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- Space Science
- Materials Research & Structural Mechanics
- Intelligent Systems, Advanced Computer & Electronic Technology, & Automation
- Measurement & Nondestructive Evaluation of Materials & Structures
- Engines, Fuels, Lubricants, & Vehicle Systems
- Geology & Nuclear Waste Management
- Fluid & Machinery Dynamics
- Electronic Systems & Instrumentation
- Chemistry & Chemical Engineering

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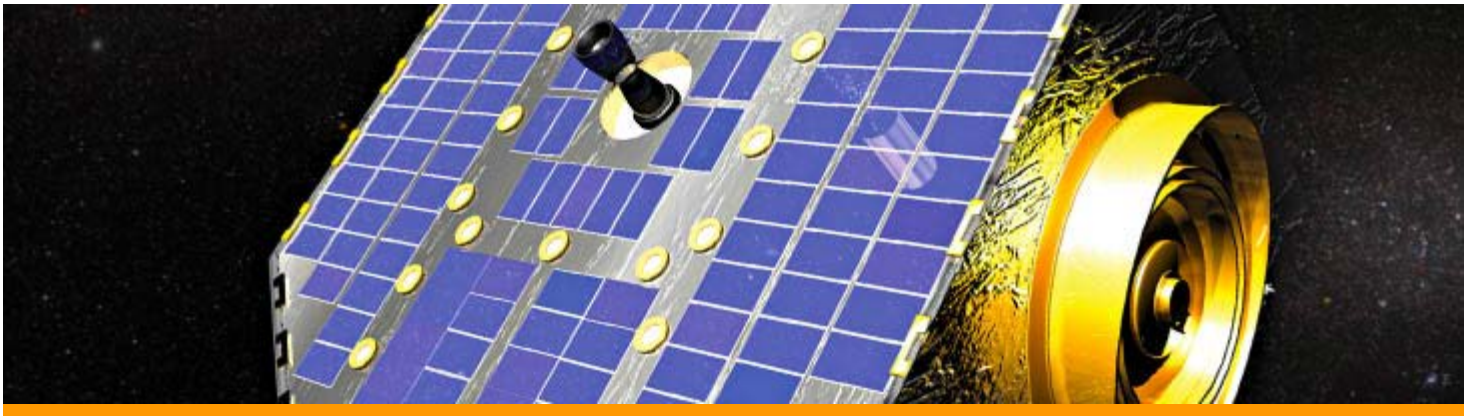
SwRI IR&D 2011 – Space Science



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- Capability Development and Demonstration for Next-Generation Suborbital Research, 15-R8115
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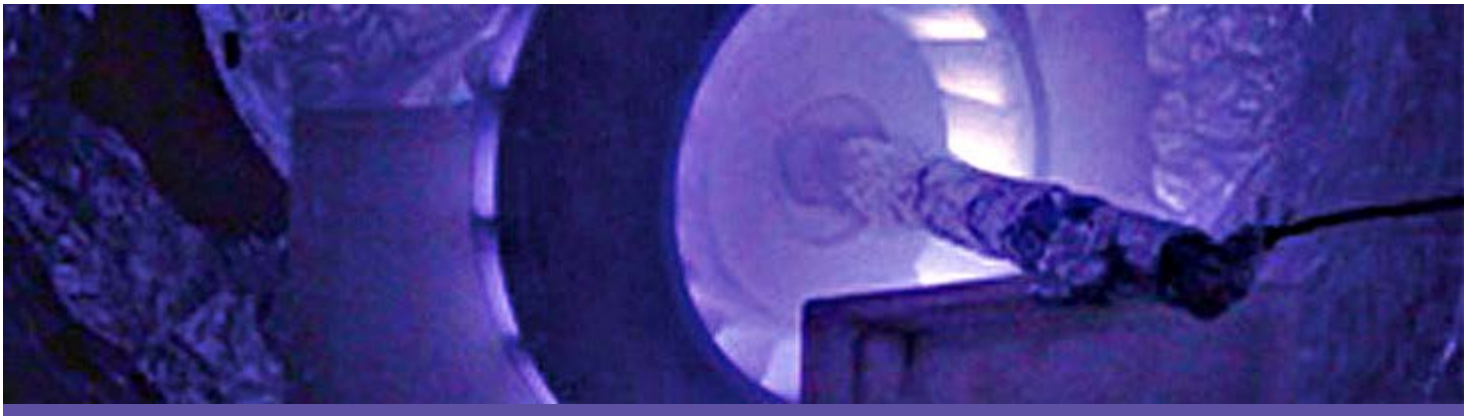
SwRI IR&D 2011 – Materials Research & Structural Mechanics



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Development of a Simple Instrument for Measuring Ionospheric Low Energy Electrons using a Delta-Doped CCD as Electron Detector (LEES), 15-R8053

Principal Investigators
Raymond Goldstein
Bill Tomlinson
Nick Alexander
Rudy Frahm

Inclusive Dates: 04/01/09 – 04/01/11

Background — SwRI has a long and successful history of designing and building instruments using specialized detectors for a variety of applications. In space applications, it is desirable to reduce the power, weight and complexity of the detector and supporting electronics. Reducing weight and power aids in meeting the spacecraft resource limitations for the instrument. For instrument operation, the less complicated the detection electronics, construction is easier and fewer things can go wrong. In a previous project, SwRI researchers successfully demonstrated that a new type of detector known as a delta-doped CCD developed by the Jet Propulsion Laboratory is capable of detecting charged particles. The chief advantage of this type of detector is that it does not require high voltages for its operation, in contrast to conventional particle detectors that require typically a few thousand volts. Eliminating this requirement will help simplify instrument design and fabrication, and reduce cost. This feature also allows its use under conditions (such as certain atmospheric/plasma pressure regimes) in which the presence of high voltages would result in dangerous arcing.

Approach — This project seeks to design, build and test a simple instrument that could be used for measuring electrons in a planet's ionosphere. Upon successful completion of this project, a valid science instrument will result. The basic design of the instrument is a standard retarding potential analyzer (RPA) combined with a Faraday cup. The RPA uses a set of grids, one of which has a variable negative voltage applied that then repels electrons of energy lower than the voltage at a given time. The Faraday cup houses the detector to measure the electron current passing through the grids. The instrument covers the energy range from 10 to 350 electron volts. This potential is swept over its range on the repeller grid.

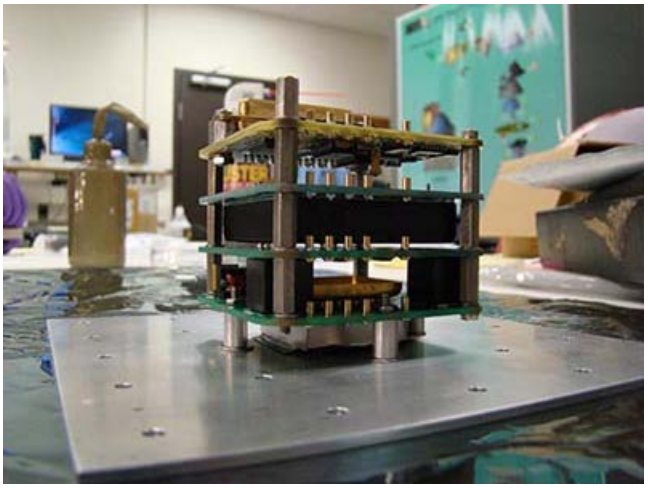

Figure 1. SwRI Developed LEES instrument without outer shell.

Accomplishments — The LEES (Low Energy Electrons) instrument has been designed and built. A photograph of LEES without its outer aluminum shell is shown in Figure 1. (The entrance aperture faces through the aluminum support plate to the bottom of the assembly. Most of the structure consists of the electronic circuit boards.) LEES is approximately 2.5 in. x 2.5 in. x 2.5 in., consumes 2.5 W electrical power, and has a mass of approximately 650 g. The CCD detector was delivered by the supplier and has been installed in LEES. The project team has also designed, built and tested the electrical control system,

based on a laptop computer and commercial control software. The setup, arranged on a table-top, is shown in Figure 2. The LEES instrument is designated by the red circle in the figure. Preliminary tests of the instrument were conducted in the SwRI electron test chamber. LEES appears to be operating as designed, but the output has a high level of noise, apparently the result of some internally generated interference. Because the project has terminated, researchers are unable to continue the development. However, NASA funding has been received that will allow researchers to test LEES on a suborbital rocket flight in early 2012.

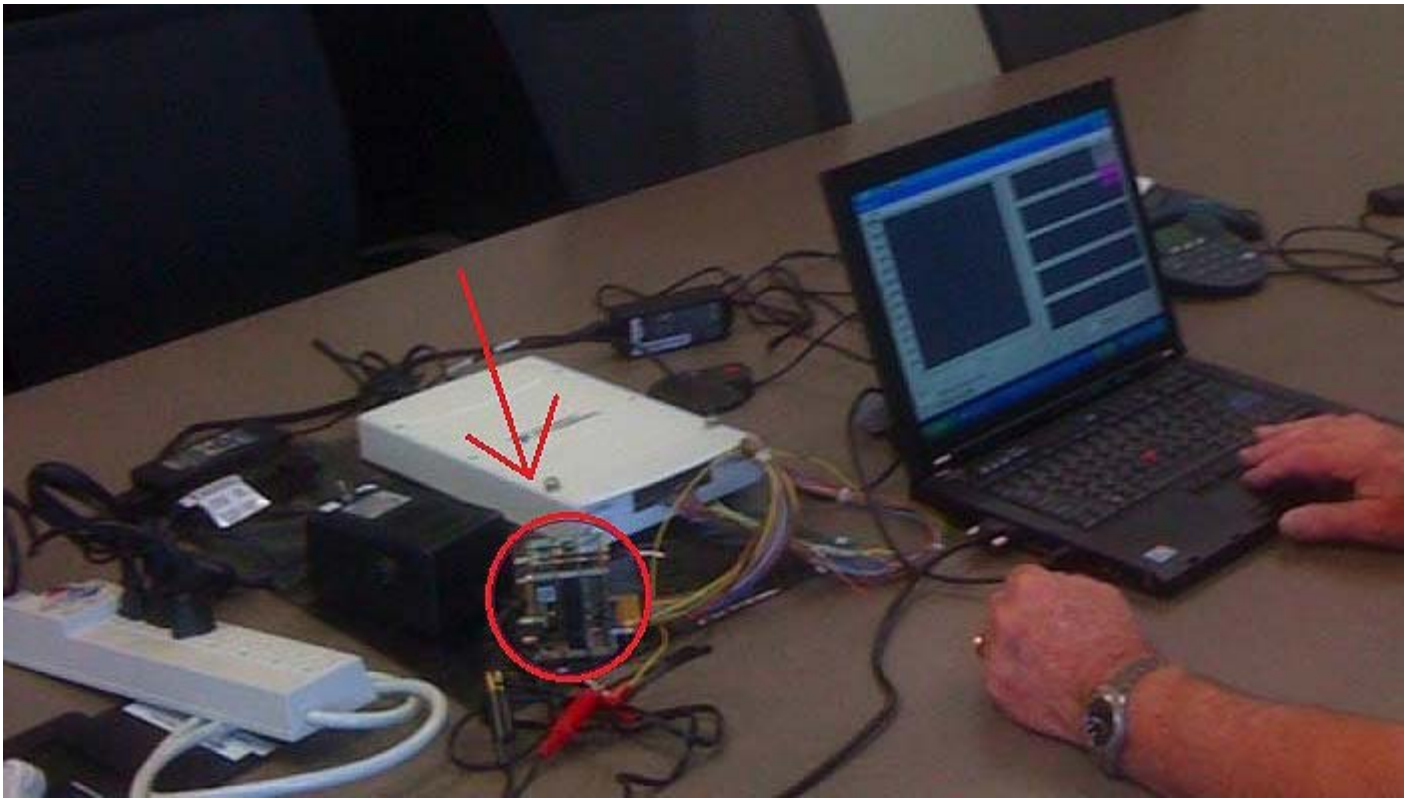

Figure 2. LEES instrument electrical control system.

Capability Development and Demonstration for Next-Generation Suborbital Research, 15-R8115

Principal Investigator
S. Alan Stern

Inclusive Dates: 01/01/10 – Current

Background — Research applications for new-generation suborbital vehicles include, but are not limited to, microgravity sciences, space life sciences, Earth and space sciences, land use, education and public outreach (EPO), technology development and demonstration/space systems development, and demonstrations (including TRL raising). The primary research advantages of these vehicles include better launch affordability compared to conventional sounding rockets, capability for human operator presence, better experiment affordability, more frequent access to the space environment, gentler ascent and entry compared to sounding rockets, extended periods of turbulence-free microgravity, and increased time in the 250,000 to 400,000 ft (80 to 120 km) region of the atmosphere (the "Ignorosphere").

Approach — SwRI's long-term business interests in these vehicles are:

- To exploit them for planetary, microgravity, aeronomical and auroral research.
- To provide research-related common systems (flight computers, data recording racks, etc.) and payload integration services to NASA and/or vehicle providers.
- To provide instrumentation, payload specialists and flight project expertise to research groups, both domestic and overseas, working in this area.

Therefore the overarching objective for this project is to put SwRI in the lead of the burgeoning suborbital research field using next-generation, manned vehicles by becoming one of the first, and quite possibly the first, organization to fly payloads with research payload specialists on these vehicles. This will open up to SwRI a series of new business opportunities including new funded research projects, new hardware development projects, ground and flight system task order contracts associated with next-generation suborbital work, and the provision of payload specialists for next-generation suborbital work.

Accomplishments —

- Completed and announced flight reservation agreements with Virgin Galactic and XCOR Aerospace for a total of nine seat launches.
- Completed a second set of F-104 training flights with focused, in-flight investigations to (1) evaluate the wearability and function of the AccuTracker II biomedical harness with standard crew flight suits and life support equipment during typical g-loads, and (2) test the design concept for the BORE microgravity experiment during zero-g parabolas.
- Completed a zero-g training flight and team exercises to refamiliarize/practice personal mobility and experiment handling operations in

zero-g conditions.

- Made technical presentations on the SwRI Suborbital Program and SwRI's three suborbital experiments at the Next-Generation Suborbital Researchers Conference (Orlando, FL).
- Completed construction of the BORE microgravity experiment.
- Passed vibration testing of the Blue Origin configuration of the BORE microgravity experiment.
- Continued refurbishment and testing and early calibration of SWUIS-A.
- Made invited oral presentations on the SwRI Suborbital Program at Spacefest III (Tucson, Az.), to a University of Colorado class, and at the NASA Marshall Space Flight Center.

Figure 1. A sign in New York's Times Square announces the agreement between SwRI and XCOR Aerospace.

- Completed FAA Class II and Class I medicals for each SwRI payload specialist to maintain expected suborbital flight medical qualification standards.
- Designed and released the SwRI payload specialist team mission patch with press release.
- Initiated discussions with David Clark Company and NASTAR on a collaborative effort to test/evaluate the CHAPS pressure suit under launch g-loads.
- Made flight assignments for personnel and experiments.
- Completed space suit familiarization training at the Dave Clark company.
- Created a payload specialist experiment training plan.

2011 IR&D Annual Report

Development of Near-IR Spectroscopic Techniques for Mineral Detection at the Surface of Venus, 15-R8128

Principal Investigators
Mark A. Bullock
Victoria Hamilton
Constantine Tsang
Erik Wilkinson

Inclusive Dates: 01/01/10 – 07/01/11

Background — The clouds and dense atmosphere of Venus prevent the kind of infrared remote sensing required to identify minerals at its surface. Furthermore, the high temperature and pressure of Venus' surface alters the interaction of visible and infrared light with mineral crystals. Therefore, the infrared signatures of common rock forming minerals are unknown under Venus surface conditions. Below the clouds, visible and infrared light is absorbed at most wavelengths by CO_2 and H_2O vapor absorption bands. In addition, scattering of light by atmospheric molecules is much more vigorous in Venus' atmosphere than in Earth's since Venus' is 60 times denser. This kind of scattering is highly dependent upon wavelength, so it is possible to calculate spectral regions that are optimal tradeoffs between atmospheric scattering and atmospheric transparency. In addition to reflecting sunlight during the day, the hot surface of Venus glows at near-infrared wavelengths. Calculations of the scattering and absorption of solar radiation, as well as the surface emission, are necessary to model the appearance of the surface within the best spectral windows. These calculations drive the design of a camera system optimized for acquiring images on descent through the atmosphere of Venus.

Approach — SwRI researchers adapted a computer package originally developed by the project manager for calculating the radiative energy balance of the Venus atmosphere. This 1-D climate model primarily calculated fluxes and heating rates in the Venus atmosphere. Researchers used the HITRAN and HITEMP spectral databases to calculate the line-by-line absorption coefficients for the nine known absorbing gases in Venus' atmosphere from 0.6 to 2.5 μm. Researchers then calculated the upward and downward radiation in the five most transparent bands at 0.65, 0.85, 1.02, 1.10, and 1.18 μm. This was done by solving the radiative transfer equation at 80 levels in the atmosphere, including absorption, scattering, and emission by both the atmosphere and surface. The theoretical results compared favorably with atmospheric *in situ* data from the Soviet Venera 13 and 14 spectrophotometers. In addition to the optical challenges, the exposure time constraints imposed by motion of a descent vehicle through the atmosphere of Venus were investigated.

Accomplishments — Even within the spectral windows, calculations show that light scattering by atmospheric molecules – Rayleigh scattering – swamps the signal from the surface at short wavelengths. Venus' sky is very bright, in part because light within the transparent windows is reflected several times between the surface and the bottom of the clouds. Just beneath the clouds, the sky is 200,000 times brighter than the surface at 0.65 μm. However, at 1.02 μm, the sky is only 38 times brighter than the surface. The exposure time is tightly constrained by descent vehicle motion. Venus descent probes have exhibited rotations as fast as 20 °/s. To ensure sharp images from a high-resolution descent camera, exposures must be shorter than 10 msec. To observe the Venus surface on descent, therefore, a long wavelength-enhanced fast CCD camera with a deep well depth and high dynamic range (24 bits) will be necessary.

2011 IR&D Annual Report

Establishing Astrophysics at Southwest Research Institute, 15-R8141

Principal Investigators
Peter W.A. Roming
Randall J. Rose
Gregory S. Winters
Robert A. Klar

Inclusive Dates: 04/01/10 – 03/31/11

Background — SwRI has a long history of excellence in heliophysics and planetary physics instrumentation and science missions. SwRI would like to expand into astrophysics instrumentation and science missions. The NASA Science Mission Directorate's most recent Science Plan (2010) and the Astrophysics Decadal Survey (2010) highlighted the importance of Balloon- and Explorer-class programs for astrophysics. Of necessity, this requires that current and new technologies for accomplishing the goals of the astrophysics community become more compact, low mass and low cost while maintaining high reliability and facilitating high-performance science. One such potential technology is a stabilized dispersive focal plane system (SDFPS) that allows a wide-field spectroscopic survey to be accomplished while simultaneously stabilizing the image field with only a single detector. This cost-effective technology would have a tremendous impact on future dark energy, low- and high-z quasar, large-scale structure and brown dwarf surveys, just to name a few.

Approach — A component of establishing astrophysics as an area of focus at SwRI is bringing the SDFPS technology to a high technical readiness level (TRL). The method for raising this technology to a TRL 6/7 is: defining the interface between the application-specific integrated circuit and the control electronics, building a prototype SDFPS, testing the system with a representative light source in a relevant environment thus raising the technology to TRL 6, and investigating balloon demonstration opportunities that would allow the technology to be raised to TRL 7.

Accomplishments — All interfaces between the application-specific integrated circuit and the control electronics have been defined and connected. A prototype SDFPS was built and run in both direct and dispersed modes with a jitter source moving the beam every two seconds. In both the direct and dispersed modes the SDFPS stabilized the beam. The basic concept of operation was been demonstrated. Balloon flights are being investigated.

Risk Mitigation of the SIDECAR™ ASIC System Interface in Focal Plane Array
Space Science Instruments, 15-R8160

Principal Investigators
Yvette D. Tyler
Mark A. Johnson

Inclusive Dates: 07/12/10 – 11/12/10

Background — The SIDECAR™ (System Image, Digitizing, Enhancing, Controlling and Retrieving) ASIC (application-specific integrated circuit) device is a compact, low-power solution for focal plane array applications. The interface to the SIDECAR™ ASIC represents a current general design challenge for space system electronics, which is handling an increase in performance while reducing power and maintaining reliability. The current system electronic design architecture cannot handle the maximum data output from the SIDECAR™ ASIC and will lead to data loss.

Approach — The main purpose of this project is to improve the design architecture of SwRI space system electronics. A trade study was initiated to evaluate possible solutions to accommodate the demanding performance requirements of the SIDECAR ASIC. Key parameters within the trade study were performance (power, speed and complexity) and expandability, as well as radiation hardness. The results of the trade study showed that two field programmable gate arrays (FPGA) technologies were capable of meeting the basic interface needs of the SIDECAR ASIC and were selected for further evaluation. FPGA code was developed and implemented in the two selected FPGA devices, and the board design architecture was developed for both devices.

Accomplishments — The first FPGA evaluated has lower power consumption and requires fewer components, which generates lower board power consumption. However, the first FPGA barely meets the speed requirements, with only 12 percent of the available logic used. The second FPGA evaluated meets the speed requirement with adequate margin while using 9 percent of the available logic. The second FPGA consumes more power and requires more components so the overall board power consumption is higher. The estimated power difference between the two board designs is approximately 700mW. The FPGA and the voltage regulator supplying the FPGA core voltage account for the majority of the power difference. The second FPGA was chosen for the prototype board because it meets the performance requirements of the SIDECAR™ ASIC and has more capabilities for further design development. The prototype board was built and tested for use in a proposal demonstration. The prototype board will continue to be used for further familiarization with the SIDECAR™ ASIC interface and to provide a platform for improvement of the overall performance of the system electronics.

2011 IR&D Annual Report

Automated Granulometric Analysis of High Spatial Resolution Images for Application to *In Situ* Martian Sedimentology Studies, 15-R8191

Principal Investigator
Victoria E. Hamilton

Inclusive Dates: 10/18/10 – 02/18/11

Background — Sediments form by the mechanical and/or chemical breakdown of their parent rocks. Physical properties of sediments, such as their particle size distribution and particle morphology, are indicators of mineral composition, distance transported and depositional environment. A geologist can make the observations needed to determine the above characteristics by simple visual inspection of sediments (or sedimentary rocks) in the field, but this is clearly not possible on Mars or other planetary surfaces. An Earth-bound geologist must rely on photographic images of the sediments and rocks to determine particle size and distribution (granulometry) characteristics. Published granulometric analysis of Martian sediments using images acquired by the Mars Exploration Rovers (MER) *Spirit* and *Opportunity* have relied on painstaking manual analysis of a very small subset of all available data. The primary objective of this effort was to test whether commercial, automated particle-counting software (designed for mining applications) may enable more rapid, comprehensive and quantitative analyses of granulometry from images. If so, such software could allow the analysis of a larger fraction of all data, leading to better statistics, and thus better constraints on the processes that produce and modify sediments. The immediate application is to granulometric studies of Mars during the upcoming NASA Mars Science Laboratory (MSL) mission, which has multiple cameras designed to image the surface of Mars at spatial resolutions down to ˜20-30 μm.

Approach — SwRI researchers conducted lab work to produce and image control samples as well as field work to collect images of natural sedimentary materials under a variety of illumination conditions and from a variety of natural geologic settings. Researchers also selected images of Martian sediments from recent rover missions for re-analysis. A subset of these lab, field and Mars images was subsequently processed using an automated image processing software package to determine how well particle shape and particle size distributions can be retrieved, depending on the amount of user intervention and the image quality.

Accomplishments — The following goals were accomplished:

- Collected a high-resolution data set of sediments from different geologic environments under varying observation conditions.
- Demonstrated the use of automated granulometry software.
- Determined optimal observations for automated analysis.
- Demonstrated automated analysis on images of Martian sediments.

Despite finding that automated analyses needed a greater amount of user intervention than initially estimated (largely due to user inexperience), it was found that the amount of time required to analyze an image could be decreased by up to 50 percent over manual methods, enabling a doubling of productivity and data analyzed. The influence of image processing on results was not investigated, but based on the results, some image processing (e.g., reduction of contrast, image filtering) could lead to additional increases in efficiency of the automated particle analysis process.

Developing a Foil Mask for the Janus XCAT Instrument Entrance Aperture, 15-R8198

Principal Investigators
Kelly Smith
John Roberts

Inclusive Dates: 11/15/10 – 03/15/11

Background — A spaceborne X-ray coded aperture (XCAT) instrument is being proposed as a complement to the Joint Astrophysical Nascent Universe Satellite (JANUS) instrument suite. The mission of XCAT is to detect gamma ray bursts (GRBs) and provide the necessary pointing information to the spacecraft to train the observatory's infrared telescope in the same direction for more detailed observations. An integral component of the XCAT instrument is the entrance aperture mask. Typically, these masks are constructed of very thin foils with significant flatness requirements. The foils are of a porous design that uses a random grid pattern to achieve the required transmissibility. SwRI is proposing the JANUS mission to the NASA Explorer Program Announcement of Opportunity (AO), announced November 1, 2010.

This project proposes to test the ability of the foil to withstand launch acoustic loads. Several candidate foil mask designs and configuration permutations were tested. With the completion of the acoustic testing, resources allowed additional thermal and random vibration testing to further characterize the foils in the expected launch and space environments.

Approach —

- Test masks were mounted into frames as would be expected in a flight design. Two frame styles were considered for this study. One design included interior pane support ribs, while the second frame style omitted the interior pane support ribs, which would be preferable from a science viewpoint, and was thought to be the worst-case mask support condition.
- A test enclosure was design and fabricated to provide a cavity similar in volume to the expected flight design (see Figure 1). While the volume was flight-like, the wall thickness of the enclosure was significantly thicker than the expected flight design. This was deemed necessary because of the lack of actual flight design details and a desire to minimize the variables affecting the mask response. The assembly included a back panel and mounting provisions for attaching of the test article to the acoustic chamber as well as the vibration facility.

