only used but not used in carbon dioxide in steel implementation Fred W. Ramirez 1998 syllabus lata from two plants plants cost High - Created High-Water & CO2 a Green used in reactions rather Chao Jun Li 1999 Chemistry class than harmful chemicals No industrial support Yes High- Eliminates hexavalent chromium Not yet - waiting from aluminum metal until current DOE grant is almost coatings, replaces them 1999 None with zeolites No industrial support complete Yushan Yan Medium - Use of IT in Not in the United waste management States, but similar makes disposal and Medium - Mobile methods are collection of trash more Automation, Motorola, already used in 2001 None Valerie Thomas efficient. OxLoc Europe Medium - Replaces Very high some harmful Two courses Very High - Working made from feedstocks with Richard P. Wool 2001 research with 10+ companies composite materials

### Appendix Y: Impacts Overview for 10 PIs Table 19: Impacts Overview for 10 PIs

# **US EPA ARCHIVE DOCUMENT**