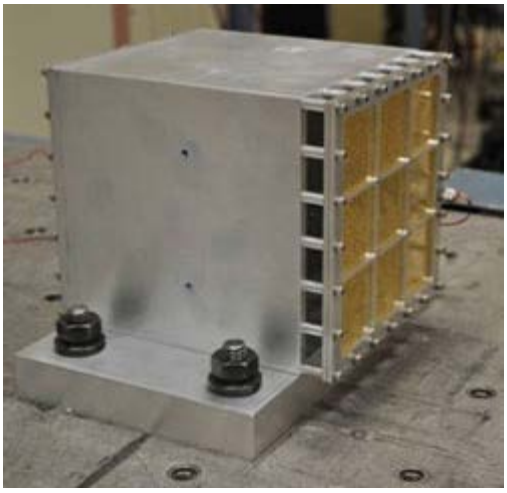

Figure 1. Test Assembly (shown mounted on vibration table).

- Another fixture was developed to use in random vibration testing of the test articles.
- Finite element modal analyses were performed to determine the response of the enclosure to the environmental testing and to ensure coupling would not occur between the enclosure and the mask.

Accomplishments — Several candidate foil mask designs and configuration permutations were tested to determine their ability to withstand launch and orbit environments. Multiple mask variants were tested with positive results in all cases. Even post-structural damage caused by a handling mishap proved to not lead to acoustic failure. The proposed JANUS coded aperture mask design appears to be quite tolerant of Taurus level acoustic loading. This is likely because of the perforated nature of the mask.

Thermal testing was conducted on a sample mask. While not suffering a catastrophic failure, the masks did exhibit unacceptable behavior in the thermal testing. Permanent deformation occurred in the foil section of the mask. It should be noted that the thermal test was very much an extreme temperature excursion test that was not necessarily indicative of the actual expected performance on orbit. Further thermal environment definition will likely also indicate a much smaller temperature range will reduce the thermally induced strain on the mask.

The mask was exposed to standard launch vehicle random vibration as well. The result of this test was structural failure prior to reaching the two minute planned test time. Additional work on better characterizing the vibration and thermal environments, along with actual flight foil assembly design, will be required to demonstrate survivability for these types of loads. Some limited characterization of the masks was conducted using a laser velocimeter while exposing the mask to low-level vibration. This data could be used in further development efforts of a flight mask support design.

As to the original intent of this project, the screens have been shown to be capable of surviving exposure to the expected acoustic environment. Additional work on better characterizing the vibration and thermal environments, along with actual flight foil assembly design, will be required to demonstrate survivability for these types of loads.

2011 IR&D Annual Report

Leadership and Capability Development in Suborbital Space Research, 15-R8207

Principal Investigators
Glenn T. Laurent
Donald M. Hassler

Inclusive Dates: 01/01/10 – Current

Background — The Rapid Acquisition Imaging Spectrograph Experiment (RAISE) sounding rocket payload is an extremely high-speed scanning-slit imaging spectrograph designed to observe the dynamics and heating of the solar chromosphere and corona on time scales as short as 100 ms, with 1 arcsec spatial resolution and a velocity sensitivity of 1 to 2 km/s. The maiden flight of RAISE (Flight 36.219 US) was launched August 23, 2010, with all subsystems working properly, but suffered from an alignment shift at launch that resulted in missing the targeted active region and pointing off-limb by several arcminutes.

Approach — The primary objectives of this project are to:

Identify and correct the causes of alignment and/or focus failures associated with the maiden flight of the RAISE sounding rocket.

Once the issues associated with the alignment/focus failures have been identified, use this knowledge to correct the problem to have a successful re-flight.

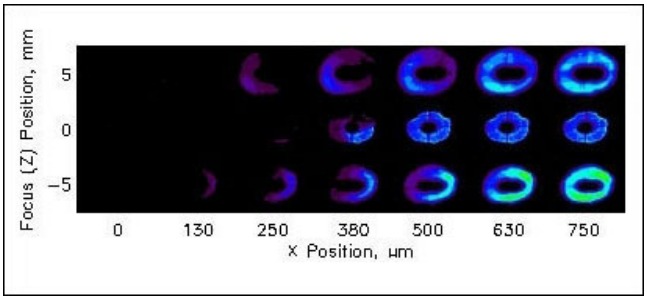

Figure 1. An image from the RAISE spectrograph.

Analyze the data and publish the scientific results from this second flight to be in a good position to win future sounding rocket programs and other instrument development program funding.

Secondary objectives include developing leadership experience and visibility of an SwRI staff member as a viable principal investigator, with publishable data and a success record leading to future rocket program funding and science opportunities.

Accomplishments — Considerable progress had been made during the initial nine months of funding. All calibration equipment (UV vacuum collimator, Zybian camera) needed for final alignment and focus verification has been fully tested and calibrated. Final testing of replacement flight vacuum skins and a flight chromospheric slit-jaw camera (prior to delivery) is under way.

Alignment Shift Identification – Post-flight alignment tests of the RAISE payload have revealed a significant alignment shift of the nominal primary mirror position relative to the SPARCS LISS sensor, causing the telescope pointing to be shifted off of the solar limb.

Flight Skin Design – New flight vacuum skins have been manufactured with removable vacuum doors for each of the flight optical hardware components (primary mirror, grating, detectors) to facilitate adjustments during the alignment procedure.

Zybian Camera – A Zybian (low-light) optical camera has been procured for calibrating the RAISE payload. The camera will be temporarily mounted on the RAISE optical payload to monitor the slit plane focus in real time during optical alignment.

Chromospheric Slit-Jaw Camera – A replacement chromospheric slit jaw camera has been designed and

ordered for the purposes of risk mitigation of future misalignments in flight.

UV Vacuum Collimator – Development of a UV vacuum collimator is nearing completion for use at SwRI's facility in Boulder, Colo., for end-to-end alignment and focus checks of the RAISE instrument. The vacuum collimator has been autocollimated in air using a knife-edge technique, with the Zybian camera monitoring the out-of-focus spot.

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Lighter than Air Vehicle Gas Leak Rate Measurement, 15-R8212

Principal Investigator
James Noll

Inclusive Dates: 03/11/11 – 07/11/11

Background — Stratospheric airship development efforts under SwRI's HiSentinel program have yielded a recent flight of a quarter-million cubic foot displacement vehicle to an altitude of more than 60,000 feet. The airship hull structural integrity was maintained throughout ascent and during float. Prior to flight, the hull underwent leakage rate testing over multiple days. It was instrumented and inflated to a differential pressure of several inches of water while stationed at ground level. The rate measured during this testing predicted the inflation gas leakage observed during flight. Improvement in the flight duration of subsequent similar lighter-than-air platforms will be realized by reducing the overall leakage rate of the airship hull and requires corresponding improvement of the leak qualification testing itself.

Approach — State-of-the-art sensor technology and leak-assessment methodology have been researched to understand the best approach to quickly and inexpensively quantify the leaks in an airship hull. The completed research investigated a modified pressure decay leak testing methodology for determining overall leakage rate in a large inflatable structure. This methodology was tested via a prototype instrumentation system. The system was calibrated against a fixed volume test article with known leak rates and was used to test an inflatable structure.

Accomplishments — The research has produced specifics on the sensor precision, sensor configuration and test duration required to quantify small leakage rates with a high degree of confidence. The methodology developed during this effort will make future testing more accurate and cost-efficient.

2011 IR&D Annual Report

Development of a Comprehensive Two-Dimensional Gas Chromatography and Mass Spectrometry Research Thrust at SwRI, 15-R8223

Principal Investigators
Mark Libardoni
Kristin Favela

Inclusive Dates: 04/06/11 – Current

Background — Volatile and semi-volatile organic compounds are some of the most widely studied samples. Traditional analytical methods rely on single dimension gas chromatography (GC) coupled to selective detectors or mass selective detectors (MS). More recently, the use of comprehensive two-dimensional gas chromatography (GCxGC) as an advanced analytical tool has gained significant popularity for complex sample analysis, target species in a heavy matrix, and screening of difficult samples compounds below traditionally reported LODs. Recent advances to GCxGC instrumentation have made this technique more robust to routine analysis, complex sample screening and the simultaneous quantitative detection of compounds found within. This multi-year project will introduce GCxGC to SwRI and explore the opportunities that make it a viable analytical tool for advanced analysis of complex mixtures, trace level detection of target compounds and future hardware development for space applications.

Approach — The development of a GCxGC thrust at SwRI is divided into two sub-projects. The first is establishing GCxGC as a routine analytical tool, thus increasing the outreach exposure and analytical capabilities of the Institute to provide advanced separation techniques to current and future clients. Application avenues in the field of metabolomics (small molecule metabolites for healthy and diseased states) as well as environmental screening are being investigated and pursued. The second sub-project involves developing advanced GCxGC methodology and space flight hardware. Sample inlet systems, thermal and valve-based modulator development to support portable and flight-ready GCxGC systems as well as advanced detectors are being investigated.

Accomplishments — Researchers successfully demonstrated the use of GCxGC in metabolomic and environmental samples. A GCxGC developmental laboratory has been established where students and scientists are working on advanced methodology and hardware support projects. Both efforts have let to establishing contacts with clients, resulting in collaborative projects.

Measuring Ultraviolet Sensitivity of New Detectors: Capability Development for the NASA Planetary Instrument Definition and Development Program, 15-R8234

Principal Investigators
Michael W. Davis
Thomas G. Greathouse
Kurt D. Retherford
Gregory S. Winters

Inclusive Dates: 06/27/11 – 10/27/11

Background — SwRI has a nearly 20-year history of building ultraviolet spectrographs for NASA sounding rocket and satellite payloads. Every one of these successful instruments contained a core detector consisting of a microchannel plate (MCP) stack operated at high voltages of 4,000 to 5,000 V. The dependence on high voltages means building a custom high-voltage power supply for each instrument, adding undesirable mass, cost and complexity to the design.

A leading manufacturer of astronomical sensors is developing CMOS detectors that are sensitive down to EUV wavelengths without the use of an MCP or high voltage. Their detectors, while still in the prototype stage, have greater than 40 percent sensitivity to light at wavelengths as short as 200 nm. However, this manufacturer lacks the test capability to measure the sensitivity of these CMOS detectors at shorter wavelengths (100 to 200 nm) of high scientific interest to our UV group.

Approach — The main objective of this experiment was to verify the vacuum ultraviolet sensitivity of the silicon detectors. This measurement was made by directing a known intensity of ultraviolet light at discrete wavelengths onto the test detectors and reading out the resulting photocurrent. The sensitivity of the detector to light of the given wavelength was then calculated from the intensity and wavelength of the input light and the active area of the test detector.

Accomplishments — SwRI demonstrated that the detectors are sensitive to UV light at levels ranging from 9 to 22 percent at 1216 Â to 20 to 40 percent at 1600 Â. These detectors meet the initial criteria of 10 percent sensitivity in the vacuum UV for their use in future spaceflight instrument concepts. Indeed, approximately 40 percent sensitivity at 1600 Â greatly exceeded expectations for the potential suitability of these devices for SwRI UV studies. Further development and UV-optimization of these devices are warranted.

2011 IR&D Annual Report

Stabilized Dispersive Focal Plane System, 15-R8236

Principal Investigators
Peter W. A. Roming
Robert A. Klar
John M. Roberts
Randall J. Rose

Inclusive Dates: 07/01/11 – Current

Background — As the cost of space missions continues to rise, the demand for compact, low-mass, low-cost technologies that maintain high reliability and facilitate high-performance science is increasing. One such technology being investigated at SwRI is a novel approach to provide image stabilization, spectroscopic, and direct-imaging functionality using only a single optical path and detector. Typical systems require multiple expensive optical trains and detectors, often at the expense of performance. SwRI's approach, known as the Stabilized Dispersive Focal Plane System (SDFPS), is ideal for performing wide-field, low-resolution, space-based spectroscopic and direct-imaging science surveys. SwRI's low-mass, low-volume, cost-effective design has enormous potential for impacting future large area space-based science surveys.

In a previous effort, the SDFPS concept was integrated into the necessary hardware and facility infrastructure, algorithms and software for image stabilization were developed, and the system was tested in simplified dispersed and direct-imaging modes. Although the overall concept was validated, this early version of the SDFPS only demonstrated the basic idea. Its technical readiness level (TRL) is not suitable for proposing as a low-risk technology. In this current effort, the focus is on the remaining development necessary to bring the SDFPS to a low-risk TRL focus on increasing the detector data transfer rate sufficient for use in the stabilization algorithms, and creating a mechanism to switch the optical path between spectroscopic and direct imaging (i.e.: a rotating prism mechanism).

Approach — The objective of this investigation is to build and ground test a prototype SDFPS that will concurrently eliminate unwanted image blurring caused by the lack of adequate platform stability, while producing science images in both spectroscopic and direct-imaging modes. The overall approach is to develop the rotating prism mechanism and new science image data handling software, and then retrofit them into the SDFPS. The system will be tested and verified in an Institute Image Stabilization Lab. Demonstrating the prototype SDFPS in the lab will raise the entire system's TRL to a level sufficient to enable flying the system on a suborbital balloon.

Accomplishments — All software and hardware requirements have been defined. Software and hardware peer reviews have been completed. Software coding has begun including the guide mode assembly to be integrated into the H2RG SIDECAR. Optical and mechanical components are being ordered. Manufacturing of the mechanical components will now commence.

Polar Regolith Environment Molecular Impact Simulation Experiment (PREMISE), 15-R8241

Principal Investigators
Edward L. Patrick
Ben Teolis
Gregory P. Miller
Scott Anderson

Inclusive Dates: 07/01/11 – Current

Background — The need for this project was based upon recent discoveries of volatiles sequestered at and near the lunar poles. If cometary impacts are the source of these sequestered volatiles, what local pressures, exposure times and temperatures are necessary to produce a detectable inventory of compounds detectable by a landed mass spectrometer instrument?

Approach — The main objective of this work is to produce a laboratory simulation of the lunar surface conditions in a chamber containing a sample cup containing a measured quantity of JSC-1A lunar soil simulant. The soil sample cup is cooled to cryogenic temperatures and selected gases leaked into the chamber over a fixed period of time. After the period of time allotted, the cooling will be reversed and the temperature of the soil sample increased to a level above that typical of lunar noon temperatures. A thermogram of the evolving gas will be recorded using a residual gas analyzer and ionization gauge. To characterize the experimental setup, the experiment will first be performed with nitrogen both with and without lunar simulant present, before moving on to the important volatiles, water vapor and carbon dioxide. After the basic volatile gas entrapment experiments are completed, a UV source, ion source and mechanical rod will be used to disturb the gas-laden soil simulant for the purpose of establishing the best combination of soil preparation techniques for the prototype inlet of a landed mass spectrometer. An existing cryotrap inlet system (CIS) will be used as a means to collect and store volatiles evolved by the three above-described methods for probing the lunar soil.

Accomplishments — To date, a prototype soil sample chamber has been designed and assembled. A solid copper soil sample cup has also been designed and fabricated and is awaiting assembly after fitting with thermocouples and temperature loggers has been completed.

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2011 IR&D Annual Report

Design and Fabrication of Multi-Component Scaffolds for Bone Tissue Engineering, 01-R8078

Principal Investigators
XingGuo Cheng
Gianny Rossini

Inclusive Dates: 07/07/09 – 01/07/11

Background — The ideal bone scaffold should have a modulus match to that of bone, while also biodegradable, tough, cheap, easily processable and biocompatible. Moreover, the scaffold itself should be able to stimulate bone-like tissue growth and accommodate intrinsic or external osteo-inductive factors. In light of these requirements and challenges to repair and regenerate bone defect, this research project aims to develop Mg alloy-based scaffolds to stimulate bone growth.

Approach — To develop an ideal bone scaffold, SwRI researchers have developed a three-dimensionally coated, cylindrical, wrapped Mg alloy scaffold with interlayer spaces and lumen (Fig. 1a); *in-vitro* biocompatiblity testing methods using mesenchymal stem cells (MSCs, Fig. 1b) and *in-vitro* corrosion testing (electrochemical corrosion, mass, pH, etc.); and *in-vivo* testing methods using both rat and rabbit models. X-ray radiographs and micro-CT imaging, blood CPK measurement, SEM/EDX analysis and biomechanical testing have been used to characterize the implantation outcome.

Accomplishments — Without any external osteoinductive factors (BMP2, thrombin peptide TP508, gene transfer of BMP-6, platelet-rich plasma, stem cells and anabolic drugs), SwRI's Mg alloy scaffolds resulted in partial-to-full regeneration of rabbit critical-size ulna defects within 12 weeks. The statistical analysis showed that, on average, the intact ulnae and the implant-treated ulnae exhibited a similar biomechanical performance in one group. Radiograph (Fig. 1c-d), SEM/EDX and Micro-CT analysis (Fig. 1e) indicated that bone-like tissue grows inside and outside the scaffold. This study suggests the SwRI-designed and fabricated Mg alloy scaffold is promising for bone regeneration.

Figure 1. (a) 3D coated biocompatible Mg alloy scaffold (3.5 mm diameter x 15 mm length); (b) Image of live MSCs on coated Mg alloy; (c-d) Mg alloy scaffold implantation resulted in repair of a critical sized ulna

defect; (e) Micro-CT image of radio-dense bone-like tissue (red arrow) in and surrounding Mg alloy scaffold.

2011 IR&D Annual Report

Development and Characterization of a Novel Ceramic Membrane for CO_2 Separation in Coal-Fired Power Plants and Energy Industries, 01-R8148

Principal Investigators
Francis Y. Huang
Vladimir Gorokhovsky

Inclusive Dates: 04/01/10 – Current

Background — Carbon dioxide emission from coal-fired power plants constitutes a large portion (~40 percent) of total CO_2 emission to the environment. The cost, or energy penalty, for CO_2 emission prevention (usually called carbon capture and sequestration in the literature) can be up to 50 percent of energy budget of a power plant. The major portion for the penalty for CCS is the energy wasted in cooling the flue gas (typically up to 750 °C) to a low temperature (100 to 300 °C), tolerable to the CO_2 separation system. Considering that using absorbents for CO_2 capture requires sophisticated engineering for the adsorption and regeneration cycles, membrane technology provides an attractive CCS alternative. However, to date no commercially available membrane system exists that can effectively and economically capture CO_2 at high temperature. These facts motivate the present research effort to identify a workable membrane system for CO_2 capture at high temperature. This project is anticipated to deliver an economic solution for the CO_2 separation market to minimize the energy penalty, possibly down to 20 percent to 30 percent of power plant output from the current estimates of 40 percent to 50 percent.

Approach — A novel lithium metal oxide-based CO_2 separation ceramic membrane is proposed. The novel aspects include (1) use of porous ceramic substrate and lithium metal oxide solid sorbents allowing operation in the 500 to 700 °C range, (2) a dual-phase system consisting of a solid framework and molten carbonate outer layers on the sorbents facilitating CO_2 diffusion, (3) a thin, dense, metal oxide interlayer between the sorbent and the substrate forming a barrier to prevent any other gases except CO_2 from transporting through the membrane, and (4) a ceramic inert metal oxide layer deposited on the dual phase lithium metal oxide sorbent framework improving the mechanical strength of the membrane. This novel membrane is fabricated by spray- and plasma-deposition methods, as illustrated in Figure 1. With an integrated approach of identifying new materials, economic production methodologies, engineering process, and performance evaluation of the membrane system, the project is anticipated to deliver a radically improved solution for CO_2 separation from flue gas at existing coal-fired power plants and the new Integrated Gasification Combined Cycle (IGCC) power plants. The project will also develop testing methodologies to prove the function of the candidate membranes.

Accomplishments — In the first two quarters of the project, the synthesis and characterization of the novel metal oxide sorbent have been completed. The efforts in the next two quarters will focus on deposition methodologies and testing the fabricated membrane. An intellectual property filing, "Composition and Fabrication Process for High Temperature CO_2 Separation Ceramic Membrane," was submitted May 18, 2010.

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2011 IR&D Annual Report

Post-Implantation Analysis of 3D Mg Alloy Scaffolds, 01-R8211

Principal Investigators
XingGuo Cheng
Todd Bredbenner

Inclusive Dates: 03/01/09 – 07/01/11

Background — In response to the clinical need for synthetic scaffolds for bone repair and regeneration, SwRI has recently completed an internal research project to develop multifunctional Mg alloy scaffolds for bone repair and regeneration. Two types of coated, three-dimensional, wrapped cylindrical AZ31 Mg alloy scaffolds were evaluated in a critical size rabbit ulna defect model. X-ray radiograph, gross examination and biomechanical testing indicated that significant radio-dense material formed at the bone defect site, resulting in partial to full biomechanical restoration. The objective of this project is to further investigate the bone repair and regeneration capabilities of the SwRI-designed Mg alloy scaffold.

Approach — To investigate the bone regeneration capabilities, four major tasks have been proposed: 1) ESEM-EDX analysis and mapping of Mg alloy implanted ulna defect, 2) Histology analysis, 3) Image analysis of micro-CT data, and 4) Blood c reactive protein analysis of rabbit serum after implantation by using an enzyme-linked immunosorbent assay (ELISA).

Accomplishments — SEM-EDX analysis of the Mg alloy implant surface indicated that a highly mineralized bone-like organic-inorganic matrix was formed on the surface. EDX mapping indicates close integration of the Mg alloy degradation product with the bone-like tissue. Methods were successfully developed and implemented to analyze the spatial distribution of tissue surrounding Mg AZ31 scaffolds in a rabbit ulna defect model. Two-dimensional analyses of tissue adjacent to scaffolds were quantified, and variation in the three-dimensional structure of the tissue density distributions was qualitatively demonstrated between the scaffold groups. The CRP protein level after implantation was less than 100 fold, indicating there is no acute-phase inflammatory response of biocompatible Mg alloy implants. This study confirms the formation of new bone-like matrix due to Mg alloy, suggesting the SwRI-designed Mg alloy bioactive scaffold is promising for bone repair.

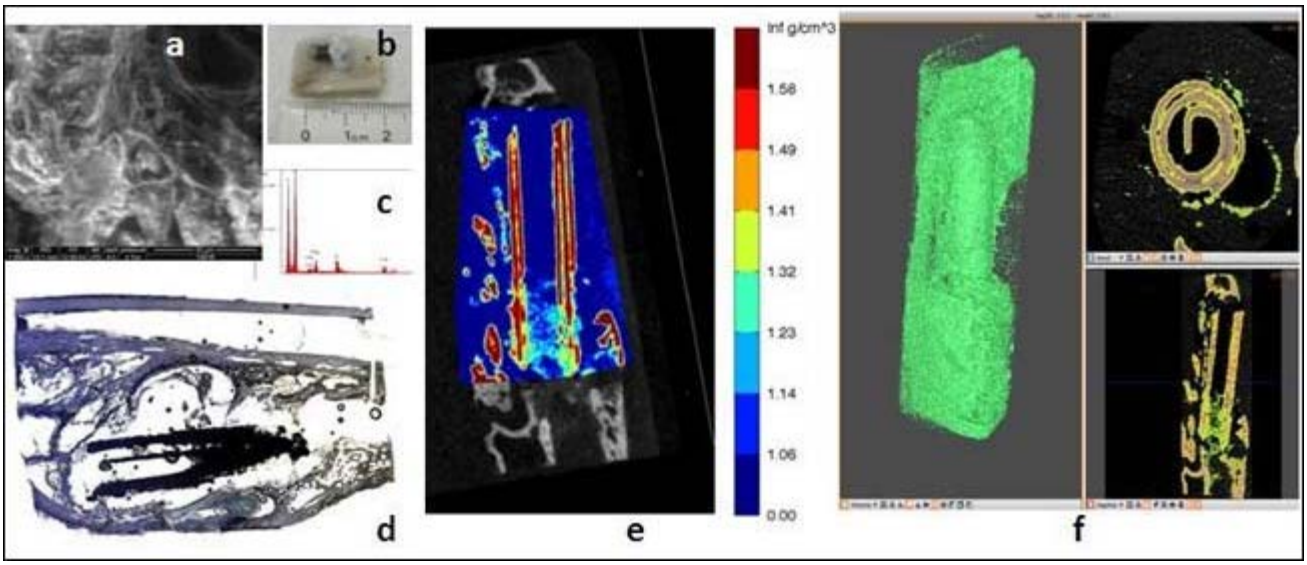

Figure 1. (a) SEM image; (b) Optical image of implant; (c) EDX spectrum indicates formation of bone-like matrix; (d) Histology indicates collagen deposition; e) 2D tissue distribution; f) 3D tissue distribution of radio-dense bone-like tissue in and surrounding Mg alloy scaffold.

2011 IR&D Annual Report

Design, Modeling and Fabrication of Metamaterials, 14-R8008

Principal Investigators
A. Leigh Griffith
Diana L. Strickland
Michael A. Miller
Jeremy R. Pruitt

Inclusive Dates: 12/03/08 – Current

Background — Metamaterials are engineered structures consisting of the arrangement of artificial elements of different materials (usually metallic and dielectric) designed to exhibit specific and often unusual properties not found in natural materials when they interact with electromagnetic (EM) fields. The artificial elements consist of inclusions (structures much smaller than a wavelength) placed within a host background (e.g., polymer, ceramic or air). The EM properties of metamaterials are controlled by the spatial arrangement and shape of the inclusions, and by the selection of materials of which the host and inclusions are composed. Surface plasmons (SPs), which may also be known as surface plasmon polaritons, are intense surface-bound EM waves that propagate in a direction parallel to a metal/dielectric interface. They are often elicited in these structures and are key to the unusual properties exhibited by certain types of metamaterials.

Metamaterials have emerged recently as a subject of intense research by the physics, chemistry and materials science communities because they promise to become the building blocks for novel device applications, such as optical components not limited by diffraction, future-generation microprocessors based on the propagation of light or surface plasmons (instead of current), small radio-frequency antennas, high-sensitivity chemical sensors and optical cloaking, among many others. In this project, SwRI is developing theory, modeling tools and fabrication processes to explore high-consequence applications of metamaterials in two areas of interest: small, high-performance radio-frequency antennas and surface plasmon generation in structures to mediate chemical interactions for catalysis and for chemical sensing.

SwRI is employing metamaterials to reduce the size of electrically small antennas while maintaining an impedance match to their power source. Additionally, metamaterial surfaces or "metasurfaces" are being used to improve the performance of antennas by reducing lossy surface waves and also to improve gain, directivity and element isolation in arrays.

SwRI's interests are further directed toward the fundamental question of whether surface plasmons can be elicited from metamaterials at infrared (IR) frequencies to effect the binding, repulsion or chemical transformation of adsorbed molecules when the frequency of the surface plasmon is matched to molecular vibrations (i.e., resonance conditions).

Approach — A novel, electrically small patch antenna incorporating metamaterials as the key component was selected from the literature for the feasibility study. The goal was to determine whether metamaterials improve electrically small antennas and whether they are practical to implement. SwRI designed, built and tested this metamaterial antenna at several frequencies and compared its antennas to conventional, electrically small antennas. Additionally, we tested the effects of various metamaterial surfaces to improve antenna performance using a broadband simulation test bed.

In an effort to understand the fundamental requirements and potential limitations of mediating the outcome of surface-plasmon-molecule interactions, quantum mechanical and classical computational techniques

were applied to study the resonant coupling between low-frequency SPs evinced from nano-scale artificial elements of metasurfaces and the vibrational harmonics of simple molecules. Experimental validation of plasmon-mediated chemical binding and catalysis effects was accomplished by establishing a framework for modeling the electromagnetic scattering properties of two- and three-dimensional periodic structures and exploring suitable techniques for fabricating the structures. A laser-induced, thermal desorption, mass spectrometry (LTDMS) technique was then refined to enable measurement of the interaction energies between these metasurfaces and small molecules (e.g., H_2, CO) adsorbed on them.

Accomplishments — SwRI researchers found that antenna resonance can be tuned independently of antenna dimensions. Excellent impedance match was achieved for antennas as small as a 30th of a wavelength (λ/30). The types of metamaterials used to load the antenna included spiral ring resonators printed on circuit board, an array of barium strontium titanate cubes, and Sievenpiper (or mushroom-shaped) structures on printed circuit board. The SwRI team is one of the first to report results for this innovative antenna.

SwRI researchers were also able to reduce the mutual coupling between antenna array elements and improve the gain and bandwidth of individual antennas through the use of metasurfaces. These metasurfaces were printed on the same substrate as the antenna. This can be done on the same layer as the antenna itself, or on an inner layer of the substrate, depending on the desired results and end application.

In the plasmonics research, SwRI demonstrated via systematic computations that free-standing (three-dimensional) wire grids of cubic symmetry can be tailored to evince surface plasmons with infrared frequencies. It was further shown that the oscillating EM field of these plasmons may directly couple with the ground-state fundamental vibrations of adsorbed molecules. However, fabrication of these structures via advanced techniques such as proximity nano-patterning and optical phase-mask lithography was found to be exceedingly difficult and not commercially practical. In its place, two-dimensional devices consisting of simple, pad-like periodic structures surrounded by nanowires, as well as three-dimensional "log pile" devices, were designed to evince SP modes in the infrared near 60 THz. Under a Cooperative Research and Development Agreement with Sandia National Laboratories, Albuquerque, NM, these devices were successfully fabricated and are currently being evaluated using the LTDMS technique to measure the coupling strength between SPs and adsorbed molecules, such as carbon monoxide. If strong enough, this coupling may be exploited to control the structure of surface matter at the nano-scale, opening the door to important opportunities in nano-engineered devices for photocatalysis, quantum control of structure, optical sensors and, possibly, molecular levitation.

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2011 IR&D Annual Report

Plasma Processing of Micro-Screen Supported Ultra-Thin Carbon, Ceramic and Metal Foils for High Energy Particle Detection and Beyond, 15-R8190

Principal Investigators
Edward L. Patrick
Greg Miller
Vladimir Gorokhovsky
Tom Booker
Craig Engel
Rick Johnson
Royall Cox

Inclusive Dates: 10/11/10 – 01/11/11

Background — The motivation for this project was based on the use of thin carbon foils as secondary electron emitters (SEE) in the detection of high-energy particles by time-of-flight (TOF) mass spectrometry in high-energy physics and space research. For these applications, carbon foils as thin as 1 nm, or less than 0.1 mg/cm^2, are required. Foils must also be strong enough to sustain mechanical deformation during handling, defects (pinholes) must be low and durability against high energy particles must be considerable. At the same time, the structure and morphology of the ultra-thin foils must provide maximum SEE at the lowest possible energy of detectable particles. Diamond-like carbon (DLC) fulfills this material requirement for particle detection applications. Conventional free standing unsupported carbon foils made by thermal evaporation of carbon and condensation of carbon vapor do not meet these criteria and are extremely difficult to handle during installation. It is well-known that ion bombardment by energetic ions during the deposition process can substantially improve coating structure and morphology, reduce the density of defects, and improve coating mechanical and thermochemical stability.

Approach — Phase I of the effort was to use physical-vapor deposition (PVD) or chemical-vapor deposition (CVD) to fabricate the micro-screen support and carbon foil as an integrated process, to microscopically inspect the foil, and to test its SEE properties for particle TOF instruments. The deposition of carbon on a silicon wafer was followed by the deposition of a nickel layer. Lithography was then used to etch the nickel foil support layer into a microscreen, then separate the foil attached to the reinforcing metal screen that will constitute the final product: microscreen-supported functional thin foils having thicknesses ranging from 2 nm to 10 μm. The microlithography process involves the following steps: spin coating and baking a layer of resist on top of the nickel layer; UV-exposing the resist through a mask to cross-link the resist monomers in the hole areas; using a development chemical to remove the resist from these areas; etching the nickel out of the hole areas; and then stripping the remaining resist from the nickel surface. Finally, the Si substrate is stripped away, leaving the DLC foil on its reinforcing metal screen. This was accomplished by soaking the structure in a silicon etch (which will not attack the nickel or carbon) until the carbon layer is microscopically clear of any residual silicon.

Accomplishments — Microscopic inspection of commercially available carbon foils identified numerous defects and holes that were the impetus for this effort. A prototype "proof-of-principle" fabrication process succeeded in creating an integrated silicon-carbon-nickel wafer coated with a layer of resist. Lithography of the nickel and subsequent stripping of the resist was successful and produced a microscreen in the nickel foil layer. However the attempt to etch the Si substrate from the carbon foil caused curling and warping of the carbon layer even after a number of etchants and conditions were employed. Though this

"no-go" condition terminated the effort, the need for uniform and defect-free carbon foils remains, and an improved etching or deposition process is needed to produce intact carbon foils with microscreen support.

2011 IR&D Annual Report

Development and Validation of a Shock Tube Apparatus for High-Fidelity Blast Wave Generation, 18-R8132

Principal Investigators
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Walt Gray
Thomas Z. Moore
Larry Goland
Trenton Kirchdoerfer

Inclusive Dates: 01/01/10 – Current

Background — SwRI has identified blast and blunt impact trauma as an emerging market opportunity well suited to its impact and blast physics expertise. SwRI's current blast loading method of using high explosives presents limitations in experimental fidelity and repeatability and has been met with skepticism by proposal reviewers in the medical community. Although trauma research using explosives is still being conducted, the shock tube method has become the *de facto* standard. Large shock tube apparatuses are currently under development at other organizations conducting blast trauma research. Without such a device, a gap will soon appear in SwRI's research capabilities that may severely limit its ability to maintain a viable research program in blast trauma. For that reason, SwRI researchers proposed to design and build a high-fidelity shock tube apparatus.

Approach — The goal is to design and develop a shock tube test apparatus with sufficient flexibility to achieve the range of shock pressure conditions required to study a broad spectrum of blast trauma mechanisms. The apparatus will be unique. It will include an adjustable length high-pressure gas reservoir section allowing for independent tailoring of the shock peak pressure and pulse width (impulse) with a single device. In current shock tubes, the peak pressure and impulse are coupled, and tailoring usually requires changing hardware. This approach has not been attempted before and will require a significant research and design effort. The validity of the apparatus for trauma studies will then be demonstrated experimentally.

Figure 1. SwRI-designed shock tube system.

Accomplishments — A new shock tube system has been designed and fabricated, see Figure 1. The system consists of four primary components: an adjustable length high pressure driver section, a dual burst diaphragm section, a modular expansion section and a test section. The driver section consists of a 4.9-inch internal diameter tube rated at 6,000 psi. The adjustable length is achieved by sliding a movable piston in the tube bore to the desired location along the tube's length. This effectively changes the length of the driver section without having to change hardware. The piston location is infinitely adjustable using a

specially designed system. The diaphragm section is a dual diaphragm design allowing for more precise control over shock tube firing and allowing higher driver load pressures to be obtained. The internal diaphragm holder can be quickly accessed by removing a single clamp device and moving the entire driver section away via a roller system. The test section currently consists of a 36-inch diameter, 12-foot long pipe. With the current test section, it is expected that shock pressure up to 20 psi and durations up to 20 milliseconds can be obtained. Much higher shock pressures can be achieved by limiting the diameter of the test section. The modular design of the expansion section will allow for various test sections to be easily installed.

Along with the mechanical design of the system, a complete electronic control system was developed and is currently being installed. The system consists of a control console with various pressure readouts and controls, which actuate the high speed valves used to fill and fire the shock tube.

A Bone Fracture Risk Metric Based on Statistical Shape and Density Modeling (SSDM), 18-R8162

Principal Investigators
Todd L. Bredbenner
Daniel P. Nicolella
Robert L. Mason

Inclusive Dates: 06/29/10 – 04/04/11

Background — The problem of increased risk of skeletal fractures caused by bone mass loss in aging or disease is a major clinical problem leading to estimated health care costs of nearly $17 billion in the United States. Notwithstanding the economic burden, non-vertebral fractures, particularly of the hip, are a significant cause of morbidity and mortality in the aging population. More than 4 percent of hip fracture patients die during the initial hospitalization following fracture, and 24 percent will die within the first year. At present, clinical fracture risk assessment is most often based on areal BMD (aBMD) and accurate identification of at-risk individuals may be compromised because three-dimensional structural factors are not assessed by aBMD. The structural integrity of an individual bone in any mechanical loading environment is dependent on the bone mineral density (BMD) distribution and the macroscopic morphology of the bone, as well as complex and interrelated cortical and trabecular bone characteristics.

Approach — The goal of this research project was to generate the fundamental knowledge required to develop and implement a risk assessment tool that is easily accessible in the clinic. Innovative risk assessment methodology was developed based on statistical shape modeling methods, which have been used to describe variability in the morphology of a population of anatomical structures. Statistical shape models capture the variability of biological structures by projecting a high-dimensional representation of the structure onto a lower dimensional subspace of possible shapes constructed from a population of training shapes. In this study, researchers retrospectively investigated the use of fracture risk classifiers derived using statistical shape and density modeling (SSDM) methods, which describe both the multivariate geometry and BMD distribution variation contained implicitly within 3D imaging data for a set of bones. The performance of SSDM-based fracture classifiers in predicting fracture risk was compared to that of BMD alone.

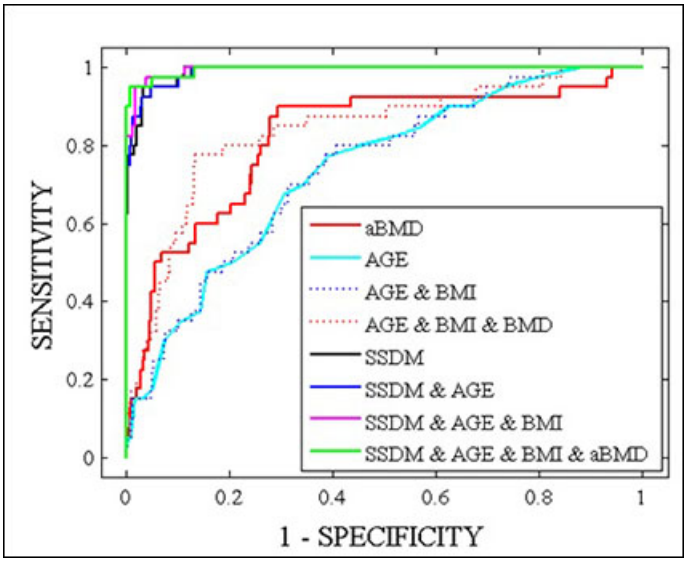

Figure 1. Area under the Receiver Operating Characteristic (ROC) curves demonstrated that fracture classifier reliability increased substantially with the inclusion of SSDM weighting factors over that of individual characteristics alone or of combinations of individual characteristics.

Accomplishments — A new fracture classifier based on statistical shape and density modeling (SSDM) was developed to predict the future risk of bone fracture with significantly greater sensitivity and specificity compared to current clinical fracture risk assessment methods. This new bone fracture risk classification

method will provide the basis for a revolutionary and more reliable clinical and research tool to predict future fracture risk in individuals. In addition, researchers demonstrated that the new method significantly outperforms a competing emerging method, which is based on using finite element models to compute a measure of bone strength in predicting future fracture. Using prospective data from a large National Institutes of Health clinical osteoporosis fracture study, SSDM-based fracture risk classifiers correctly classified 62.5 percent of individuals who would go on to suffer a hip fracture (fracture cases) whereas current density-based clinical methods only identified 7.5 percent of future fracture cases. Additionally, using previously collected cadaver femur data, SwRI researchers demonstrated that statistical shape and density modeling predictions of bone fracture strength are statistically equivalent to current clinical (bone density based) and emerging (finite element modeling based) methods of fracture risk assessment.

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2011 IR&D Annual Report

Dynamic Modeling of Knee Mechanics, 18-R8167

Principal Investigators
Daniel P. Nicolella
W. Loren Francis
Travis Eliason
Baron Bichon

Inclusive Dates: 07/01/11 – Current

Background — Osteoarthritis (OA) is the most common form of arthritis and, as the major cause of activity limitation and physical disability in older people, is a tremendous public health concern. Arthritis causes pain, swelling, and reduced motion in joints caused by the breakdown or degradation of the articular cartilage covering the joint surfaces. While it is generally accepted that differences in knee mechanics or alterations in knee mechanics due to certain risk factors lead to knee OA, the precise dynamic mechanical environment of the knee and its anatomical structures during routine physical movements is largely unknown. Thus, a remaining unmet, technically difficult challenge in musculoskeletal research, and the focus of this project, is determining the detailed dynamic mechanical environment of the healthy knee joint and understanding alterations in knee mechanics caused by injury, aging or disease.

Approach — The primary objectives of this project are:

Develop a dynamic, finite element model of the lower human body driven by neuromuscular control and active contraction of the major muscle groups of the lower body.

Determine the dynamic neuromuscular control parameters for: i) leg extension, ii) standing squat, iii) single gait cycle and simultaneously determine the mechanical environment within the knee.

Determine the changes in knee mechanics resulting from known OA risk factors.

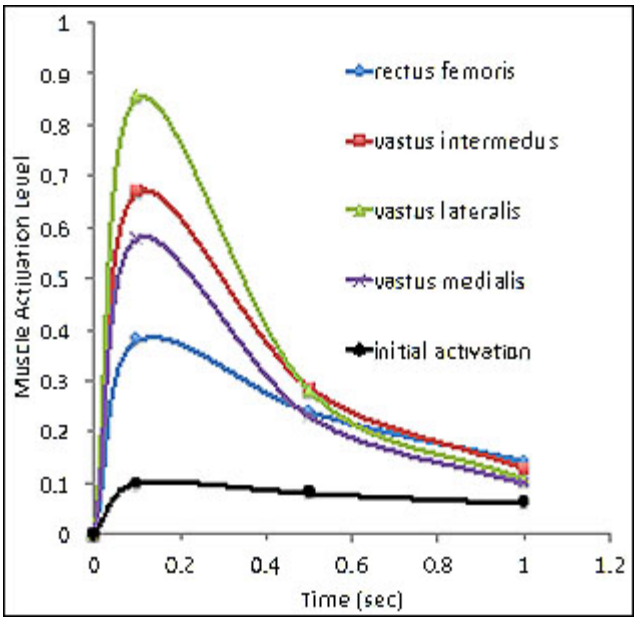

Figure 1. Initial and final muscle activations. The optimally determined muscle activations required to perform a leg extension compared to the initial muscle activations.

Accomplishments — In this project, SwRI researchers have used multibody dynamics, active muscle modeling, and detailed finite element modeling to generate a high fidelity dynamic model of the human lower body. Researchers explicitly modeled the lower limbs (pelvis down to the foot), including a detailed representation of the knee, using finite elements. Motion at the knee joint is controlled explicitly via deformable surface contact at each articular surface (rather than idealized as simple revolute or ball and socket joints). The major muscles activating the lower limb are explicitly modeled using anatomical muscle insertion points and geometric wrapping. The dynamic muscle forces, joint kinematics, contact forces, and detailed (*e.g.*, continuum) stresses and strains within the knee (cartilage, meniscus, ligaments and bone) were simultaneously determined for a neuromuscularly controlled seated leg extension with a weight of 30 pounds added to

the ankle. The simultaneous prediction of multibody dynamics and detailed continuum mechanics of the knee (or any other biological structure) under self-actuation (*e.g.*, muscle activation) has not been previously performed.

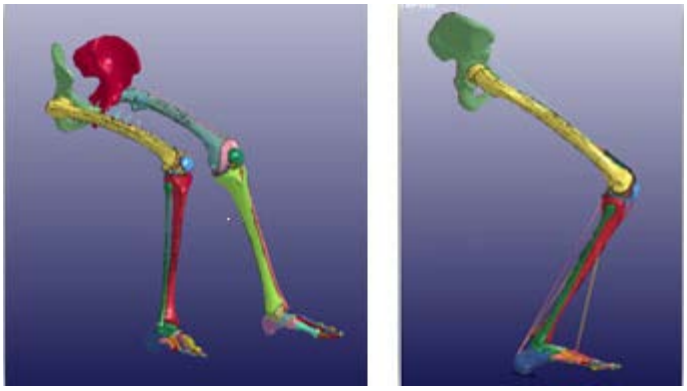

Figure 2. The lower limb dynamic finite element model (left) was used to simulate a standing squat (right). Active time varying muscle forces were applied using a Hill-type muscle model for the quadriceps muscles (vastus lateralis, vastus medialis, rectus femoris, and vastus intermedius), tibialis anterior, gastrocnemius and soleous muscles.

2011 IR&D Annual Report

Improving Model Prediction Accuracy by Reducing Uncertainty in Model Components, 18-R8169

Principal Investigators
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John M. McFarland
Todd L. Bredbenner
Daniel P. Nicolella
Barron J. Bichon
Don Moravits

Inclusive Dates: 07/01/10 – Current

Background — Numerical models such as finite element analysis are routinely used to predict the performance of engineered systems. Government and industry now routinely rely on model predictions to make such decisions as to when to retire system components, how to extend the life of an aging system, or if a new design will be safe or available. The validity of many models used to predict the performance of existing engineered systems has been assessed through historical data, but this type of validation is not possible for new designs or designs used in different environments. The validation of new models using experiments becomes more difficult and costly as the complexity and reliability requirements increase. For example, a highly reliable aircraft engine component is difficult to test to failure under operating conditions due to the high reliability. In addition, it may be cost prohibitive to actually test an expensive component to failure. Other systems are impractical to test such as the *in vivo* measurement of performance measures in human subjects or animals. Valid model predictions become increasingly important as the cost, reliability and experimental complexity of the engineered system increases. Therefore, effective approaches for model validation are needed to assess and improve model predictions. A general and consistent approach for model validation has not been developed for complex problems. Determining the uncertainty on the model predictions is a critical element in the validation process and is a main focus of this research.

Approach — The primary objectives of this program are to:

- Develop model precision methodology for different types of model uncertainties (e.g., model form, limited data) and approaches and methods to compute model component uncertainty and their contribution to the total model uncertainty.
- Demonstrate the methodologies and approaches by developing validated finite element models of mouse ulnae.

Accomplishments — Variance decomposition methods as described by Saltelli, et al., have been implemented, extended and exercised to model different types of uncertainties and identify their importance to the model prediction uncertainty for the model precision methodology. The approaches were evaluated via the reliability analysis for the deflection of a statically indeterminate beam. The example problem illustrates the distinction between aleatory and epistemic uncertainty, as the aleatory distributions for the model inputs are estimated based on limited sample data, which introduces epistemic uncertainty about the distribution parameters such as the means and standard deviations. It is shown that the variance decomposition approach can successfully identify a data-rich input as having a negligible contribution to variance, even though the deterministic model is highly sensitive to that input.

The model precision methodologies and approaches will be demonstrated during the validation of finite

element models of the mouse ulnae. A validated model will be developed for the wild type (WT) mouse to predict strain for an *in vivo* loading protocol. The validated model will be used to predict strains for the BMP2 conditional knockout mouse (cKO), which has different geometry and material properties. The project team has acquired eight wild type and nine cKO mice for the validation experiments. Material testing, validation experiment and boundary condition calibration test protocols are being developed and finalized.

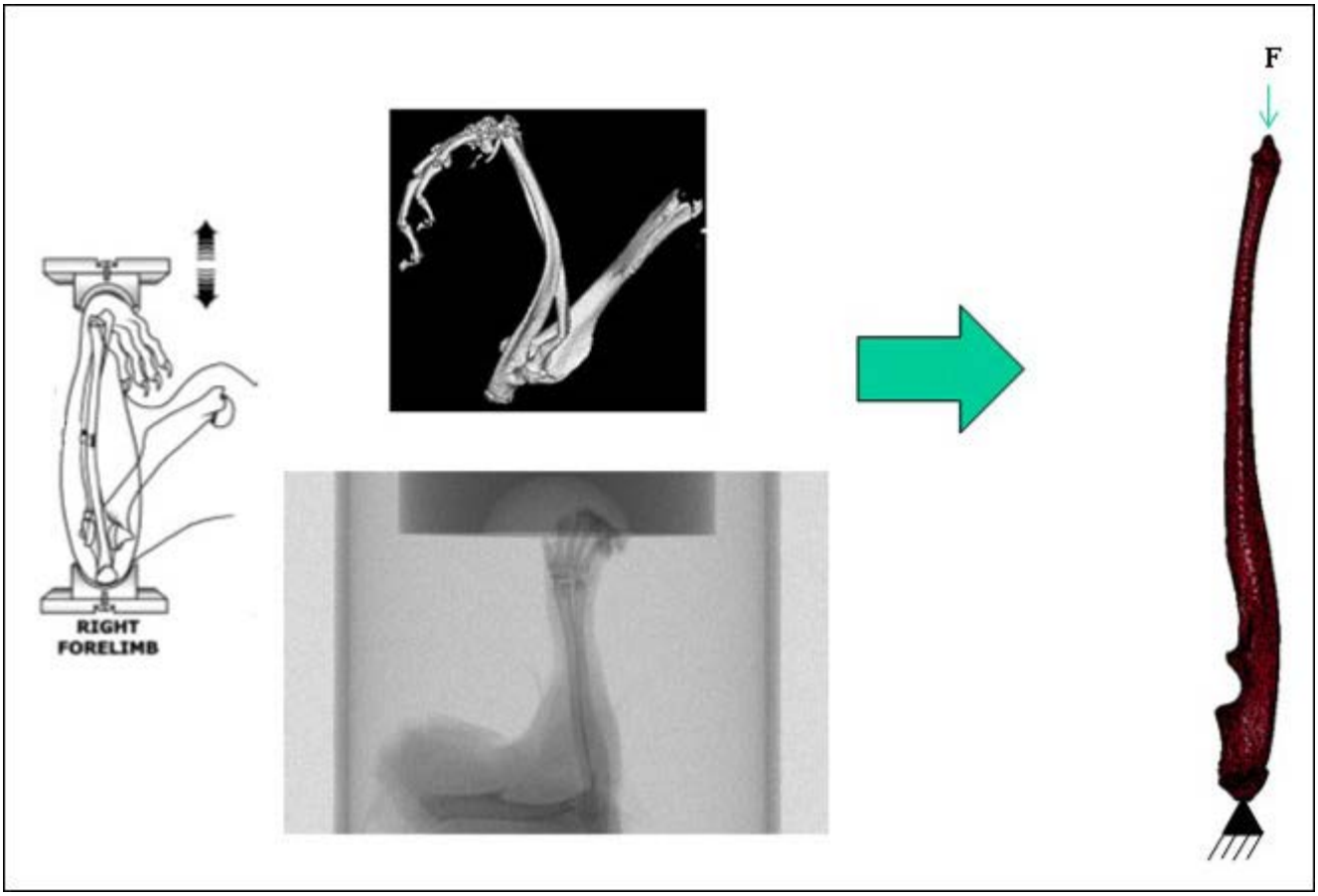

Figure 1. Finite element models will be developed to simulate the Robling-Turner en vivo experiment (left). The validation and calibration experiments are performed in a micro-CT where geometry, displacements, and bone x-ray density can be measured to obtain the calibration and validation data. The protocol includes imaging the mouse arm in the load stage (lower middle), applying a specific load (upper middle), and converting the unloaded and load image to finite element models (right).

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Development of Solution-Based Diamond-Like Carbon Coatings, 18-R8177

Principal Investigators
Vasiliki Z. Poenitzsch
Kent E. Coulter

Inclusive Dates: 07/14/10 – 11/14/10

Background — Because of their excellent mechanical and tribological properties, diamond-like carbon (DLC) coatings are widely used as protective overcoats in various industries ranging from medical to automotive sectors. However, the vacuum deposition processes traditionally used to prepare DLC coatings considerably limit the realization of many applications. The limitations of these common vacuum deposition techniques include (i) high costs, (ii) slow rates of film production, (iii) limited ultimate film thickness, (iv) limited areas based on the size of the reaction chamber, (v) restricted vacuum-compatible substrate choices, and (vi) inability to combine with reinforcing materials. This project investigated an innovative non-vacuum-based process of fabricating DLC coatings that addresses these limitations.

Approach — The primary objective of this research project was to develop an atmospheric solution-based processing technology for fabricating diamond-like carbon (s-DLC) coatings. Another objective was to obtain preliminary data to convince potential clients that such a processing technology is a promising candidate for depositing DLC on components with large dimensions.

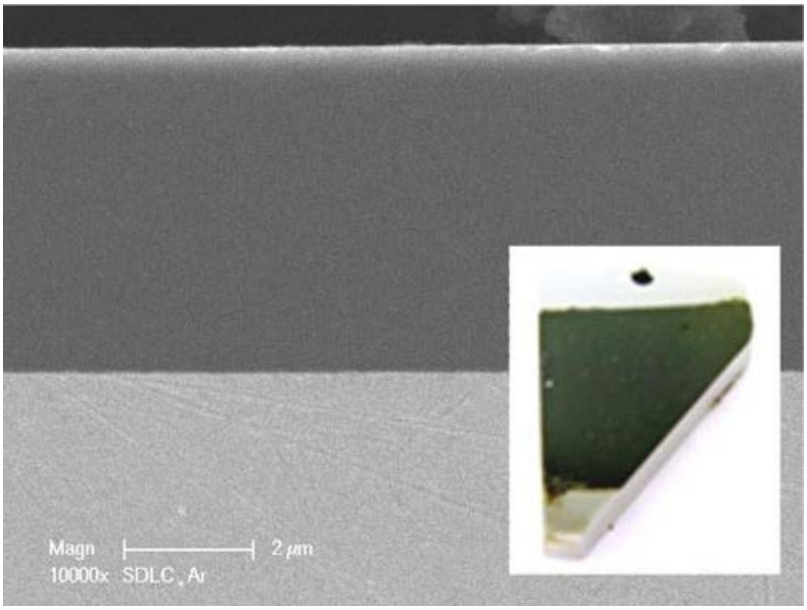

Figure 1. Cross-section SEM image and photograph (inset) of machined edge of sDLC coated steel substrate.

Accomplishments — This project has resulted in the proof-of-concept development of an atmospheric solution-based processing technology for fabricating DLC coatings. This method used chemical synthesis of hydrocarbon polymers possessing diamond-like structure at the atomic level and the subsequent pyrolysis and potentially photolysis to convert the polymers to diamond-like carbon. A scalable and affordable method was established to reproducibly synthesize carbon polymers possessing a diamond-like structure by reducing α-α-α-trichlorotoluene at room temperature and normal atmospheric conditions. A post-synthesis purification procedure was developed to further refine the raw polymer products. The conversion of the polymer precursor to s-DLC was investigated as a function of temperature. A deeper understanding into the process-property relationship for preparation of sDLC coatings was obtained. Finally, the chemical composition, microstructure and properties of the s-DLC coatings were examined with and compared to those of traditional DLC using FTIR and Raman spectroscopy, electron energy loss spectroscopy (EELS), scanning electron microscopy (SEM), electrical impedance and nanoindentation

measurements. These resultant sDLC coatings exhibited properties akin to those of traditional vacuum-prepared DLC. This new solution-based processing route opens doors for many applications of DLC films (e.g. protective coatings, friction reduction, corrosion resistance, etc.) with substrates previously impractical due to their size, geometry or incompatibility with vacuum processes.

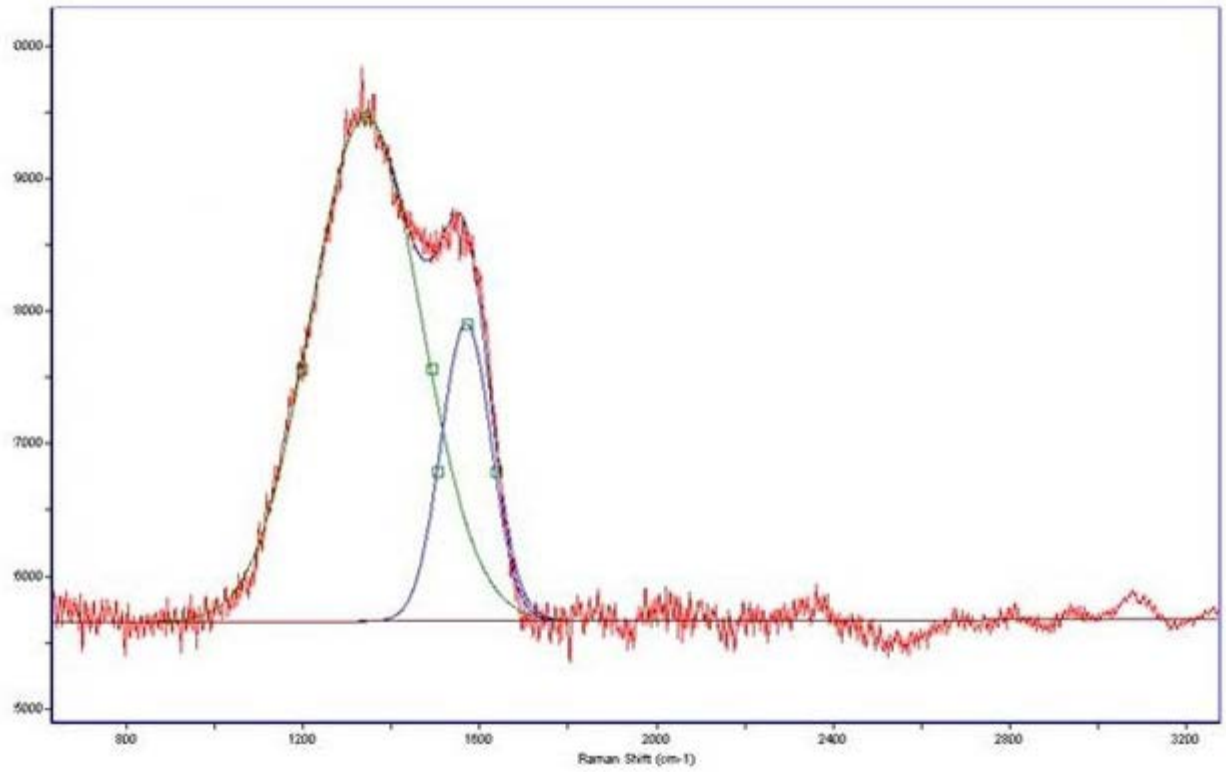

Figure 2. Raman spectra of sDLC coated steel substrate.

Pulsed-Laser Synthesis of Group IV Clatrates for Energy Storage Applications, 18-R8180

Principal Investigators
Kwai S. Chan
Michael A. Miller

Inclusive Dates: 10/01/08 – 09/30/10

Background — Energy storage and battery materials represent a major growth market for fundamental research, applied research and technology development. The U.S. Department of Energy (DOE) has established an extensive technology program to advance the development of Li-based batteries to enable a larger market penetration of hybrid electrical vehicles, plug-in hybrid electrical vehicles and electric vehicles. The pulsed-laser synthesis capability was needed to fabricate silicon, germanium, and tin clathrates, which are potential electrode materials for lithium-ion batteries. These results were needed to support a proposal to DOE.

Approach — A pulsed laser (mode-locked YAG with frequency doubling) and power supply system (Coherent Antares™, Model 76-S) were received from SP2 Carbon and installed in the Laser Raman Laboratory at SwRI. The pulsed-laser was set up on an air-suspended optical table in line with an SwRI-developed vacuum target-chamber. However, there were several issues with the laser cavity that required some repairs and alignment. The laser was repaired but the optical path could not be sufficiently aligned to cause lasing. To achieve the project goal, researchers redirected the project efforts to develop an alternative method of fabricating Si clathrates using an ionization-enhanced plasma magnetron sputtering technique.

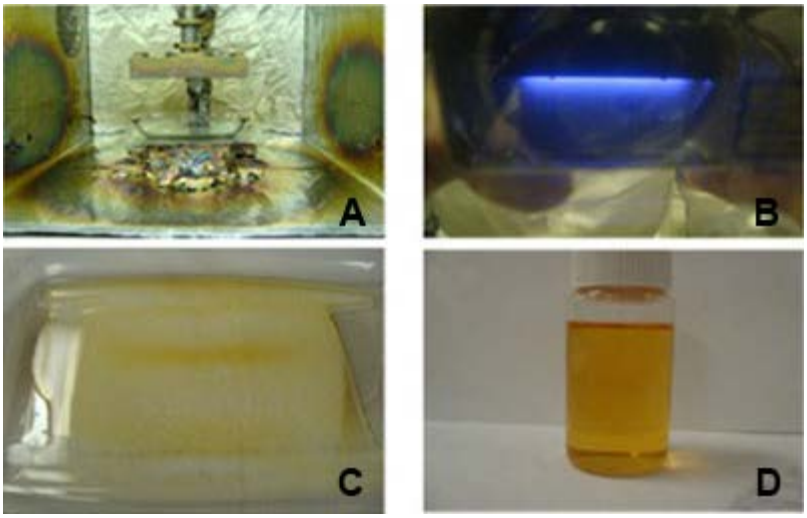

Figure 1. (A) Experimental setup for plasma magnetron synthesis of silicon clathrates. (B) Image of plasma interaction with a pool of ionic liquid. (C) As-deposited nanoparticles of silicon in pool of ionic liquid. (D) Fully dispersed nanoparticles of silicon clathrates in ionic liquid recovered from the PEMS process.

Accomplishments — A plasma-enhanced magnetron sputtering (PEMS) vacuum deposition chamber was set up to explore the synthesis of guest-free silicon clathrate particles by directing a silicon-argon plasma into a pool of ionic liquid (IL), as illustrated in Figure 1(A). This synthesis process involved purchasing a silicon sputtering target based on SwRI's design specifications. The Si target was sputtered, and the sputtered Si-argon plasma was directly deposited into a pool of ionic liquid in vacuum, as shown in Figure 1(B). The suspended particles, Figure 1(C), were then separated from the ionic liquid, Figure 1(D), and structurally characterized via powder X-ray diffraction and Raman spectroscopy. The results indicated that small amounts of empty silicon clathrates, Si_{46}, were synthesized using this technique. This technique is currently being used to make silicon clathrates in an external project supported by the DOE through the Lawrence Berkeley National Laboratory.

Development and Characterization of Nanodiamond-Containing Nanocomposite Films/Coatings, 18-R8188

Principal Investigators
Christopher Rincon
Ronghua Wei

Inclusive Dates: 10/01/10 – 10/01/11

Background — As industrial components are pushed to operate under more and more severe environments, there is a need to develop more advanced materials. Because of the difficulty of forming diamond-containing coatings using conventional physical vapor deposition (PVD) or plasma-enhanced chemical vapor deposition (PECVD), a novel approach was proposed for this project. The method utilizes a solid phase of nanodiamond particles and a gas (or metal vapor) phase to form the nanodiamond-containing nanocomposite coatings (NDNC) identified as the next generation of materials. This new type of NDNC coatings holds a very high potential for much wider applications than the coatings and films that are currently available in industry.

Approach — The primary objectives of the project were to (1) conduct a preliminary study to prove the concept that nanocomposite films/coatings consisting of nanodiamond particles can be deposited on engineering materials, (2) develop a method for nanodiamond particle dispersion into a vacuum chamber, (3) use EDS, SEM, and Raman to characterize the coating and particle dispersion and (4) characterize the tribological performance of the coatings using pin-on-disc and sand erosion test methods.

Accomplishments — Dry powders of nanodiamond, nanosilver, and micron-diamond were successfully added to a DLC coating without any change in standard process parameters. The doped DLC had an increased surface roughness as well as a visible change in appearance. The addition of various types of micron and nanometer size powder into a standard DLC coating did not result in any significant changes in tribology or erosion resistance compared to an undoped DLC in the current study. Further study should be given to examine the effects of silver or TiO_2 as an antibacterial agent in a DLC coating. Other types of previously untested powder materials could be added to a DLC coating without sacrificing wear resistance or low coefficient of friction.

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Electrochemical Studies of the Effect of Solution Impurities on the Onset of Stress Corrosion Cracking of Austenitic Stainless Steel in Pressurized Water Reactor Primary Water, 18-R8202

Principal Investigators
Florent Bocher
Todd S. Mintz
Steve T. Clay

Inclusive Dates: 12/20/11 – Current

Background — Existing nuclear reactor facilities in the United States are fast approaching the end of their operation license period. The Nuclear Regulatory Commission (NRC) and utilities are in the process of extending these licenses. This requires a better understanding of long-term deterioration of materials used in the power plant. Stress corrosion cracking (SCC) in primary water is of special interest because it has been the cause of failure of nickel-based alloys and stainless steels. SCC is a delayed fracture process divided into three stages: (1) initiation, (2) steady-state propagation and (3) final failure. A majority of the work carried out in pressurized water reactor (PWR) environments has focused on the second and third stages for Ni-based alloys. However, as the lifetime of the current PWR fleet increases, a better understanding of the initiation processes has become necessary. SCC of stainless steel in PWR is becoming more of a concerned because more than 130 SCC events have been reported since the 1980s. As a result, EPRI has classified SCC of stainless steel in primary water of PWR as a high priority issue.

Approach — The objectives of this project are: (1) to measure the effect of contaminants (chloride, sulfate and oxygen) in primary water on the electrochemical properties of austenitic stainless steels, (2) to measure the effect of those compounds on the semiconductor properties of the passive film, (3) to assess the impact of applied potential on crack initiation and growth, (4) to correlate the changes in electrochemical and semiconductor properties with the measured occurrence of crack initiation and propagation, and (5) to successfully develop a new technique to assess the early stages of stress corrosion cracking in passive materials.

Accomplishments —

Task 1 – Assemble the Experimental Setup: The experimental equipment is a once-through system based on preexisting equipment that was modified to accommodate the current program. The experimental setup was completed during the second quarter of the project.

Task 2 – Determine the impact of impurities on the electrochemical properties of the passive films. Cu/Cu_2O reference electrodes were assembled, tested and used during the high-pressure, high-temperature electrochemical testing. Electrochemical polarization scans of stainless steels 304 and 316 were performed in Cl^- (5 ppm) and $Cl^- + SO_4^{2-}$ (5 ppm each) contaminated borated water solution 3 and 4, respectively. The passive current was lower for stainless steel 304 in both solutions. Both stainless steels in solution 3 display a clear passive behavior, while their open circuit potentials and current densities in solution 4 are significantly higher. It has been reported that combinations of chloride and sulfate had dramatic impact on the SCC resistance of stainless steels in the field. The potentiodynamic scans suggest that the combination of impurities has a similar impact on the electrochemical behavior of stainless steels.

Task 3 – Effect of applied potential on crack growth rate of stainless steels. The design, manufacture and

calibration of the CT specimens have been completed. Non-instrumented CT specimens loaded at 85, 90 and 95 percent of yield stress have been added to the autoclave during the electrochemical tests performed in solution 4.

Corrosion Measurements in Fuel Systems, 18-R8203

Principal Investigators
James F. Dante
Gary Bessee

Inclusive Dates: 01/01/11 – Current

Background — Corrosion in fuel systems has become a widespread problem in recent years for underground storage tank manufacturers and operators at fuel dispensing stations nationwide as well as engine/engine part manufacturers. Some of these issues appear to be related to the introduction of ultralow sulfur diesel fuel (ULSD). One of the major difficulties in studying corrosion of metals in fuel systems is the inherent low conductivity of the fuel environment, which makes conventional electrochemical techniques to measure *in situ*, real-time corrosion rates virtually impossible. Another significant technical issue is the phase instability of ethanol/gasoline blends, such as E10, in the presence of water. As low as 0.5 vol percent water in the dispensing line can cause phase separation leading to severe corrosion and off-spec blend. This phenomenon has been found to be very sensitive to the composition of the blend, water content and temperature, but no operating boundaries for phase stability have been established. While several hypotheses have been developed to explain the corrosion failures observed in the field, no confirmed root cause has been established to date.

The objectives of the project are to 1) validate a method for measuring corrosion rates in fuel systems, 2) investigate the effect of dew points, water content and fuel chemistry on the corrosivity of ULSD, and 3) determine some of the parameters that lead to phase separation in ethanol/gasoline blends.

Approach — This project addresses the measurement issues by employing a recently developed corrosion sensor technology to measure corrosion rates in fuels. The sensor system (SwRI® multielectrode array sensor, MAS) is able to measure corrosion rates in thin electrolyte layers, such as ones forming in a fuel containing very small amounts of water. This sensor technology has never been used in non-aqueous environments. Carefully selected model fuels of known composition will be used to investigate the environmental effects that increase the corrosivity of ULSD compared to other diesel fuels. Two approaches will be employed to study the phase separation of ethanol/gasoline blends. Thermodynamic calculations will first be carried out using a mixed solvent electrolyte model to define parameter boundaries of phase instability. Then, the corrosion properties of different blends will be measured using MAS technology.

Accomplishments — A corrosion test cell and multi-electrode probe were fabricated. Corrosion currents in a surrogate fuel with varying amounts of "aggressive" ethanol were measured. Data indicated a significant increase in corrosion current with increasing ethanol concentration. Initial testing to measure corrosion currents in diesel fuel has begun. Data indicates that corrosion currents are very small in systems with small amounts of contamination in the water phase. Investigations continue in an attempt to understand the levels of ionic contaminants and the effect of diesel fuel composition on corrosion currents.

2011 IR&D Annual Report

Effect of Aging Concrete on Seismic Performance of Shear Wall Structures, 20-R8090

Principal Investigators
Biswajit Dasgupta
Ken Chiang
Luis Ibarra

Inclusive Dates: 10/01/09 – 10/01/11

Background — Concrete aging can cause deterioration of the mechanical properties of concrete and affect the seismic performance of the existing reinforced concrete (RC) structures. The consequences from failure of aging infrastructure (e.g., bridges, dams, and nuclear power plants) in the United States and other countries are a major concern. As concrete ages, its properties change as a result of continuing microstructural changes (i.e., slow hydration, crystallization of amorphous constituents, and reactions between cement paste and aggregates); however, under aggressive environments, the degradation process may accelerate. In addition, physical challenges, including freeze and thaw cycling, thermal exposure and thermal cycling, abrasion, erosion or cavitation, fatigue or vibration, and corrosion of steel reinforcing rebars, are significant contributors to the overall degradation of structural resistance. Several experiments reported in the literature have evaluated the potential effects of aging and temperature on the mechanical material properties (e.g., compressive strength and elastic modulus). The effect of long-term degradation of concrete, however, has not been comprehensively addressed in seismic performance evaluations. In this research, investigators developed a methodology to assess the effect of concrete aging on the seismic performance of structures in which RC shear walls are the main lateral resistance components.

Approach — A large number of studies have evaluated the effect of high temperatures on concrete, but data regarding concrete performance under long-term, high-temperature exposure are limited and do not take into account the strength gain that concrete may have experienced at room temperature. Moreover, previous data do not consider widespread use of admixtures, such as plasticizers. The compressive strength of concrete cylinders was tested at 28 days and then at regular 90-day intervals over 24 months for a moist-cured specimen. Additionally, cores were exposed to 90 to 95 °C [194 to 203 °F] over the same period, and compressive strength was tested to study exposure of concrete to temperature. Petrographic analysis was performed to assess the deterioration of concrete at high temperatures. Concrete core tests were performed on samples taken from existing buildings. Additionally, threshold chloride levels for localized corrosion of carbon steel rebar material have been studied in three types of simulated concrete pore solutions.

A new approach was developed to generate fragility curves of structural systems that account for aging of concrete. The structures evaluated in this project consist of representative systems commonly used in the nuclear industry, which include thick, RC shear walls as the main lateral resistance component. Structural response was evaluated for concrete aging factors caused by loss of steel area, changes in concrete compressive strength and loss of concrete area caused by cracking and spalling. The separation of variables method used in seismic probabilistic risk analysis for nuclear power plants was used to develop fragility curves for the non-degraded and degraded shear wall components. The variability of parameters for fragility of non-degraded and degraded shear wall components were concrete strength, stiffness, and strain at ultimate strength, and yield strengths of steel. The probability of unacceptable performance or seismic failure was computed by convolving the fragility and hazard curve.

Accomplishments — The compressive strength of concrete mixes containing admixtures to accelerate strength development was tested at standard moisture content and elevated temperatures close to the boiling point of water. The results indicated that long-term compressive strength of concrete cured in a standard moisture environment is not significantly affected by the presence of water admixtures. The water-reducing admixture in the concrete contributed to early strength development because it accelerated the cement hydration; however, the long-term compressive strength has not been significantly affected after 1.5 years, and the concrete strength has stabilized with a gain of 10 to 15 percent with respect to compressive strength at 28 days. The effect of continuous exposure to temperatures resulted in a loss of compressive strength of less than 10 percent. Petrographic analyses suggest that deterioration of concrete compressive strength at these temperatures was mainly caused by physicochemical changes in the cement paste. The localized corrosion of carbon steel experiments demonstrated that if the chloride concentration is greater than certain pH levels, high-corrosion rate is estimated to cause a 20-percent reduction of the rebar cross-sectional area.

The seismic performance evaluation used experimental data on the corrosion of steel reinforcement and variability of concrete parameters as a function of time. To obtain the variation in the system capacity caused by concrete aging, detailed numerical models of RC shear walls were developed using the finite element method. The deterioration effects of RC are accounted for in the material properties of concrete and steel rebar in the shear wall model for evaluation of fragility curves. Failure probability increases with aging of RC because the increase in the concrete compressive strength with time does not overcome the degradation of the seismic performance caused by concrete cracking and corrosion of steel rebars. Aging effects increase the probability of failure of RC shear walls subjected to lateral loading. The increase is about four times of magnitude when all sources (demand and capacity) of variability are considered.

Investigation of Model-Based Diagnostic Methods, 09-R8104

Principal Investigator
David A. Ogden

Inclusive Dates: 09/28/09 – 04/01/11

Background — This project explored various diagnostic techniques using empirical data and physics-based models. Previous internal research projects addressed anomaly detection technologies. This project is related to those previous efforts by addressing diagnostics, which is the next step in the detection, diagnostic and prognostic process that enables a condition-based maintenance (CBM) system. In improving and automating the diagnostic process, project team members developed a configurable physics-based model to be fused with empirical sensor data acquired from in-flight data. The improved and automated methods developed for this project represent advancement beyond the state of the art for aerospace propulsion engine diagnostics.

Approach — The main objectives of this project were to create a configurable physics-based model and to develop analysis methodologies that fuse the physics-based information with sensor data to provide a high level of diagnostic automation and precision.

Accomplishments — With this approach, pattern/regime recognition and classification algorithms and particle swarm intelligence-based diagnostic algorithms were created and tested. The pattern recognition algorithms proved reliable for operational regime classification and sensor validation. The particle swarm diagnostic algorithms fuse the formerly disparate data sets of empirical data and physics-based models. These algorithms reduce diagnostic time by automatically directing maintenance personnel to the failed module, even if the failure is not predefined as a fault.

Future efforts for this project will address using the pattern recognition algorithms as a diagnostic tool for alerting users to previously defined failures, using the particle swarm optimization algorithms for selecting an optimal set of features to be used for diagnostics, and using the physics-based model to calculate and test using additional health parameters that are available once the model and data are fused.

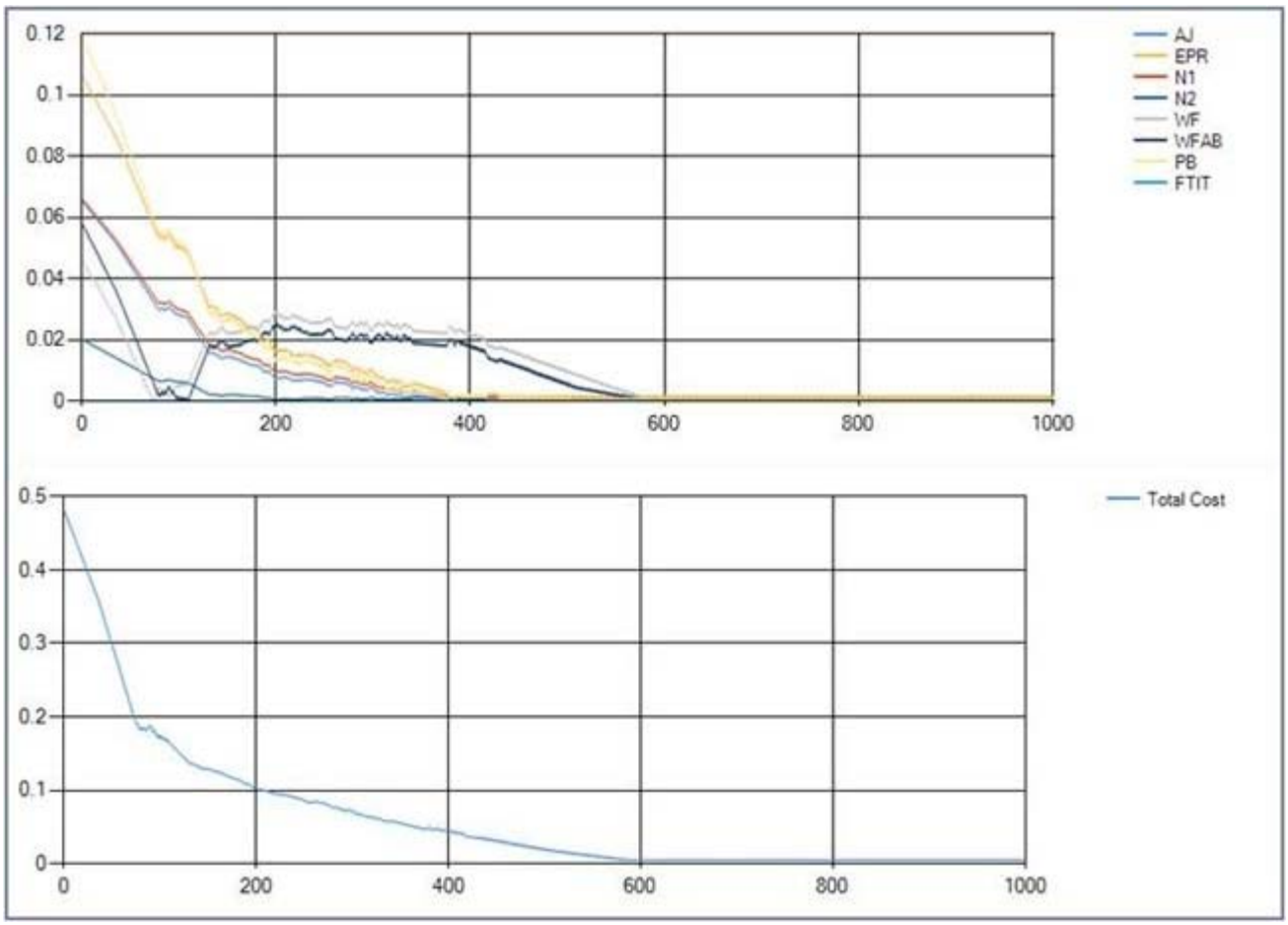

Figure 1. Cost Information Associated with One Particle during a Diagnostic Analysis.

Evaluating the Efficacy of a Criteria Model for Selecting Mobile Augmented Reality as a Learning Tool, 09-R8200

Principal Investigators
Randall Standridge
Jenifer Wheeler

Inclusive Dates: 01/03/11 – Current

Background — Mobile devices are becoming an increasingly important and strategic component in the delivery of learning content. To a large degree, this is driven by the ubiquity of these devices, as well as the increasing capabilities of the technology. Thus far, most learning applications have focused on the delivery of training content and courses. However, mobile devices are now capable of supporting a wide range of content delivery including applications such as simulations and mobile augmented reality (MAR). While anecdotal evidence indicates strong potential for using mobile platforms in training and performance support, more empirical data is needed to begin truly defining the best use for this technology. For instance, when is it most appropriate to use MAR for learning as opposed to alternatives such as two-dimensional animation or three-dimensional simulation? Understanding the criteria for selecting MAR will aid in its effective application as well as the application of other approaches.

Approach — This research effort consists of the following phases:

Develop and analyze selection criteria for a MAR learning application based on human performance and learning theories.

Design a task for study that is tailored to the MAR selection criteria. That is, based on the criteria established in the first phase, design a task that is optimally suited for a MAR application.

Implement three different mobile learning solutions (i.e., 2D, 3D simulation and MAR) that are each intended to teach or support the task created in Phase 2.

Collect and analyze data from three different groups of participants, each using a different mobile learning application, to perform the task to draw conclusions regarding the validity of the selection model as well as key usability insights for each type of solution.

Accomplishments — Thus far the project team has developed a criteria model for selecting mobile augmented reality as a learning delivery tool based on skill type, task characteristics and task execution variables. This model was subsequently used in selecting a study task, which will use a three-dimensional assembly problem to study the relative performance of different mobile learning technologies. Technology evaluations have been conducted to select the most appropriate mobile software development tools including those required for developing augmented reality applications. Based on the technology selections, the application requirements and software designs have been completed for the three different mobile learning applications.

Investigation into Idling Reduction Technology Using Intelligent Traffic Signal Controller Algorithms, 10-R8105

Principal Investigators
Steven W. Dellenback
Karl Kreder
Mark A. Workman

Inclusive Dates: 09/28/09 – 09/30/11

Background — Many industrialized countries are enacting (or considering) greenhouse gas (GHG) reduction legislation. Within the United States Senate, this legislation is called the "American Clean Energy and Security Act of 2009." Currently, transportation is the second largest source of GHG emissions within the U.S. (second to electric generation). As a result, public and private transportation entities must prepare for cap-and-trade or similar regulations to reduce GHG emissions. As part of these preparations, the transportation community must investigate steps towards reducing transportation-related GHG emissions. One opportunity to lessen GHG emissions within the transportation arena is to reduce idling time at signalized intersections. Anytime a vehicle slows, stops, idles and accelerates in relation to a signalized intersection, time is wasted, fuel is consumed and excess GHGs are emitted from the vehicle. By eliminating unnecessary speed variances and idling time generated by vehicles interacting with the traffic signaling system, the transportation community can reduce GHG emissions, improve fuel efficiencies and reduce traffic-related congestion and delays.

Approach — The objective of this research effort was to evaluate both actuated and non-actuated signal controller algorithms and their effect on GHG emissions. These evaluations are carried out through state-of-the-art commercial and SwRI-proprietary microscopic computer simulations. These simulations evaluate different signal control types and configurations under different traffic flow volumes. The simulation results provide comparative analysis for traffic signal algorithm effectiveness towards GHG reductions.

Accomplishments — Through sophisticated software simulation, a signalized traffic signal system was evaluated under real-world traffic signal controller types, vehicle sensing technologies and diverse traffic flow conditions. The traffic signal simulations generated individual driving profiles for each vehicle within the system. Each driving profile was evaluated for its corresponding GHG emissions. The outcome of this research demonstrates that effective traffic signal design and implementation involve many tradeoffs. A traffic signal algorithm may implement a strategy that increases positive traits such as traffic travel time and throughput, but it may also have a negative effect on queue wait times and/or GHG emissions. Before this research, such comparative analysis of GHG emissions relating to traffic signal systems was not possible. This research provides an approach to manage traffic based on emissions as opposed to the traditional method of optimizing on speed and occupancy.

Manipulating Traffic System Dynamics Using Smartphone Technology for Improving Public Safety, 10-R8126

Principal Investigators
Paul A. Avery
John Whipple
Thomas Dietzel

Inclusive Dates: 01/01/10 – 12/31/10

Background — Modeling traffic system dynamics can be very complex, considering a number of factors that affect the aggregate flow, such as vehicle density, road width, bend radii, obstructions, detours, etc. Approaching traffic system modeling at a macro level and applying averaging assumptions, the model results will only be valid within the bounds of the averaging assumptions and will not give the modeler flexibility to investigate system-level effects that emerge from individual vehicle capabilities. To effectively model traffic system behavior as it relates to the capabilities and behaviors of individual vehicles requires an understanding of how internal dynamics of complex systems interact to produce system-level phenomena. This research modeled traffic system dynamics at the micro level to understand the effect on the system when some vehicles have access to supplemental information through a smartphone application regarding elements of their environment and exit route, and developed the application on physical smartphones for hardware-in-the-loop testing.

Approach — This project developed an agent-based model to simulate traffic flow on urban road networks to understand the traffic system macro-behavior, which is a complex nonlinear problem with adaptive interactions among its elements. The model was constructed by specifying the physical characteristics and the rules of behavior for individual vehicles, the road network in which the vehicles operate, and the goals or objectives for individual vehicles. A smartphone application was also developed using a freely available smartphone emulator, and then moved to actual smartphone platforms. The application subscribed to a notification service and provided specific optimal routing information to the user through a Google Maps interface.

Accomplishments — An agent-based model was developed including vehicle behaviors, such as route selection and following, and vehicle following. The vehicles can also modify their route selections based on local congestion. A road network was constructed based on the San Antonio major highway network using map data from Google Maps. A specific population of vehicles has the capability to receive the evacuation notification, which emulates the smartphone capability. An XMPP communications protocol was implemented to enable the physical smartphones to communicate with the evacuation data server and the agent-based model. Routing information is delivered to the phones using a Google Maps interface, where an origin location is provided by the phone's GPS position, and a destination location is selected based on an effective evacuation route.

2011 IR&D Annual Report

Development of an Automated Laser Depaint System, 10-R8155

Principal Investigators
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Michael P. Rigney
Michael O. Blanton Jr.

Inclusive Dates: 06/03/10 – 03/01/11

Background — Laser paint removal has the potential to become the process of choice for a number of industries. The advantages of laser coating removal include reduced waste stream volume, lower maintenance and lower power consumption. Although these advantages were recognized two decades ago, the ability to deliver sufficient laser power to the end effector of an extended-reach robotic system, suitable for whole-aircraft paint removal, has only recently become feasible with the maturity of fiber lasers. In addition, this type of laser offers power control capability appropriate to prevent damage to sensitive substrates and enable selective coating removal. Though manual open-loop testing is showing good results, the key to the success of an automated system is closed-loop sensing/control of the process.

The purpose of this project was to develop a control solution comprised of sensors and data analysis software to measure the coating removal state and provide real-time feedback to modulate laser power. This closed-loop control system was then integrated with a commercial fiber laser into a custom robotic platform.

Approach — This project developed a real-time, closed-loop control system that used machine vision to characterize the target surface, and then provided a control signal to modulate a laser power source. A high frame rate color camera and a filtered monochrome camera were used to provide RGB and NIR spectral data for real-time analysis of the coating removal process. The two cameras were optically aligned via a beam splitter, and software controls allowed for fine-tuning to match the field of view of both cameras. Images were acquired at twice the rate of the laser raster period. This allowed alternate analysis of the left and right image fields, which were synchronized with the laser position. Subsequent analysis and spectral classification were used to identify coating versus substrate and to modulate the laser power to precisely control the coating removal process.

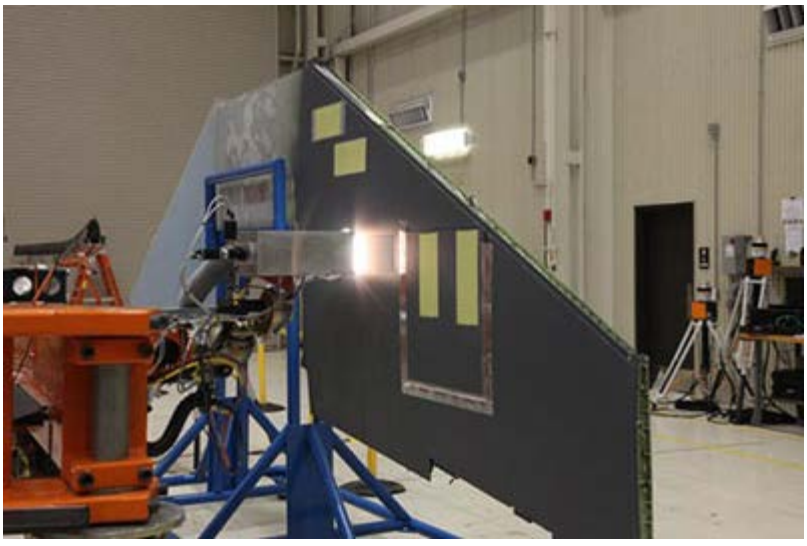

Figure 1. Paint Stripping Demonstration Using Custom SwRI Robotic Platform.

Work was executed in two phases. Phase 1 developed and validated the sensor/control system, and Phase 2 integrated the new technology into a large-scale coating-removal robotic platform at SwRI to validate and demonstrate system capability.

Accomplishments — This program successfully developed a sensor package that provided operational coating/substrate discrimination for high-contrast combinations in the presence of brightly incandescing laser/coating interactions and smoke. Using commercial-off-the-shelf equipment, acquisition and analysis of image data and communicating laser control data at rates of 600Hz and 300Hz were achieved.

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Investigation into the Usage of Bluetooth® Signals for Roadway Speed Calculations, 10-R8164

Principal Investigators
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Adam Clauss
Meredith Wright

Inclusive Dates: 07/02/10 – 11/02/10

Background — With Bluetooth®-enabled devices becoming more prevalent in vehicles, a few companies have developed proprietary solutions for determining travel times over roadway segments. While Florida and Texas Departments of Transportation (DOT) districts are interested in obtaining this functionality, a turnkey solution is undesirable. The DOTs require data be incorporated into their existing traffic management software rather than invest in multiple solutions that are not integrated. However the DOTs are under some pressure from the various districts to implement a solution that can be put in place where little to no infrastructure exists.

Approach — The objective of this project is to investigate potential issues with Bluetooth technology used for the purpose of traveler information. Some of the concerns with using Bluetooth technology for this purpose include validating that an adequate number of data points can be gathered from devices at high speeds and what mode a device must be in to read a signal.

This research includes investigating various Bluetooth device capabilities. The assortment of evaluated devices includes end-user products such as cell phones, personal digital assistants (PDAs), MP3 players, headsets and cars with Bluetooth technology. The other end of the product spectrum includes Bluetooth adapters for connecting to devices and range extending antennas. Scanning capabilities were ascertained to determine the feasibility of using this technology for the purpose of determining traffic speeds and travel times.

Accomplishments — One of the initial limitations investigated was whether the end-user devices must be in discoverable mode to be detected. Prototype software was developed to scan for devices. Bluetooth adapters were used in conjunction with both focused and omni-directional antennas to determine effective ranges. Some adapters are capable of ranges up to 250 feet without an attached antenna, which is adequate for scanning end-user devices on roadways with 20 lanes of traffic. Determination was made that only discoverable devices can be detected, which limits the use of this technology for the purpose of travel time generation.

2011 IR&D Annual Report

Information Framework for Transportation Applications, 10-R8175

Principal Investigator
Steven W. Dellenback

Inclusive Dates: 07/01/10 – 06/30/11

Background — In the transportation domain there are a large number of sources from which decisions are made. Consider the following examples:

- A traditional manned vehicle 20 years ago: a driver had to rely on his vision and wits to determine the safest and most direct path to get between two points.
- A traditional manned vehicle today: a driver has navigation systems, radio feeds, real-time traffic conditions on their PDA and/or Internet connection as well as potentially other sensors in their vehicle to assist in the safest and quickest path between two points.
- An unmanned vehicle of several years ago: uses sensors on the vehicle to determine the "state" of the world around the vehicle and navigates between two points utilizing pre-programmed "way points."
- An unmanned vehicle of today: utilizes data from other vehicles and/or the roadside to more accurately determine the optimal path.

While the Global Positioning System is important to locating a vehicle, there is a major push by the military to have their intelligent vehicles (whether manned or not) operate in "GPS-denied" environments, that is, use their surroundings to determine their location and not rely on specific GPS data. This project developed the algorithms and techniques to create a world-view model combining a number of data sources, both static and dynamic, to create a world model. Because of the huge amounts of data, an important component of the research was developing an algorithm that extracts regions of interest that are limited to what data is required by the application requesting data.

Approach — Sources of data (i.e., the proposed research is not creating this data) that are placed into the model include:

- Data generated from processing the data from sensors on vehicles.
- Navigation data.
- Traffic condition data available as data from Internet sources, radio broadcasts (available on a data feed in parallel with voice data).
- Traffic management center data.
- Landmarks such as buildings, stadiums, etc.

The internal structure of the model is based on a coordinate system, but the data can be extracted either in spatial (feature) or geolocation form.

Accomplishments — The program has successfully demonstrated the extraction of features from vision and LIDAR data to determine relative position of the vehicle.

2011 IR&D Annual Report

Temporally Coherent Communications, 10-R8194

Principal Investigators
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Inclusive Dates: 11/01/10 – 11/01/11

Background — Current communications systems do not have time coherence between sender and receiver (a common sense of time) and must perform significant amounts of signal processing to identify whether a signal is present and to synchronize with it (bit synch). This processing requirement drives the size, weight, and power (SWaP) of the implementations higher. The Defense Advanced Research Products Agency (DARPA) Chip Scale Atomic Clock (CSAC) program has developed small, low-power atomic clock technology. Highly coherent atomic clocks are now available that are sufficiently small and power efficient that they can be used in mobile wireless communications. This research has developed methods for leveraging the CSAC to reduce the amount of synchronization-related processing that must be done in radios. It has also developed a new media access control (MAC) scheme that leverages time coherence, which promises to have low probability of intercept/low probability of detection (LPI/LDP) properties.

Approach — The primary objective of this project was to investigate the concept of temporally coherent communications (TCC) and to characterize the performance parameters of a novel temporally coherent waveform that leveraged the CSAC devices. Consequently, researchers were also able to obtain hands-on experience with CSAC devices that positioned the team as knowledgeable early adopters with actual device performance results to substantiate waveform development. The focus of this effort was to characterize and evaluate the CSAC technology and apply it to developing a set of waveforms for low-power, covert and interference-tolerant communications.

The technical approach was two pronged. The project team experimented with actual CSAC development boards and developed a waveform based on the model of the CSAC derived from real-world experimentation. The CSAC was leveraged to develop the TCC architecture and waveform. The approach was to develop a waveform that varied the encoding, modulation, transmit frequency, power, and time patterns in a novel way. The transmit and receive radios would each have an integrated CSAC, meaning they were temporally coherent within the bounds derived from the CSAC experimentation and modeling.

The project team designed and built a custom dual mixer time difference measuring system that mixes two CSAC time sources with the same reference signal. The CSAC timing model and clock drift values were empirically derived from multiple experiments using the dual mixer time difference measurement method. The research team used the captured test data to develop a model of the CSAC's drift with respect to temperature and time since discipline. The propagation delay can be estimated by sending custom "sounding" messages between the pairs of radios. The proposed solution operated with very low power by executing a time-synchronized, media access scheme. To functionally validate the team's research claims that the coherent waveform was feasible, base functionality was implemented in the Gnu's Not Unix (GNU) Radio framework. In both the transmitter and receiver, a CSAC model was used to

simulate the clock that drives the scheduler.

Accomplishments — As a result of this research, several practical use cases were developed that led to consideration of various potential application areas and customers. Researchers conducted numerous experiments with CSAC development boards and developed a model of the clock drift over time and across temperature. These experiments were used to simulate CSAC-enabled communication and develop the temporally coherent algorithm and waveform. Several promotional opportunities have been pursued throughout the past year. The team has many promising leads and already has successfully won a Small Business Innovative Research (SBIR) directly related to the work done on this project. The team aims to transition the technology into use in Department of Defense (DoD) applications.

Metrology Referenced Roving Accurate Manipulator Phase 2 (MR ROAM 2), 10-R8205

Principal Investigators
Glynn Bartlett
Paul Hvass

Inclusive Dates: 01/01/11 – 01/01/12

Background — Modern industrial robots are generally monolithic assemblies, either floor-mounted or gantry mounted, whose accuracy is largely determined by the error stack-up through each joint and link from a ground reference to the robot's end effector. The fact that the systems rely upon a physical link to the ground reference means that there is limited robot market penetration both for large-scale applications and for operation at remote sites. However, the recent availability of large-scale metrology systems to provide real-time non-contact position data enables a signal-based link to ground reference that can replace the physical link. The robotics industry is ripe for rapid expansion using off-the-shelf manipulators on mobile platforms in conjunction with an external metrology system for large scale and remote site tasks where accuracy and repeatability are required over large working envelops.

Approach — A demonstration system was developed using a commercially available platform and manipulator. The first step was to port the software developed during phase 1 and update it as necessary to match the new robotic manipulator and mobile platform. The next step was to incorporate the new external metrology system. The metrology system provided was a six degree-of-freedom (DOF) base pose correction to the mobile platform position, implemented at specified rates. Software was developed to correct the tool point based on the feedback from the metrology device. The robotic manipulator was corrected to a world path plan using an incremental real-time correction implemented through the robotic controller. The project ported from phase 1 the closed loop control developed for the mobile platform motion using an external metrology device. The closed-loop path control of the mobile platform maintained the manipulator tool point within reach of an independent tool path. Once the MR ROAM 2 system was integrated, empirical testing was conducted to determine the repeatability and capability of the system. The experimental variables consisted of the tool-point velocity at one specific update rate and two different part locations within the field of view of the metrology device. Metrology receivers were attached to the mobile platform to track its position for the feedback loop. Metrology

Figure 1. Integrated MR ROAM 2 System.

receivers, mounted on the end effector, were used to both make real-time path corrections, and track accuracy and repeatability of the complete system to follow a specified world path.

Accomplishments — The basic integration of the three individual systems occurred over the first two quarters. This integration included mechanical, electrical and software components. During the third quarter, calibration of the system and different control algorithms were tested to evaluate performance. Final testing finished at the end of the third quarter, and analysis was completed during the fourth quarter. Data indicates the positional accuracy is less than one-half inch and repeatability is one-quarter inch according to ISO standard 9283. The system maintained a standard deviation of less than one-quarter inch in all coordinate directions.

2011 IR&D Annual Report

Using Extreme Value Theory to Eliminate Binary Thresholds in Anomaly Detection, 10-R8209

Principal Investigator
Sandra G. Dykes

Inclusive Dates: 12/22/10 – 07/06/11

Background — Anomaly detection (AD) algorithms are central to machine learning and data mining, with application to a wide range of areas such as malware detection, image processing, fraud detection and fault analysis. Although AD is potentially powerful, current methods are prone to high false positives, sensitive to training data, inconsistent over different data sets and provide little insight into results. One root cause of these problems is the use of binary thresholds. A binary threshold creates a discontinuity in the detection function, regardless of whether the detection method uses a statistical, classification or clustering algorithm. Consider two data points that are approximately equal, x_1 and x_2, with x_1 slightly above the threshold and x_2 slightly under it. Despite this small difference, x_1 would be considered an anomaly and x_2 would not. A binary threshold therefore couples false positive and false negative error rates — shifting the threshold reduces one at the expense of the other.

Approach — SwRI researchers introduced a new approach to anomaly detection called extreme value theory-anomaly detection (EVT-AD) with two novel concepts:

- Applies *extreme value theory* to replace binary thresholds with continuous scores.
- Constructs *mathematical functions of behavior patterns* from natural-language descriptions of the model.

The SwRI approach of applying formal extreme value theorems is unique. This method enables a more accurate model of the tail of the distribution where anomalies reside. Our second innovation is a method for constructing mathematical functions to represent behavior patterns. Behavior functions are constructed by mapping descriptive natural language terms onto mathematical variables and operators, where variables are the extreme value scores. This approach provides insight into *why* an entity was detected. Insight into results is critical because it provides contextual and supplemental information about significant underlying events.

SwRI researchers developed EVT-AD for use in insider threats and credit card fraud detection; however, it can be applied to a wide range of problems. Insider threat and fraud detection are particularly difficult because there may be no distinctive indicators. For insiders, the majority of their activities may be legitimate and normal; that is, there are no indicators for any single event. Instead, it is the *pattern* of activities that is unusual. Similarly, for credit card accounts, there may be no indicator of fraud for a single transaction. Fraud is detected by looking for differences in historic patterns or from average behaviors of a peer group.

Accomplishments — Phase I of this project developed the basics of EVT-AD, implemented a prototype version in software, and used simulation studies to evaluate its detection performance compared to a standard statistical anomaly detection method used in commercial products. Experiments in Phase I focused on insider threat models. In Phase II, we applied EVT-AD to credit card fraud detection with feature data generated to match parameters of known credit card usage. Experimental results showed that EVT-AD far outperformed the binary-threshold approach for both insider threat and fraud detection, providing the same detection rate with substantially fewer false positive errors. Results suggest that EVT-

AD offers a significant contribution in the field of anomaly detection.

Adaptation Layer for SpaceWire Plug-and-Play Protocols, 10-R8216

Principal Investigators
Paul Wood
Allison Bertrand

Inclusive Dates: 04/01/11 – Current

Background — Network solutions to support rapid development and deployment of space assets and satellite plug and play (PnP) concepts are currently of great interest to the space community. The European Space Agency (ESA) and U.S. Air Force Research Laboratory (AFRL) both have PnP initiatives. Although gaining some ground, network-enabled devices such as sensors are currently rare. Network attached storage (NAS) is an anticipated early need for SpaceWire (SpW) PnP.

Approach — An adaptation layer suitable to allow an application program to operate in a network conforming to either PnP standard is the main goal of this project. A simulated NAS is being used as a challenge task to accomplish proof of concept for the adaptation layer. To this end, an SpW network consisting of a simulated producer, consumer and NAS device will be assembled. In this context, relevant elements of the two competing PnP protocols (ESA and AFRL) will be evaluated.

Accomplishments — A hardware setup consisting of the following was assembled: three Pentium® 4 computers running a Linux Ubuntu distribution, three SpaceWire cards, four SpaceWire cables and two SpaceWire routers. An additional computer connects the routers over a universal serial bus (USB) and is used to configure the SpW routers and monitor the SpW network.

SwRI researchers analyzed the protocols described in the Spacecraft Onboard Interface Services (SOIS) and the Space Plug-and-Play Architecture (SPA) standards produced by ESA and AFRL, respectively. The SPA standards are much more mature than those of the SOIS. The SPA has undergone more iterations of refinement and has a second generation software reference implementation nearing completion. No reference implementation is available for the SOIS.

The project team acquired a current copy of the SPA reference implementation and was able to host it on the development environment. The reference implementation was modified to use the SpW driver to communicate over the SpW hardware. The existing SpW interface driver was modified to provide necessary support for the SPA Services Manager (SSM). Researchers defined an Application Program Interface (API) for the adaptation layer and developed the simulated producer and consumer applications and the simulated NAS. These components are communicating in a proof-of-concept configuration that uses an implementation of the adaptation layer API to provide access to the underlying SSM.

2011 IR&D Annual Report

3D Imaging for Behavior Classification, 10-R8221

Principal Investigator
Chris Lewis

Inclusive Dates: 05/01/11 – 09/01/11

Background — The automated interpretation of the movement of bodies is a broad field with applications in robotics, surveillance, traffic management, healthcare and homeland security, among others. This project leverages the recent advancement in low-cost three-dimensional imaging technologies, which generate high-resolution, colored point clouds to develop a behavior recognition capability.

The first objective of the project was to track a body in motion using the 3D colored data. The second objective was to recognize the subject's behavior using its motion history. Researchers showcased SwRI's ability for customized tracking and behavior recognition using a healthcare application that monitors disabled children being treated for severe self-abuse behavioral problems.

Approach — The approach for tracking the body state assumes there is an underlying kinematic model for the subject that constrains the relative motion of the 3D linkages. At each instant in time, the kinematic model is fit to the observed 3D data and the resulting measurement is smoothed using a state estimation filter. This provides a time history of the body's motion to the behavior classifier. The behavior classifier operates with two layers of classification. First, basic actions are detected, and then the subject's behavior is ascertained from histograms of basic actions. A pitcher's basic actions might include the positions of his pitching and glove hand, a back step, a weight shift, head nods, sideways glances, the length of his stride and the height of his kick. SwRI's hypothesis is that these basic actions are predictors of the pitch thrown.

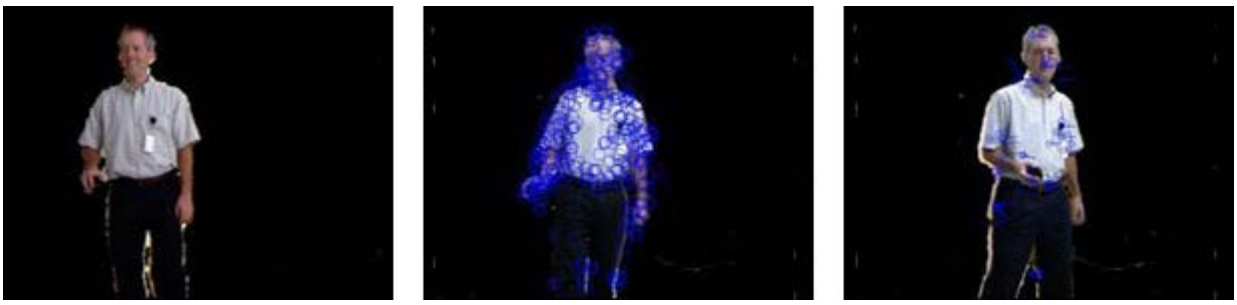

Figure 1. Colorized clouds of data from Microsoft's Kinect sensor are processed by a ROS node to first remove the background data (left). Then, a node detects and characterizes salient features (middle). Correspondence of features in subsequent frames helps estimate the subject's pose (right).

Accomplishments —

- Evaluated the kinematic results returned directly from the Microsoft™ Kinect.
- Developed software for subtracting the background.
- Developed software for automatically detecting and tracking features in the foreground data.
- Developed architecture for a multi-layered behavior classifier from body motion statistics.

Investigation of Intra-vehicle Location Finding using Inexpensive Sensors, 10-R8222

Principal Investigators
John G. Whipple
Ted R. Wilmes
Brian K. Anderson

Inclusive Dates: 04/04/11 – 08/04/11

Background — Distracted driving is a growing problem that expands with the increasing role that smartphones play in day-to-day activities. Many solutions exist that attempt to curb this problem by first detecting when the user is in a moving vehicle and then disabling distracting functionality. These solutions lack the ability to determine if the smartphone belongs to the driver or a passenger and thus, every smartphone in the vehicle has reduced functionality. This research focused on finding a solution to this problem by data mining the accelerometers that already exist in smartphones.

Approach — Vehicles generate forces that act on objects differently based on their position in the vehicle. Accelerometer sensor technology can be used to detect these variations. This research began by using SwRI's test track to record driving actions such as turning, accelerating and braking from several different vehicles using a custom accelerometer recording device. Multiple instances of the device were placed in each vehicle to facilitate recording acceleration data from multiple locations within the vehicle at the same time. This data was then analyzed using statistical software to extract features that could be used to determine driver or passenger. Digital signal processing was used to filter and identify relevant features of the data. Machine learning techniques such as neural networks and genetic algorithms were then used to model the data. A classification of "driver" or "passenger" could then be determined by feeding the models previously unseen data.

Accomplishments — This project confirmed that the accelerometer sensor can be used to deduce its own location within a mobile frame of reference. This solution does not rely on any external infrastructure and is not limited to automobiles. The same process that was used to develop the automobile models could be applied to container ships, passenger ships, train cars and tractor trailers. The wide applicability of the solution has prompted the investigators to file a patent application.

2011 IR&D Annual Report

A Senior Staff Renewal IR&D Project at Willow Garage, 10-R8224

Principal Investigator
Shaun M. Edwards

Inclusive Dates: 05/16/11 – Current

Background — The "Robot Operating System" software, better known as ROS, is an open source project that provides a common framework for robotics applications. ROS is being heavily used by the research community for service robotics applications, but its technology can be applied to other application areas, including industrial robotics. ROS capabilities, including advanced perception and path/grasp planning, can enable industrial robotic applications that were previously technically infeasible or cost prohibitive.

SwRI has already utilized ROS for several industrial and advanced manufacturing projects (see illustration for an example). Its use has enabled rapid development and overall lower cost. However, ROS use in these projects has been narrowly defined and one goal of the ROS Industrial program is to generate a framework for broader applications.

Approach — The principal researcher for this project is working closely with ROS developers at Willow Garage to develop an open source ROS software stack (software suite) to support the use of ROS for industrial applications. The software will provide a standardized interface for a variety of robot controllers, thus enabling robot-agnostic ROS software to be used on a variety of robotic platforms. The resulting software developed under this project will be released as open source. This is an ongoing project scheduled to be completed in March 2012. An initial version of the software has been released and is available at http://code.rosindustrial.org

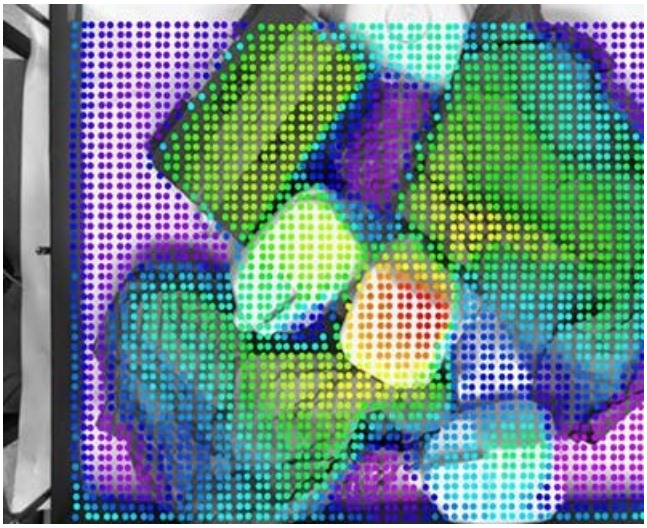

Figure 1. Image shows 3-D pointcloud data overlaid on a camera image for an industrial sorting applications.

Accomplishments — The project has completed the following milestones:

- Proof-of-concept code demonstrating remote control of an industrial robot via the ROS software.
- Development of a platform independent messaging structure will allow ROS to interface with a variety of industrial robotic platforms.

2011 IR&D Annual Report

Special Purpose IP Routing, 10-R8243

Principal Investigators
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Maria Araujo

Inclusive Dates: 07/01/11 – Current

Background — Network solutions permeate all domains, from our homes to cars and industry, and to space. The success of networking stems from the growth and standardization of the Internet Protocol (IP), which provides a universal open transport. The openness of this protocol makes it such that multiple vendors have fielded interoperable devices. Almost every company has network closets filled with blue boxes (Cisco® routers) and nearly every home has a network connection including a router and wireless access point. This openness in standardization comes with a cost. Special purpose and flexibility beyond the envelope of support is very hard to reach. For example, simply adjusting a home router to better handle overload in the Voice-over-IP scenario is a serious challenge. Consequently, most networks are used only in their default settings with performance accepted and the functionality left as a mystery.

The ubiquitous nature of networks has led to a desire to leverage networking technologies in special communications arenas. Unfortunately, not all of these scenarios are well served by "default setting" networking. At times, for the small volume specialized scenarios, the existing vendors are unwilling or unable to adapt or adjust their products.

Approach — The goal of this project is to create a framework for rapid development and deployment of special purpose IP routers. This can be achieved by adjusting settings on standard routers (rather than using the typical "default settings") and combining with embedded computer nodes. The embedded computer nodes can leverage knowledge about the inner workings of the commodity devices and manipulate data flows such that the overall specialized scenario needs are achieved.

The approach to this project is to research, define and characterize the virtual router concept and to evaluate its suitability to solving the types of problems similar to flight-test telemetry networks. This required evaluating open-source router source code to determine portions that can be leveraged for creating the router virtualization and adding the distributed concepts necessary to implement a virtual router. A series of challenge problems will be developed to evaluate the virtual router concept. Baseline performance will be measured using standard routers with both default and optimized configurations. The virtual router will then be evaluated using the same challenge problems and compared to the baseline performance. The virtual router implementation will be successively revised and reevaluated to determine performance gain over baseline.

Accomplishments — The team evaluated a number of open-source routing packages to determine which looked most promising for a starting point in developing the virtual router concept. Based on this evaluation, the team selected the Click® Modular Router package for further development of the virtual router framework. The team has built up standard routers with Click and is beginning to explore the appropriate code modifications needed for the virtual router capabilities. The team has begun setting up the laboratory environment by implementing multiple virtual router nodes using a combination of SwRI network lab resources. These nodes will be modified and replicated as needed to execute the challenge problems. Initial planning has begun for the challenge problems that will form the basis for evaluating virtual router concept performance.

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2011 IR&D Annual Report

Mobile Autonomous Robotics Technology Initiative (MARTI), 10-R9648

Principal Investigator
Steven W. Dellenback

Inclusive Dates: 07/24/06 – 08/01/11

Background — Technology needed to facilitate the autonomous control of cars, trucks, tractors and military vehicles has made dramatic advances in the last few years led by defense science programs such as the Defense Advanced Research Projects Agency (DARPA) Grand Challenge, DARPA Urban Challenge, and Office of Energy Management (OEM) car and truck industry advances in active safety systems and associated sensors. The Mobile Autonomous Robotics Technology Initiative (MARTI) was initiated to improve safety in urban traffic environments. MARTI is charged with developing new sensor, computing and mobile technologies to augment vehicle platforms and provide autonomous vehicle capabilities.

Approach — MARTI is fusing the latest technology from multiple industries to meet the challenges associated with autonomous control of cars, trucks, tractors and military vehicles. Through the incorporation of technologies and design methodologies from multiple industries such as unmanned aerial systems, intelligent transportation systems, cognitive multi-agent systems, machine vision, engineering dynamics, hardware and software in-the-loop simulation, large-scale multi-function robotics, and safety and reliability systems, SwRI is developing a full-scale autonomous ground vehicle platform to be used for advanced engineering of intelligent vehicle systems and applications development.

Accomplishments — The project has completed with the following accomplishments:

- Concept development and validation that the program is a viable business area for SwRI.
- Initial technology development, with a demonstration at the ITS World Congress in New York City in November 2008. The demonstration included navigating five blocks of 11th Avenue in an autonomous fashion that included other moving vehicles and significant intersection negotiation as well as interacting with pedestrians.
- Repackaging using lower cost hardware as well as adding cooperative vehicle functionality. The functionality to perform convoy operations as well as leader/follower operations was added so that MARTI could be demonstrated at the 2009 Robotics Rodeo at Ft. Hood performing military convoy operations. This functionality included taking the lead position in navigating through city streets.
- Functionality was added to support personnel tracking, tele-operations and seamless switching

Figure 1: The SwRI-developed MARTI fuses the latest technology to meet the challenges posed by autonomous control of vehicles.

between modes so that SwRI could demonstrate military maneuvers that were not included in previous demonstrations. MARTI's ability to interact with pedestrians/soldiers is unique and of significant value to military applications. These capabilities were demonstrated at the 2010 Robotics Rodeo at Ft. Benning.

- The initial hardware component cost nearly $500K. At the end of the program the cost of the hardware required was reduced to approximately $130K. The hardware was packaged in a manner that is deployable in a wide variety of vehicles.

Quantitative Broadband Ultrasound Techniques to Assess Fracture Risk in Bones, 14-R8082

Principal Investigators
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Qingwen Ni
Todd Bredbenner
Adam Cobb
Daniel Nicolella

Inclusive Dates: 07/07/09 – 12/30/10

Background — The state of the art of modeling ultrasound wave propagation in bone cannot explain the intrinsic attenuation caused by wave-induced flow. This is one of the main motivations to implementing more appropriate poroelastic mechanisms to understand the attenuation of broadband ultrasound propagation in bone. A quantitative understanding of ultrasound interaction and attenuation in bone would provide new capabilities for characterizing osteoporosis. Osteoporosis is a widespread public health problem; in the U.S. alone, 20 million individuals already have the disease and an additional 40 million have low bone mass. Currently, there is no cure for this disease. Early diagnosis of osteoporosis with a technique that can monitor bone quality and predict fracture risk is extremely important for both the treatment and prevention of osteoporosis. The proposed effort is based on advanced models of poroelastic mechanisms. These models have been applied to ultrasonic interrogation of saturated clean sandstone, which has similar properties to cortical bone, and has been successful in predicting observed attenuation. To assess the presence of micro-cracks caused by micro-damage, the Biot squirt-flow mechanism will be applied for the first time to evaluate attenuation measurements in either cortical or trabecular bone, and the estimation of bone permeability from attenuation will be a significant advance in the state of the art. An experimental research program of *in vitro* ultrasonic measurements of bone samples will support developing modeling and related signal-processing techniques. Ultrasonic measurements with both longitudinal and shear modes of propagation will be made and compared to the predicted values. Micro-damage will be induced in the cortical bone and trabecular bone samples to provide a baseline for a correlation between microscopic structural properties and the modeled and measured quantitative ultrasound data.

The purpose of this research project is to develop a method based on broadband ultrasonic measurements, processing and modeling to assess bone quality based on frequency-dependent attenuation. The overall goal will be to relate wave attenuation/dispersion and wave signal characteristics to bone mechanical properties, effective micro-damage, and permeability in trabecular and cortical bone. The long-term goals of this project will be to develop a methodology to assess bone quality and fracture risk *in vivo*. Successful execution of this project may provide a basis from which existing clinical bone health diagnostic techniques can be improved or new techniques developed.

Approach — SwRI researchers will perform broadband ultrasound experiments using p-wave and s-wave transducers in bone tissue, without and with induced micro-damage. Ten cortical and 10 trabecular bone samples will be selected to extract mechanic properties and wave attenuation. These properties and attributes will be complemented with other physical properties such as density, dynamic permeability and porosity. The result of the measurements (i.e., attenuation, phase velocity and the wavefield) and physical properties will be cataloged, and will be analyzed qualitatively and statistically and with computer models. The goal is to develop a methodology to assess bone quality from wave attenuation data by relating local-

flow length to the effective bone porosity, pore size distribution and induced micro-damage. The results will be verified using NMR data.

Accomplishments — SwRI researchers have demonstrated the use of poroelastic modeling to successfully simulate spectral and attenuation signatures of bones and to show how the displacement of water relative to the bone structure can affect the wave spectrum. The amplitude spectrum will be strong in highly permeable and porous bones, and small in low porosity and low permeability bones. As a result, the wave attenuation for normal bones is greater than the wave attenuation for damaged bones. The theoretical results agree with the observed spectral responses, ultrasound signatures and attenuation curves. This suggests that a procedure can be implemented to process ultrasound data to identify damaged bones using this concept. To implement such a procedure will require improving SwRI's existing ultrasound system.

Computer simulations to calculate attenuation signatures can be improved by having the experimental source (transducer) function response. This will allow a better fit between observed and calculated attenuation curves. Based on the ultrasonic results, further work needs to be performed on the measurement system to improve future results:

- Redesign the fixture to include simultaneous ultrasonic measurements, both with and without the bone in place (reference waveform). Measurements performed in this fashion would completely eliminate any issues related to temperature.
- Include both pulse-echo measurements (with the two transducers acting as transmitters and receivers, in addition to the pitch catch configuration used for attenuation). This would allow for additional ultrasonic measurements of bone thickness.
- Switch to a smaller transducer diameter to reduce the beam width of the ultrasonic waves. This would further protect against diffraction effects.
- Discontinue examination of the shear wave measurements. While interesting in a research sense, the practicality of measuring attenuations and velocities *in vivo* is limited, given that the sound must propagate through a large amount of water, which does not support shear wave propagation.
- Improve the degassing procedure to ensure that trapped air bubbles do not affect measurements.

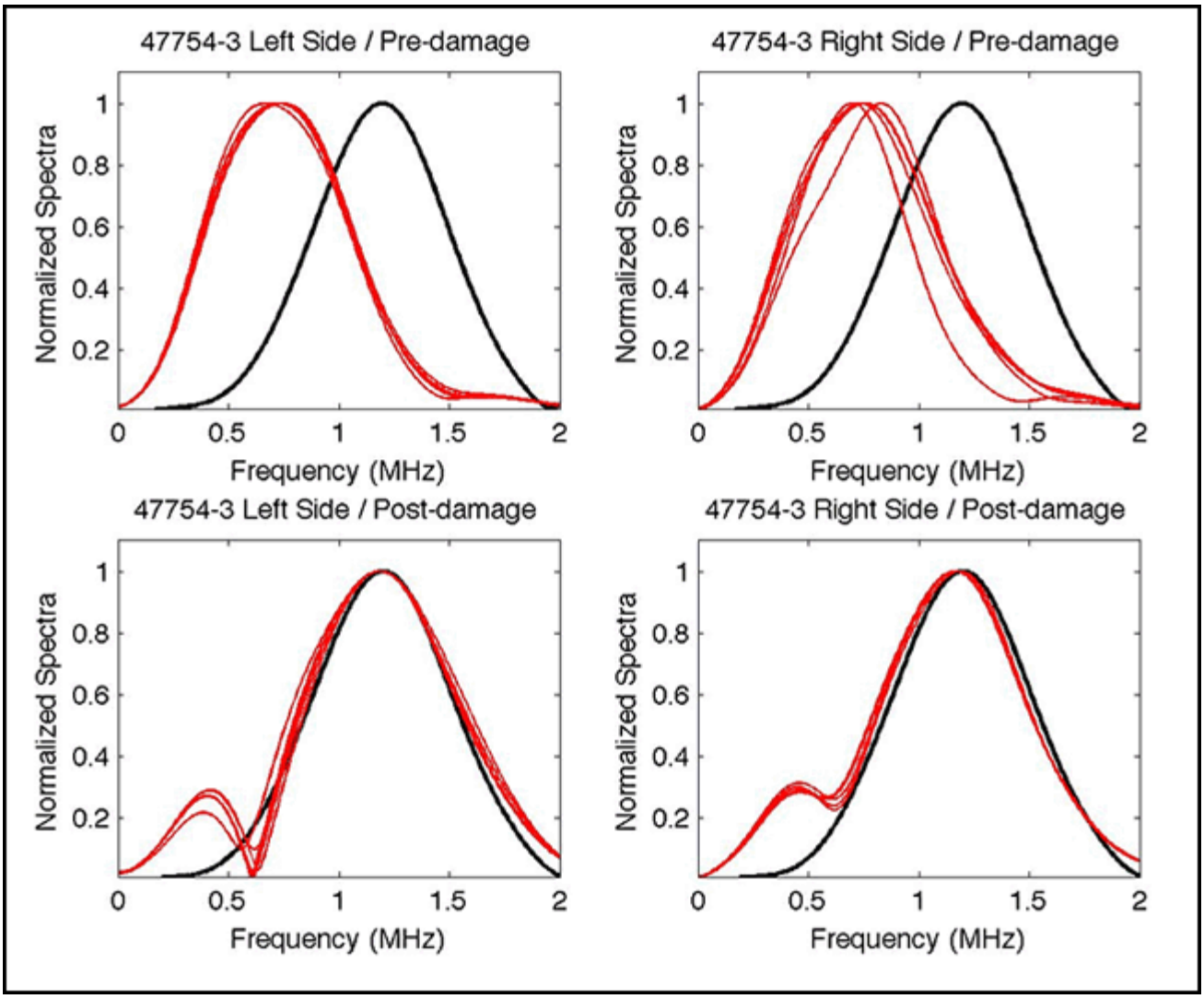

Figure 1. Amplitude spectra of bone sample 47754-3 compared with the water-only spectral response (black line). The amplitude spectrum of the pre-damage sample is shifted toward the low frequencies, and the amplitude spectrum of the post-damage sample follows the amplitude spectrum of the water. This represents the change in velocity between the normal and the damaged bone.

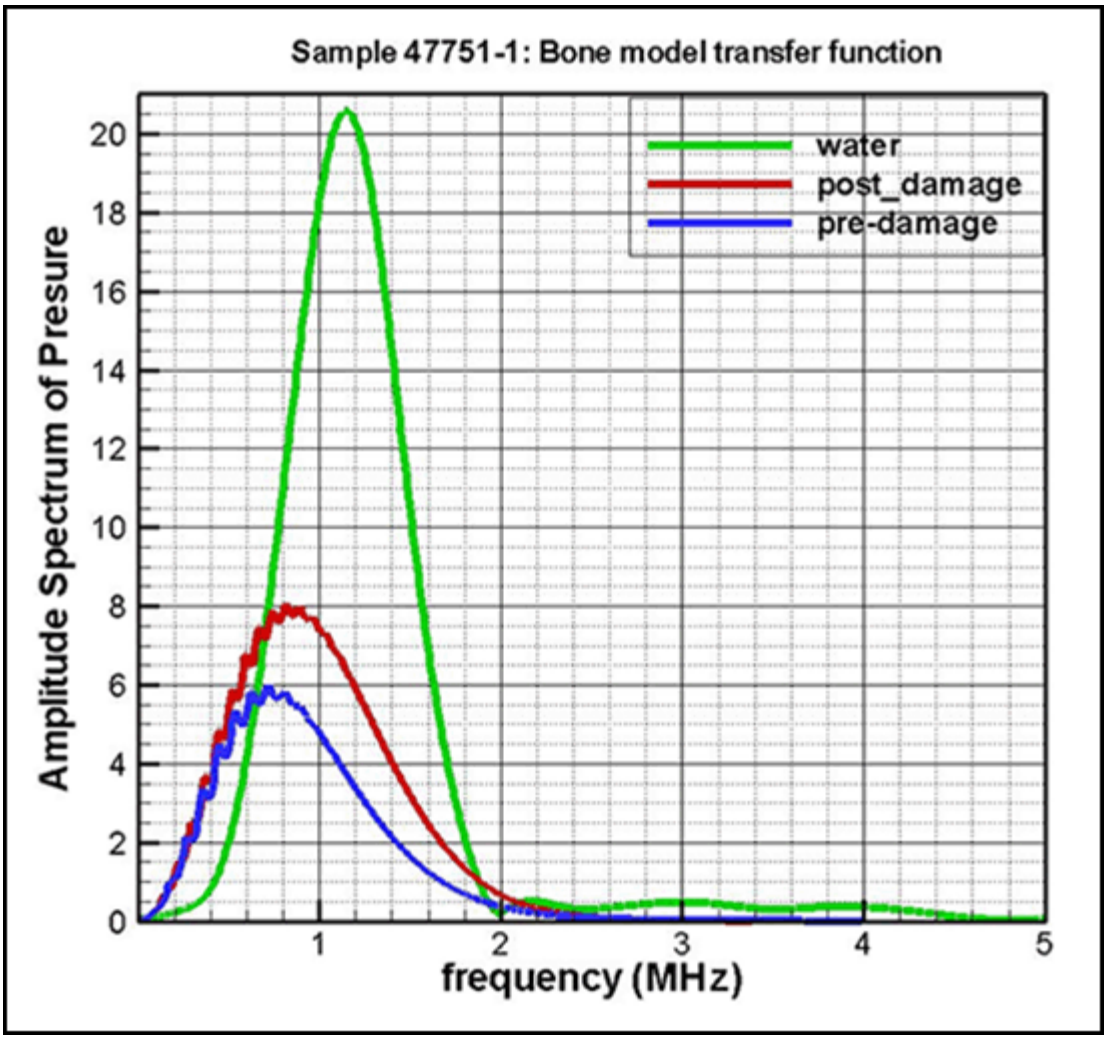

Figure 2. As the bone becomes damaged (i.e., higher porosity and permeability), its spectral signature approaches the water amplitude response (green curve). The trabecular bone samples have permeabilities of several Darcies and porosities more than 80 percent. Thus, as the bone becomes damaged, the wave-induced fluid pressure increases toward the water pressure. In the case of a normal bone (lower porosity and permeability), the wave-induced fluid pressure decreases.

2011 IR&D Annual Report

EDAS® Hardware Renewal, 18-R8163

Principal Investigators
Jay L. Fisher
Ronald H. Peterson

Inclusive Dates: 07/06/10 – 12/31/10

Background — The Enhanced Data Acquisition System (EDAS) includes SwRI-proprietary hardware and software, designed to support ultrasonic inspection of commercial nuclear reactor pressure vessels and piping. To meet customer requests for improved performance and smaller and more portable systems, and to allow long-term support of existing systems that are in current use, it was necessary to redesign the EDAS hardware. The proprietary hardware is primarily the "channel board," which is a digital ultrasonic testing (UT) instrument on a printed circuit board. This UT instrument is specialized to meet the high-speed and thick-wall inspection requirements of nuclear reactors.

Approach — The channel board architecture was redesigned to be compatible with the same bus (VME) as most existing EDAS systems, but also be useable in a smaller chassis as well as existing chassis and to improve performance in the areas of amplitude linearity and maximum bandwidth and digitization rate.

The specific goals of the redesign were to:

- Maintain the ability to manufacture the boards in the future
- Improve performance and enhance capability
- Reduce physical size and manufacturing cost
- Establish intellectual property ownership of the new boards

Figure 1. First delivered EDAS-MS Channel Board.

Accomplishments — The channel board redesign, including basic firmware, was completed. Two portable systems using the new design have been delivered to external customers, and one system was manufactured for internal use.

2011 IR&D Annual Report

Development of a Selective Noncatalytic Reduction (SNCR) System for Stationary NO_x Emission Control, 01-R8213

Principal Investigators
Maoqi Feng
Reggie Zhan

Inclusive Dates: 04/01/11 – 04/01/12

Background — Nitric oxides (NO_x), including nitric oxide (NO) and nitrogen dioxide (NO_2), are toxic pollutants formed during combustion processes. Regulations on nitrogen oxides (NO_x) emission from stationary sources are increasingly more stringent. The selective noncatalytic reduction (SNCR) does not have a catalyst, and has been used for NO_x emission control from stationary sources. It has the potential of solving the problems inherent with selective catalytic reduction (SCR) technology, e.g., high catalyst cost, high maintenance cost and sensitivity to impurities in flue gas. However, one of the disadvantages of SNCR technology is the low NO_x removal efficiency comparing to the SCR technology.

Approach — The objective of this project is to investigate the feasibility of increasing the NO_x removal efficiency of SNCR technology by optimizing the temperature distribution and increasing residence time. The project was focused on developing structured materials to tolerate high temperature with low pressure drop to achieve the objective. Computational fluid dynamics (CFD) modeling was applied to simulate the temperature and flow distributions in the SNCR reactor and calculate the pressure drops with different structured packing materials under different operating conditions.

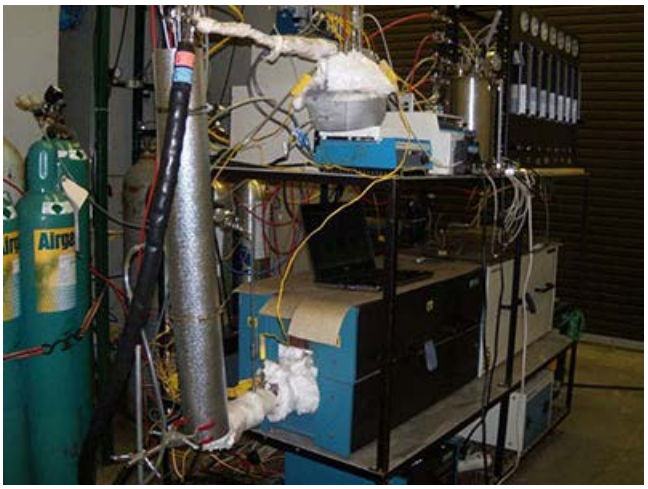

Figure 1. The SwRI-developed SNCR system.

Accomplishments — A prototype SNCR system was developed, as shown in Figure 1. NO_x concentration was measured with ASTM D5504 method (chemiluminescence GC analysis), such that NO_x reduction efficiency was calculated. CFD modeling simulated the temperature and flow distributions in the SNCR reactor and calculated the pressure drop with different packing materials under a wide range of operating conditions. Pressure drop for different packing materials was measured and compared with the CFD modeling results. The system was tested on simulated flue gas with NO_x concentrations in the range of 300 to 500 ppm and temperature from 800°C to 1,000°C. SNCR tests for different NO_x concentrations at 300 ppm, 400 ppm and 500 ppm with NH_3/NO_x = 2/1 showed that the percentage of NO_x removal was increased more than 10 percent with better temperature distribution created by the packing materials, and the ammonia slip was below 2 ppm. Hydrocarbons were also tested to be a very good reducing agent for NO_x removal. The effect of temperature on NO_x removal was also studied.

Causal Investigation of Heavy-Duty Diesel Engine Structural Limitations to Peak Cylinder Pressure, 03-R8116

Principal Investigators
Marc C. Megel
Mark A. Tussing
Barry E. Westmoreland

Inclusive Dates: 11/17/06 – 01/28/11

Background — Advances in emissions technology, fuel economy and power levels of modern heavy-duty diesel engines have increased operating peak combustion pressures to levels at or near the structural limits of the engines' designs. The relationship between design parameters and structural performance for geometrically complex engine components, like cylinder heads or cylinder blocks, is not well understood. Future improvements in the performance of the existing fleet of heavy-duty diesel engines will require an increase in the structural capability of the engine design. This project was targeted at gaining a clear understanding of the relationship between the structural performance and the key design parameters for heavy-duty diesel cylinder heads.

Approach — The approach consisted of conceptual design of a 250-bar capable production-intent cylinder head using computer-aided design solid modeling in addition to casting flow and solidification analysis related to the producibility of key novel features. Cylinder head layout was based on three key requirements. First, the feature geometry had to incorporate those characteristics previously identified in an extensive design-of-experiments analysis as being necessary for 250-bar operation. Second, the geometry needed to be compatible with a specific on-highway, heavy-duty diesel engine manufactured by a major domestic engine manufacturer with whom SwRI has partnered. Finally, the resulting design needed to be producible using available production techniques and materials.

Accomplishments — In Phase 3 of this three-part project, SwRI completed tooling design, casting, machining and hydraulic fatigue rig testing of two first-prototype cylinder heads designed in Phase 2. Test results successfully demonstrated 250-bar cylinder pressure capability with no cracking observed in the high-stress regions. Figure 1 shows the prototype cylinder head undergoing fatigue testing and Figure 2 shows a post-test section used for crack inspection.

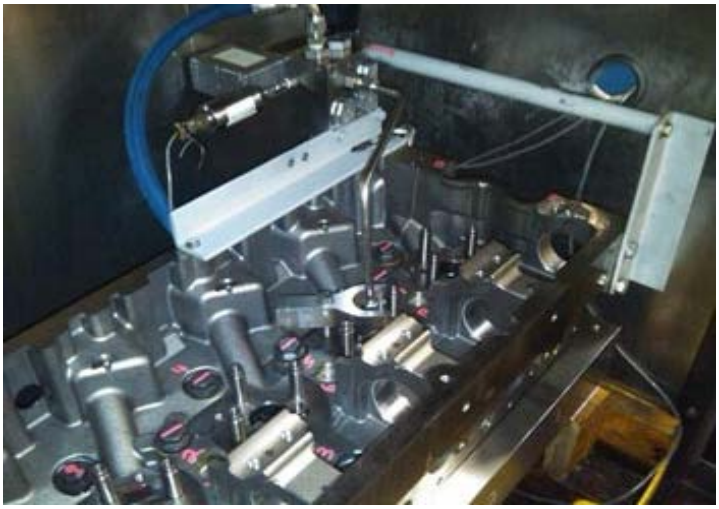

Figure 1. First Prototype Cylinder Head Hydraulic Fatigue Rig

Figure 2. Post Fatigue Test Cylinder Head Section for Crack

under Test.

Inspection.

2011 IR&D Annual Report

A Multidimensional Controls Framework for Diesel Engine Fuel-Air Management, 03-R8179

Principal Investigator
Jayant Sarlashkar

Inclusive Dates: 08/19/10 – 09/19/11

Background — Automotive emission standards continue to become stricter around the world, and industry often responds by incorporating innovative combustion and exhaust treatment technologies into new products. In this context of regulatory (e.g., emissions, diagnostics), consumer (e.g., performance), and corporate (e.g., CAFE) requirements, the automotive engine truly provides a multi-objective optimization and a multivariable control problem. The optimization problem pertains largely to operating the combustion and after-treatment system, and yields engine system characterization needed to address the control problem. However, the challenge of controlling the large number of actuators while managing interactions grows rather quickly. This increased complexity exposes the limits of the traditional method of using single-input single-output proportional-integral-derivative (PID) controllers. The main goal of this work was to develop an analytically sound and practically useful extension of the traditional PID controller to a cross-coupled multivariable form. SwRI researchers focused specifically on the diesel engine, but expected the basic results to be applicable to a wide variety of generic control challenges (including gasoline and alternative fuel engines).

Approach — The premise of the SwRI solution to the control problem is intuitively simple — manage production of pollutants and performance at source; i.e., in the combustion chamber. It is only natural that combustion can be better controlled if the conditions in the combustion chamber (also referred to as the cylinder state) are known and steered in the desired direction, and the fuel is matched to the prevailing cylinder state.

This premise naturally divided the work into three main tasks:

- Cylinder-state-based fueling. Researchers established fueling as a function of the cylinder-state: oxygen mass, oxygen concentration, intake manifold temperature, and coolant temperature. Researchers showed that such a fueling scheme could become unstable at light loads and provided an alternative solution for that region of engine operation.
- Active management of cylinder-state. The cylinder-state-based fueling manages pollutant production at source, but the cylinder-state must be managed properly to deliver the desired performance (torque response, emissions etc.). SwRI researchers spent most of the time on this part of the problem and derived a systematic method to devise multivariable PID controllers that account for and exploit the natural cross-coupling among the subsystems.
- Adaptation of standard design of experiment (DoE). Items (1) and (2) require systematic and efficient ways to collect and process experimental data. SwRI adapted the standard methods of DoE within the framework of available experiment space. For example, the gridding (or levels) normally called for in the traditional DoE cannot be applied directly to the problem at hand because the so-called "independent" variables can be controlled only indirectly.

Accomplishments — Researchers began the effort with a physically based dynamical model of the diesel engine with a dual-loop exhaust gas recirculation (EGR) system. Some elementary, but powerful ideas from network and graph theory were applied to develop a compact representation of the engine

system. Subsequently, this representation was used to develop a general method for design of controllers given a set of target states and inputs. In doing so, researchers "factored" the problem into dynamical and algebraic portions. Some ideas from the sliding mode control theory were adopted to address the dynamical portion and from multi-port network description to address the algebraic portion. Researchers developed methods to handle the issues of windup, over- and under-actuation and actuator saturation. On the fueling side, formulas were developed to compute fueling parameters suitable for the given cylinder state. The SwRI team conducted a stability analysis of the fueling scheme and showed ways to achieve stable combustion in all regions of engine operation (idle, light-load lean, lean, and rich). Over the course of the project, several dozen controllers were constructed and evaluated, and a combination of four controllers was selected to cover the entire operating range of engine including cold start.

Researchers evaluated the controller on two platforms: a 2-liter-class diesel passenger vehicle, and a 13-liter-class diesel truck. The evaluation criterion was to simultaneously meet the performance and regulated emission norms. The passenger vehicle was driven on the standard European (NEDC) and U.S. (FTP75) test cycles. At of the end of the project, the vehicle was close to meeting the NEDC standard without any NO_X after-treatment. The vehicle also showed high potential to meet the FTP75 standard with NO_X after-treatment. The truck engine was subjected to the standard U.S. (HDFTP) test cycle. The emission and performance metrics met or exceeded the standard. The method was applied successfully to two significantly different test platforms, establishing scalability of the approach.

The analytical depth of controller development and favorable results of testing allow researchers to be excited about the future of this method. SwRI expects the abstract thought process and its software implementation will form the foundation of its work in simultaneously meeting the aforementioned triad of requirements — performance for the consumer, fuel economy for the corporations and emission for the regulators. The methods are generic enough to be applicable to a large variety of control challenges.

2011 IR&D Annual Report

The Investigation of the Formation, Composition, and Durability of Zinc Dialkyldithiophosphate Films in a Spark-Ignited Gasoline Engine, 08-R8215

Principal Investigators
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Vasiliki Poenitzsch
Robert Mason
Fred Gerhart

Inclusive Dates: 03/01/10 – Current

Background — Zinc dialkyldithiophosphates (ZDTPs) are common additives used in engine lubricants to primarily improve their antiwear (AW) performance and secondarily serve as an antioxidant in the oil. Although this technology has been in existence since its invention more than 60 years ago, little is understood about the mechanism that allows ZDTPs to have such great AW performance. Past research has shown that ZDTP forms a sacrificial film that separates two metal components in relative motion to mitigate or prevent metal-on-metal contact. The film composition, formation and durability are shown to be affected by bulk temperature of the lubricant, loading on the two metal surfaces and exposure to nitric oxides (NO_x) in an aqueous solution. However, many of these experiments are restricted to bench-top test setups whose test conditions are set at coarse increments that may or may not reflect actual engine operating conditions. Also, no quantitative model exists that gives a general overview of the behavior of ZDTP films. This project seeks to study the changes in composition of ZDTP films while exposed to the harsh conditions of a fired engine test. Specifically, temperature of the oil in the valvetrain area, valve spring loads and crankcase NO_x concentration will be the test variables in these experiments. The relationship between the composition of ZDTP films and the specified test variables will be quantitatively characterized in a response surface model developed from the data obtained during the experiment.

Approach — The data required to formulate the response surface model will be obtained from the results of an experimental matrix involving three levels of variation in each of the following three test variables: oil temperature, valve spring loads, and crankcase NO_x concentration. Control over oil temperature and valve spring loads are relatively simple to achieve, but control over crankcase NO_x concentration will require a separate response surface model that requires a separate test matrix to develop. The test matrix for crankcase NO_x concentration will consist of three levels of variation in each of the following five test variables: engine load, fresh air flow to the rocker arm cover, spark advance, air-fuel ratio and piston ring gap. During the experiments, these five test variables will be independently controlled. The data obtained from this test matrix will be used to formulate a response surface model that characterizes crankcase NO_x concentration at various levels of each of the aforementioned five test variables.

Accomplishments — The investigation team has successfully established control over the test engine's operating temperatures, AFR and spark advance. A response surface model of the crankcase NO_x concentration with respect to engine load, fresh air flow to the rocker arm cover, spark advance, AFR and piston ring gap has been established. The investigation team will proceed to use this response surface model to establish operating conditions that can generate high, medium and low levels of crankcase NO_x concentrations for the main experimental matrix that tests for the effects of oil temperature, valve spring loads and crankcase NO concentration on the composition of ZDTP films.

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2011 IR&D Annual Report

An Integrated Approach for Estimating Groundwater Storage Variations in Regional Aquifers, 20-R8051

Principal Investigators
Alexander Sun
Ronald Green

Inclusive Dates: 04/01/09 – 12/01/10

Background — This project tackled a strategically important research area related to using Earth observation products for societal benefit. The availability of adequate and safe drinking water supplies has been and will continue to be critical. However, water resources are not evenly distributed. Some countries are water rich, while others are water poor. In recent years, remotely sensed data have been used extensively to monitor surface and near-surface components of the water cycle. This project evaluated the potential use of precision gravity data to measure temporal and spatial changes in the storage of water in aquifers.

Approach — The technical objectives of this project were to develop and test an integrated approach for combining GRACE (Gravity Recovery and Climate Experiment) satellite data with *in-situ* measurements and a land surface model to better constrain estimates of the water budget in regional aquifers; and demonstrate the utility of the developed approach for managing the interconnected Edwards-Trinity Plateau and Pecos Valley aquifers system in west Texas. The aquifers cover a combined area of 115,000 km^2. At the global level, several worldwide initiatives focusing on Earth observations and the hydrologic cycle have been launched. Characterizing the storage and fluxes of sub-surface water has proven less tractable to typical satellite methods. A noticeable and important exception is GRACE, a joint satellite mission launched in March 2002 by NASA and its German counterpart, Deutsches Zentrum für Luft-und Raumfahrt. GRACE comprises two identical satellites at about 500 km altitude, separated by about 220 km, in identical near-polar orbits. GRACE measures Earth's gravity field and its changes over time using range-rate perturbations between the two satellites sensed with a microwave interferometer. Over land, and accounting for atmospheric circulation, changes in the gravity field are mainly attributed to temporal variations in terrestrial water storage (TWS), which is a vertically integrated measure of water storage that includes groundwater, soil moisture, surface water, snow water equivalent and biomass water. Hence, GRACE gravity data can be used to monitor temporal (near-monthly) TWS variations.

Accomplishments — This project resulted in three main technical achievements. First, SwRI researchers, in collaboration with NASA and the National Center for Atmospheric Research, developed an algorithm for estimating aquifer storage parameters using GRACE data. Previous studies focused mainly on validating GRACE observations. This study not only showed the responses of GRACE signals to TWS in the study area, but also demonstrated for the first time the utility of GRACE data for solving groundwater inverse problems. Second, a multiobjective optimization strategy was developed to calibrate regional groundwater models using GRACE data by adjusting hydraulic conductivity, specific yield and recharge multiplier simultaneously. Finally, a webGIS prototype application was developed to visualize Groundwater Availability Model (GAM) results online.

Aquifer storage parameters play an important role in transient groundwater flow simulations and in water resources planning. However, determining representative storage values using traditional techniques (e.g., pumping test) is challenging, especially at the regional scale. To address this problem, a robust optimization method for estimating aquifer storage parameters (specific yield or storativity) using the GRACE data, *in-situ* well level observations and other ancillary information was developed. Uncertainty

inherent in the remotely sensed and *in-situ* time series can adversely affect the parameter estimation process and, in the worse case, make the solution completely meaningless. An estimation problem was formulated to directly minimize the negative impact of data uncertainty by incorporating bounds on data variations. This method is demonstrated for the interconnected Edwards-Trinity Plateau and Pecos Valley aquifers in central Texas. The study area was divided into multiple zones based on the geology and monitor well coverage. The estimated aquifer storage parameters are consistent with previous results obtained from pumping tests and model calibration, demonstrating the potential of using GRACE data for validating regional groundwater model parameters.

Previous GRACE studies highlight the importance of identifying distributed storage values instead of assuming a uniform global value for all wells in the study area. This work complements such a goal. Finally, the importance of maintaining high-quality *in-situ* monitoring networks is emphasized, which will significantly help extend the benefits of GRACE data for groundwater resources analyses.

2011 IR&D Annual Report

Development of Parallel Subsurface Multiphase Flow Simulation Capability, 20-R8087

Principal Investigators
Hakan Basagaoglu
Will L. Arensman
Stephen W. Cook

Inclusive Dates: 01/01/09 – 01/01/11

Background — Multiphase subsurface flows are important to radioactive waste repository assessments. SwRI researchers have acquired considerable experience in multiphase subsurface flow analyses, which often require computationally demanding simulations. Prior to this project, researchers developed an in-house numerical code, *xFlo*, for continuum-scale simulations of non-isothermal, multiphase flows in deep geological fractured-porous domains. Multiphase subsurface flows are also of interest in a variety of other applications including geological sequestration of carbon dioxide, geothermal energy production, compressed air energy storage in aquifers, groundwater recharge and contamination assessments, bioremediation, studies of permafrost and investigations of Mars and other solid bodies such as the moons of Jupiter and Saturn. Parallelization of *xFlo*, based on multicore computers arranged in clusters, was needed to take advantage of existing computing hardware. Hence, the main objective of the project was to parallelize *xFlo* for computationally efficient multiphase subsurface flow simulations that could be used in diverse applications.

Approach — Parallelization of *xFlo* is complicated by the need for fully implicit timestepping in the solution algorithm and the use of unstructured grids in model step-up. Researchers proposed using domain decomposition parallelization implemented with one-sided message passing interface (MPI) communication, which was added to the serial version of the *xFlo* code. In this approach, a preprocessor was used to decompose the data set into smaller, yet similarly constructed, data sets. Each smaller data set (associated with different subdomains) was assigned to different processors. With this approach, the original *xFlo* source was largely kept the same, with code introduced at key points to perform ghost cell exchanges between processors. Updates of the ghost cells (which collectively form a subdomain halo where information exchange between processors occurs) were delayed until the end of each timestep. Ghost cells were used in domain decomposition to ensure flux continuity between adjacent subdomains. By delaying halo updates until the end of a timestep, interdomain flux information was not communicated during Jacobian matrix construction.

Accomplishments — A newly proposed parallelization approach based on the domain decomposition method via one-sided MPI communication was successfully implemented in the *xFlo* code. In demonstrative one-dimensional simulations, the proposed parallelization approach resulted in 1.79 to 2.37 times speed-up on four processing cores, indicating that the proposed approach is computationally efficient. External coupling of the parallelized *xFlo* code with the existing and widely used standalone geomechanical (e.g., FLAC3D) and/or geochemical (e.g., Geochemist's Workbench) software was proposed to the U.S. Nuclear Regulatory Commission (NRC) as part of business development. The NRC agreed that coupled models would offer a new computational tool simulating coupled thermal, hydrological, mechanical, and/or chemical processes that the NRC staff can use in their independent analyses for evaluating the performance of proposed deep-geological formations for high-level waste disposal. In fiscal year 2012, development of coupled models will be conducted under the NRC Integrated Spent Nuclear Fuel Regulatory Activities program.

2011 IR&D Annual Report

Numerical Simulation of Multiphase-Flow-Enhanced Erosion-Corrosion Problems, 20-R8088

Principal Investigators
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Todd Mintz
Steve Green
Debashis Basu

Inclusive Dates: 10/01/10 – 09/01/11

Background — Fluid flow enhances corrosion by accelerated transfer of corrosion products from the reaction site. Any dissolved chemical species in the fluid also affects the water chemistry and corrosion environment by controlling the pH, electrochemical corrosion potential and reaction rate. On the other hand, erosion is a mechanical process that may take place either due to presence of a secondary solid phase such as sand in the flow or due to fluid shear that breaks away the layer of corrosion products. The detached corrosion product behaves like a solid particle and may cause further erosion upon wall impact. The erosion process can be influenced by fluid flow parameters such as velocity or turbulence. It also may depend on the physical characteristics of the solid particles, such as their diameter and shape, and their dynamic characteristic such as impingement velocity and angle. Erosion is known to enhance wall corrosion by peeling the wall protective layers and exposing the base metal to further corrosion. The combined effect of the erosion-corrosion process is greater compared to each individual process acting independently. Flow-enhanced erosion-corrosion problems are encountered in almost every engineered system including power plants, process industry and pipeline networks. The present study focuses on the erosion-corrosion encountered in the secondary cooling circuit of nuclear power plants (NPP), where a number of fatal accidents have occurred because of erosion-corrosion damage of pipelines. Modeling the erosion-corrosion process is highly challenging, as it could be affected by a large number of flow parameters that are difficult to control and quantify simultaneously. Existing system level tools are currently used to predict erosion-corrosion processes based on empirical correlations that yield reasonable results for simplified flow conditions. The objective of the present study is to develop a methodology to calculate combined erosion-corrosion damage in NPP secondary coolant circuits for relatively complex flow conditions such as occur at T-joints, expansions and bends.

Approach — In the current study, the flow field and particle motions will be solved using a commercial computational fluid dynamics package, ANSYS-FLUENT. Initially, the flow modeling will simulate a multicomponent continuous phase that includes water and the dissolved corrosive gas. Detailed simulation of water chemistry will be done to understand the effect of oxygen scavengers such as hydrazine in the wall mass transfer process. The discrete phase simulation will model the behavior of solid particles such as sand or debris. This will be useful in location-critical surface areas where the protective corrosion product layer has been removed because of erosion. The chemical corrosion process will be modeled as a mass transfer process that depends on diffusion of corrosive agents through a boundary layer and diffusion of metal through an oxide layer. Specialized water chemistry, corrosion kinetics, and erosion models are being implemented as customized field functions.

Accomplishments — A bend pipe section has been identified as the workbench for the current research, because this configuration is regularly encountered in secondary coolant circuits of nuclear power plants. Detailed hydrodynamic simulations revealed the complex secondary flow patterns that occur in the bend section and how the flow pattern affects the wall mass transfer. The study also showed the Reynolds

Stress Model to be most effective in predicting secondary flows and surface mass transfer rates. In addition, a detailed water chemistry study examined the effect of oxygen scavengers in the wall mass transfer process. Simulation showed the effect of surface reaction on the overall corrosive species distribution. Discrete solid phase sand particle trajectory calculations elucidated the solid particle impingement locations. Three different erosion models have been implemented and tested in the solver. Currently, project staff are developing the detailed corrosion model and are coupling the corrosion and erosion models.

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2011 IR&D Annual Report

Fluid-Dynamics Based Analysis of Landslides, Debris Flow, and Liquefaction Induced Ground Displacement for Hazard Assessment, 20-R8089

Principal Investigators
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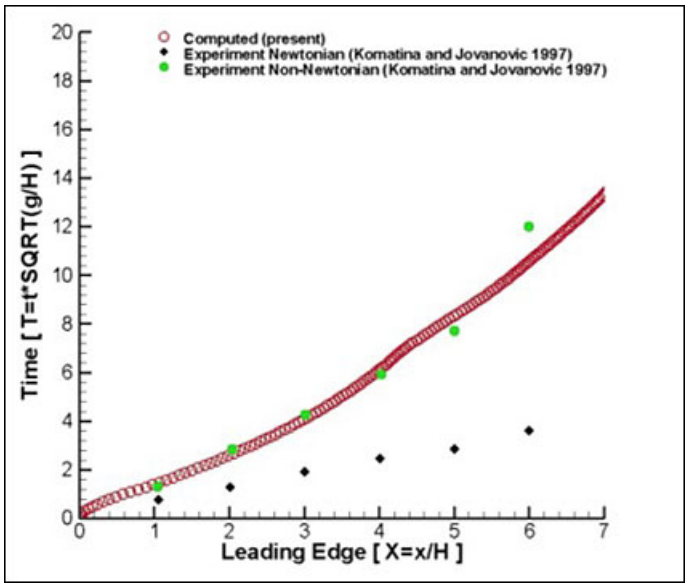
Kaushik Das
Steve Green
Ron Janetzke
John Stamatakos

Inclusive Dates: 10/01/10 – 09/01/11

Background — Landslides and debris flows are a source of societal safety hazard and economic impact throughout the world. The occurrence of a landslide depends on a number of factors including bedrock geology, geotechnical properties of surface materials, rheology and groundwater conditions. The large spectrum of landslide phenomena makes it difficult to define a single standard technique to evaluate landslide hazards and risk. However, a detailed analysis of the relationship between landslides and their various causes not only provides insight into landslide mechanisms, but can also form a basis for predicting the occurrence of future landslides and assessing the landslide hazards. A similar class of natural geotechnical hazard is the liquefaction of loose, saturated, cohesion-less soils and other granular materials during large-magnitude earthquakes. Lateral spreading induced by seismic liquefaction causes large ground displacement and shear strains that can damage and disrupt pile foundations of buildings and bridges, embankments, river dikes, pipelines and waterfront structures. Most prior analyses of debris and landslide flow and liquefaction-induced lateral spreading employed numerical techniques such as the finite element method (FEM) and discrete element method (DEM). Compared to FEM and DEM, a mesh-free computing method such as smoothed particle hydrodynamics (SPH) provides a significant advantage in handling large deformation and postfailure analysis. The broad overall objective of this research is to establish a generic SPH-based computational framework capable of solving problems in geomechanics that involve both small and large deformations.

Approach — A SPH-based computational framework is used to predict the size, shape, and runout length of debris flows, landslide flows and liquefaction-induced lateral ground displacement. The computational framework is supported by limited experiments related to the rheology of the debris and liquefied soil. Simulations are carried out for cases where experimental data and analog site data are available. The rheological characteristics are amenable to changes in the flow characteristics, geometry and material properties for flows with free-surface deformation.



Accomplishments — The Herschel-Bulkley, Bingham plastic and the power law model in the SPHYSICS code were implemented. These are the classical non-Newtonian models used in the

simulations. The models were validated against experimental data from problems involving non-Newtonian fluids. These simulations highlighted both the importance and complexity of rheology, and the effect of simulation parameters on predicted solutions. The non-Newtonian model results matched well with experimental data. A physical experiment was conducted to analyze different rheological formulations with observed data. The dynamics and motions of landslides and liquefied soils are strongly dependent on the apparent viscosity of the materials. Parametric studies of spreading of soils after liquification revealed that yield stress and viscosity play very important roles in the liquefaction process and control the extent of liquefaction. The SPH technique was found to be a very effective tool for modeling the spreading of liquefied soil.

Figure 1. Comparison of Velocity Profiles for Mud Flow with Non-Newtonian and Newtonian Models.

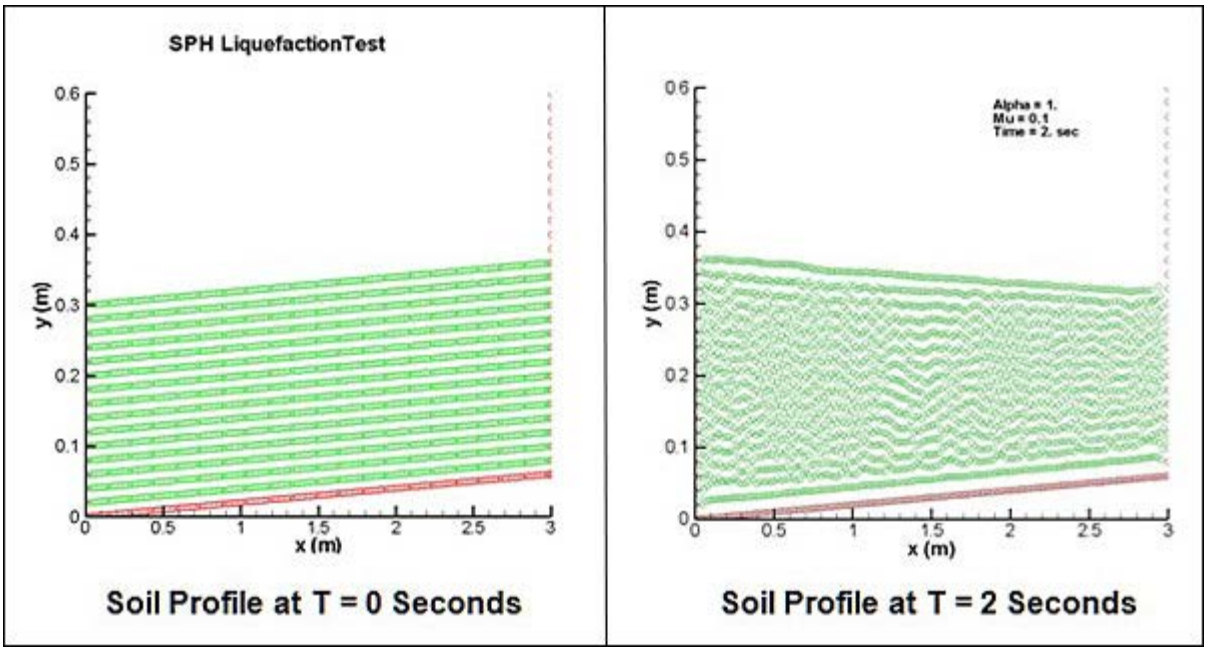


Figure 2. Soil Profiles at Initial State and at 2 Seconds After Liquefaction.

2011 IR&D Annual Report

Effects of Increased Atmospheric Carbon Dioxide on Environmental Transport of Radionuclides, 20-R8091

Principal Investigators
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Amy Glovan
David Turner
Deborah Waiting

Inclusive Dates: 09/01/09 – 04/01/11

Background — Global atmospheric CO_2 concentrations have been increasing for some time, and this change can potentially affect many Earth systems and processes, including environmental transport of radionuclides and heavy metals. Increases in atmospheric CO_2 are expected to continue such that CO_2 concentrations at long times in the future will be much higher than present values. These increased CO_2 concentrations may have particular impact on radioactive waste disposal systems, which must be capable of limiting environmental transport of radionuclides for thousands of years. This project evaluated the potential significance of such changes.

Approach — The technical approach for this project was to identify and acquire measurements of groundwater compositions from a selected groundwater system spanning recent decades and corresponding measurements of atmospheric CO_2 concentrations. The Edwards Aquifer system was selected for this work because of the comprehensive data available (e.g., thousands of wells and numerous springs sampled and measured for more than 50 years over a large geographic area). Further, because carbonates like the Edwards Aquifer respond quickly to recharge and are the aquifer host rocks most sensitive to changes in groundwater chemistry produced by variation in atmospheric CO_2, the atmospheric chemistry signal was anticipated to be clearest for a carbonate aquifer. Whatever effects were found in the Edwards Aquifer would be applicable to other types of carbonate aquifers and would be bounding for noncarbonate aquifers.

Accomplishments — SwRI researchers identified, obtained, and regularized a set of data containing 23,394 individual water chemistry records spanning from 1913 through 2009. These data were screened sequentially to identify those records that were analytically complete, charge balanced and representative of the bulk of the aquifer. Water records that did not meet these criteria were eliminated from further consideration, leaving 3,385 records. This resulting set was further refined to focus on individual wells for which there are data spanning 30 years or more and for which there are three or more analyses. This reduced the set to 1,074 individual water analyses on 89 wells. These remaining wells span six counties (with the preponderance of the wells in Bexar County) and include the years 1942 through 2009. Researchers used statistical analyses to evaluate potential trends in water chemistry for these records, with particular attention to bicarbonate because it is the aqueous component that will change most as a result of increasing atmospheric CO_2 and is potentially important for increasing contaminant transport. Fifty-four of the 89 wells were found to have statistically significant positive 30+ year trends for bicarbonate concentration. This predominance (61 percent) of positive bicarbonate trends among those wells with long-term records is consistent with what would be expected from interaction with increasing atmospheric CO_2.

Geochemical modeling of ranges of historical geochemical speciation as well as projecting future water

chemistries showed that there would be systematic effects of atmospheric forcing that could influence and reduce hypothetical radionuclide sorption. These effects are small, however, and are generally masked by complicating factors such as biological activity, equilibration with limestone, and natural spatial variability. This relatively small effect is especially true for the historical data, where changes in atmospheric CO_2 are on the order of 20 percent, but also is true even for projections of up to 2,000 ppm CO_2.

This project was successful in identifying and quantifying past groundwater chemistry responses to changes in atmospheric CO_2 concentrations over a period of decades. These changes were evaluated temporally and spatially, and ranges of potential effects were projected for the future.

Potential weakness of the atmospheric chemistry signal as reflected in the historic groundwater chemistries was recognized during planning for this project. Quantification of the signal confirmed that weakness. Starting with a very large historical dataset, screening the data for those records of highest quality, and carefully analyzing the resulting information, researchers found that though changes in groundwater chemistry resulting from increases in atmospheric CO_2 were discernable and statistically significant, the changes have limited effect on the potential for contaminant transport.

The Edwards Aquifer system chemistry is robust in response to atmospheric chemistry forcing; even larger increases in atmospheric CO_2 projected for the future are likely to produce only modest changes in contaminant transport capability. The improved quantification of the degree to which effects of changes in atmospheric CO_2 on groundwater chemistry are reflected in historic data demonstrates the resilience likely to be present in other such systems, even in response to large changes in atmospheric chemistry. As the broader climate change debate has evolved nationally and internationally in recent years, many potential climate change effects have been postulated. Some of those projections invoke dramatic scenarios. Whereas strong changes appear to be occurring in some natural systems, information from this project documents the substantial buffering capacity present in major groundwater aquifers and provides an improved basis for related decisions.

A Slope Stability Hazard Ranking Algorithm for Frozen Soil Terrains, 20-R8096

Principal Investigators
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D. Marius Necsoiu
Goodluck I. Ofoegbu

Inclusive Dates: 08/01/10 – 12/01/10

Background — The objective of this research was to develop and demonstrate an algorithm for ranking the risk of slope failures and thermokarst development in areas underlain by permafrost (ground that is continually frozen for at least two years) due to permafrost thawing. The algorithm is incorporated into a geographical information system (GIS) application that uses remote sensing data analysis, land classification mapping and geological risk assessment to identify areas susceptible to the risks of frozen soil thawing caused by climate change.

Approach — The algorithm integrates a numerical ground thawing and freezing dynamics (GTFD) model for calculating the thickness of the active layer and depth of permafrost with simple slope stability, mass wasting and thermokarst development models. The algorithm is informed by soil, vegetation and slope classification maps derived from optical and multi-polarization synthetic aperture radar imagery and existing soil and land classification maps. The algorithm is applicable to both current and future climate conditions, and can be validated by ground movement measurements derived from interferometric synthetic aperture radar (InSAR) and multispectral data displacement analysis (MDDA) methodologies.

Accomplishments — The algorithm was demonstrated using data from the Kobuk Valley in north-central Alaska developed during another internal research project, an on-going NASA-funded grant to study the Great Kobuk Sand Dunes, and soil/vegetation classification maps provided by the National Park Service. Soil thawing probability and slope failure risk maps were developed for the study area and used to illustrate the capabilities of the slope failure algorithm to assess risk to infrastructure such a pipelines.

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2011 IR&D Annual Report

Development of Computational Methodology to Assess Structural Damage in Spillway Sections of Dams, 20-R8131

Principal Investigators
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Ron Green

Inclusive Dates: 01/01/10 – 10/01/11

Background — Damage from scour and erosion of rock downstream of dam spillways is a safety concern. Spillways are overflow structures and high-velocity flows over unlined spillways can cause significant damage by erosion and headcutting of the bed rock risking instability of the dam. Examples of rock scour and erosion of hard rock from high discharges during flood inflicting severe damage are Bartlet Dam, Arizona; Tuttle Creek and Milford Dams, Kansas; Kariba Dam, Zimbabwe; Ricibayo Dam, Spain; and Srisailam Dam, India. High Flows caused significant erosion of the rock at the toe of the Midskog Dam in Sweden and on the unlined spillway at Canyon Lake Dam, Texas. Scouring of riverbed rock is induced when the erosive capacity of the water exceeds the resistive capacity of the rock mass. The erosive capacity of water is related to the flow conditions. Indicator parameters most often used are flow velocity, shear stress and stream power. The resistive capacity primarily relates to the ability of the rock mass to withstand the hydro-mechanical forces from the flowing water. During the erosion process, the rock blocks are ejected or fractured from the riverbed and swept away by the flow of water. The process stops when the energy is insufficient to cause further rock breakage or raise the broken material out of the scour hole. Currently, the dam industry relies primarily on physical model testing and empirical methodologies to predict scour potential and guide the hydraulic design of the spillways. These approaches, however, cannot accurately predict scour location, extent, and depth in the prototype structure or help understand erosion dynamics.

Approach — The dominant failure modes for erosion of unlined spillways are rock block removal, brittle fractures of rock and fatigue fracturing. All the failure modes are caused by transient water pressure in the rock joints or in preexisting closed fissures. In this research, a methodology is developed to explicitly evaluate the erosion mechanism by computational modeling. The methodology integrates fluid dynamics modeling techniques that are used to simulate the water flow with a geotechnical model that is used to assess rock damage caused by the impacting fluid. The erosive capacity of water is estimated by fluid dynamics simulation of the turbulent water flow and resistive capacity by geomechanical modeling of the rock. Computational fluid dynamics (CFD) is used to model the unsteady turbulent flow field caused by spillway discharge. Time-dependent pressure and shear stress on the spillway surface were obtained from the CFD calculations that were subsequently used in the geomechanical discontinuum model. The geomechanical model explicitly includes geologic structural features of jointed rock media, and the intact rock blocks between the joints were modeled as micro blocks by Voronoi tessellation. The hydrodynamic response of the rock caused by transient pressure and shear stress modeled the scour damage simulating block removal and brittle fracture modes. The modeling approach is a coupled process between CFD and geomechanical analyses. Therefore, after each cycle of CFD and geomechanical analysis, the geometry of the model is modified based on scour profile and the process is continued until the water jet fluctuations have insufficient energy to induce further erosion. Based on a review of the

literature and interactions with peers at conferences, a coupled approach using fluid dynamics and discontinuum modeling to predict spillway erosion has not been demonstrated before.

Accomplishments — The plunge pool of the Kariba Dam in Zimbabwe and the emergency spillway of Canyon Lake Dam in Texas were used as examples to demonstrate that the methodology can model the critical failure modes of spillway erosion. Kariba Dam is a concrete arch dam on the Zambezi River. There are six rectangular-shaped gates near the crest of the dam. The water jet emerging from these gates when open impinges on the plunge pool from a height of 75 m. The plunge pool progressively scoured from 1962 to 1982, yielding a scour profile. CFD simulations have been carried out for a single gate opening with velocity inlet boundary condition replicating the measured velocity of the water jet. The three-dimensional flow-field pattern of the jet and its interaction with the plunge pool water was simulated and pressure fluctuation from jet impact on the plunge pool rock bed was obtained. Geomechanical modeling of the erosion process of the riverbed material consists of several stages that involve initialization of the model and application of jet impact loading from CFD modeling. The analysis showed the scour depth and profile are controlled by the joint orientation, while the damage of rock is controlled by the brittle fracture.

During the record flood in 2002, the emergency spillway at Canyon Lake Dam was overtopped for the first time, resulting in excavated soil and trees as well as significant erosion and transport of rock, thus creating the Canyon Lake Gorge. The time-dependent velocity profile similar to the flood hydrograph was used to specify the inlet condition for the CFD model. The CFD model provided the unsteady pressure and shear stress distribution at several points along the spillway floor. During overtopping of the spillway, the pressure fluctuations on the spillway water rock interface were transmitted in the rock joints. The geomechanical analysis demonstrates that the block separation and removal or plucking failure modes are similar to that observed at site.

The combined approach provides a significant advantage over existing physical and empirical models because multiple full-scale numerical model analyses can be performed to study changes in flow characteristics, geometry, and material properties at a significantly lower cost and turnaround time and with greater certainty and accuracy. Additionally, geomechanical modeling provides an understanding of the dominant mechanism of scour and the extent of damage allowing study of the effectiveness of mitigation system design (e.g., rock bolts, cut-off walls). The results were presented in three conference papers. One received the Outstanding Poster Presentation Award at the U.S. Society of Dams 2011 Annual Meeting and Conference, held April 2011 in San Diego, Calif.

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Monitoring Permafrost Landscapes Using Optical and Multi-Polarization SAR Imagery. Case Study: Kobuk Valley, Alaska, 20-R8144

Principal Investigators
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Donald M. Hooper
Ronald N. McGinnis
Gary R. Walter

Inclusive Dates: 04/01/10 – 10/01/11

Background — This project was undertaken to develop an integrated methodology for using a variety of remotely sensed data to detect and monitor changes in Arctic and other cold region landscapes. The approach combined products developed from synthetic aperture radar (SAR) and optical airborne and satellite imagery. The project focused on applying these techniques to detect climate-induced changes to landforms in Kobuk Valley National Park in north-central Alaska. This target location was selected because of its ecological significance, sensitivity to climate change and its being the subject of an externally funded research project.

Approach — SwRI researchers developed and applied an integrated remote sensing based methodology to interpret and predict processes that control permafrost formation and degradation. Through well-constrained processing techniques and remote sensing data integration along with data validation, researchers analyzed elevation patterns, soil moisture, vegetation and sedimentary processes to evaluate changes in permafrost processes.

Accomplishments —

- Initiated and developed a comprehensive database of aerial and satellite remote sensing datasets pertinent to existing and future permafrost studies at Kobuk Valley (KOVA) National Park.
- Developed an integrated approach to detect, monitor and characterize changes in the permafrost environment based on state-of-the-art optical and radar methodologies.
- Developed a 2.5-m DEM of the region using optical PRISM data.
- Developed a new soil moisture retrieval methodology based on multi-temporal L-band SAR and AMSR-E data.
- Demonstrated the ability to register — with high accuracy — optical data acquired 50 years apart in the absence of stable features.
- Built successful relationships with a significant group of external collaborators who contributed to various aspects of the project. Two external scientists were appointed as non-fee consultants for the duration of the project.
- Identified new avenues of research related to arctic, arid and mountainous permafrost research with potential clients in the United States and Asia.

Antarctic Sea Ice Thickness from Airborne LiDAR and Ultra-wideband Radar, 20-R8181

Principal Investigators
Michael Lewis
Marius Necsoiu
Jorge Parra

Inclusive Dates: 10/01/10 – 04/01/12

Background — The cryosphere is intricately linked to the global climate system and the Earth's surface energy budget. Sea ice is a primary component of the polar oceans and comprises approximately 7 percent of the Earth's surface in the mean. Sea ice is important to the global climate system because of its prominent role in the 'ice-albedo' feedback mechanism that enhances climate response at high latitudes; influence on the exchange of heat, gases, and momentum between the ocean and atmosphere; and effects on buoyancy of ocean currents caused by changing fresh and saline water inputs. Despite increased research focus in recent years, the Antarctic sea-ice zone remains one of the least-known regions of the Earth's surface. The remote location, limited extent and infrequency of direct measurements, and difficulties in validation of remote sensing products have contributed to the knowledge gap.

This project involves direct collaboration with the British Antarctic Survey (BAS), Scottish Association of Marine Science (SAMS) and other international participants to obtain *in situ* sea ice measurements during the ICEBell program in November 2010. The data from this program were used to derive sea ice and snow cover thickness relationships in the Antarctic sea ice zone and ultimately will be used to improve satellite remote sensing products, allowing long term monitoring of the ice mass balance in the Antarctic sea ice zone.

Approach — The project comprises two basic tasks. The first task involves participation in ICEBell cruise aboard the *James Clark Ross* to obtain detailed snow and ice measurements that are coincident with airborne and satellite remote sensing measurements. The second task involves analyses of field campaign and airborne LiDAR and satellite remote sensing data necessary to assess statistical relationships between surface elevation, snow depth, freeboard, ice thickness, and roughness with the ultimate goal of classifying sea ice types and calculating sea-ice thickness from satellite altimetry and active radar returns.

Sea-ice measurements were obtained from the BAS icebreaker *James Clark Ross* in areas of the northwestern Weddell Sea and in the Bellingshausen Sea, Antarctica. The field program was performed in conjunction with near-coincident airborne LiDAR surveys and satellite (remote sensing) radar measurements. It was originally planned to coincide with NASA IceBridge flights acquiring both LiDAR and Snow (Ku band) radar along flight lines in the Bellingshausen Sea; however, unanticipated delays in the JCR schedule precluded the overlap of IceBridge flights.

Accomplishments —

- Successfully participated in the BAS ICEBell sea-ice cruise, collecting gridded surveys with geophysical measurements on 10 separate sites on 8 different sea-ice floes in the Weddell and Bellingshausen Seas and placing 12 ice mass-balance buoys (IMBs) that drifted with the floes for months following the cruise.

Coordinated the acquisition of 40 TerraSAR-X (X-band radar) images through the German Aerospace Agency, EnviSat radar and AMSR-E passive microwave satellite data that were coincident in time and location with IMBs during the drift period.

- Developed a methodology to analyze decomposition products from TerraSAR-X datasets in the Bellingshausen Sea to derive polarimetric parameters for sea-ice floes that may subsequently be correlated with sea-ice type.
- Co-registered overlapping terrestrial scanning LiDAR datasets for all floe sites.
- Developed geostatistical relationships and probability distributions for sea-ice floes using surface elevation, snow depth, freeboard, and ice thickness for correlation with polarimetric parameters.
- Built successful relationships with a significant group of external collaborators who contributed to various aspects of the project.
- Identified new avenues of research related to Antarctic sea ice that allow a multi-sensor approach to monitor sea-ice thickness from remotely sensed data sets with application to long-term climate change impact assessments.

2011 IR&D Annual Report

Development of a Coupled Mechanistic Model to Examine Aerosol Migration in the Atmosphere, 20-R8182

Principal Investigators
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Inclusive Dates: 10/01/10 – 10/01/11

Background — Aerosols, which are suspensions of solid or liquid particles in the atmosphere, affect Earth's climate directly by scattering and absorbing radiation, particularly by scattering incoming shortwave radiation back to space. In addition, aerosols indirectly affect Earth's climate by modifying the microphysical and radiative properties of clouds. The resulting effect of aerosols is to cool the atmosphere. Accurate estimates of the indirect radiative effects require an understanding of the role of aerosols in influencing cloud properties. This is considered one of the most uncertain aspects of current global climate models. Sea-salt aerosol emission, migration and removal also are affected by atmosphere and ocean properties. Interaction between the ocean and the atmosphere plays a crucial role in the atmosphere-ocean momentum flux exchange and heat and mass exchange. The interaction, particularly the exchange of heat, momentum and moisture between the atmosphere and the ocean, controls atmospheric phenomena such as cyclones and hurricanes. Proper understanding of the coupling among the atmosphere and ocean is essential for predicting large-scale circulation of the ocean and the atmosphere and the role circulation plays in atmospheric and oceanic transfer of momentum, heat and mass. The present work aims at developing an efficient computational tool for more accurate estimations of sea-salt aerosol effect on cloud formation by coupling ocean and atmospheric models. The efficiency of the developed computational tool is achieved through the coupling and also by modeling the effects of scattering, radiation and nucleation on cloud formation.

Approach — The project encompasses two major tasks. The first involves developing a coupled atmosphere and ocean model. At each time step, the individual models will calculate the environmental parameters and then pass this information to the other model to be used as boundary conditions. The second task will evaluate the coupled model against the uncoupled model. This will be accomplished by comparing cloud formation in the coupled model to cloud formation in the uncoupled model over the Gulf of Mexico region. The two models will be compared with actual cloud formation using satellite imagery, which can be obtained from either the National Oceanic and Atmospheric Administration Geostationary Satellite Server or the National Aeronautics and Space Administration Moderate Resolution Imaging Spectroradiometer instruments. Comparisons will include area coverage and cloud patterns. In addition to examining the fully coupled model, sensitivity analyses will evaluate the influence of coupled boundary conditions on aerosol effect and subsequent cloud formation. This will be accomplished by only coupling certain boundary conditions for a given simulation and observing the resulting outcome.

Accomplishments — SwRI researchers have successfully simulated several cases with weather research and forecasting chemistry model (WRF-CHEM) and hybrid coordinate ocean model (HYCOM) in the system. The results have been analyzed and post-processed with National Center for Atmospheric Research Command language (NCL) post-processing software. Simulations with WRF-CHEM tested the

nested grid capability. Initial simulations used a coarse grid; subsequently, the nested grid was used. The domain was chosen for the central gulf coast region. This region will be used in subsequent simulations, because observational data and prior computational data for atmospheric aerosol distributions are available. Simulations using HYCOM have also been carried out. The project team has implemented the Earth System Modeling Framework (ESMF) software to couple WRF-CHEM and HYCOM. The plan is to use the ESMF superstructure and associated coupling mechanism. Work is under way to formulate how to include the effect of nucleation on aerosol and cloud formation.

2011 IR&D Annual Report

Investigation of the Effect of Epikarst on Recharge and Storage of Groundwater in Karst Aquifers, 20-R8220

Principal Investigators
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Ronald McGinnis
Hakan Basagaoglu

Inclusive Dates: 04/01/11 – Current

Background — Increased demands for groundwater have elevated the need to better understand the hydraulics and sustainable yield of aquifers, a major source of water resources. For karst aquifers, a critical need is to better understand how the epikarst layer affects recharge and storage of groundwater. The term epikarst describes the weathered horizon at the top of the vadose zone with high porosity and permeability. Karst aquifers exhibit complex hydraulic reactions in response to recharge events caused by the development of dissolution flow pathways at the surface and at depth. The epikarst layer has a strong spatial and temporal influence on recharge of the aquifer. Epikarst layer effects vary with geographic location, scale of aquifer and the hydrogeologic characteristics of the aquifer of interest. The hydraulics of epikarst at local scales has been characterized with limited success, and formulation of a universal hydraulic conceptual model for the epikarst layer has proven elusive. This project will investigate the hydraulics of epikarst layers in karst aquifers to understand the mechanisms of recharge and groundwater storage in regional-scale karst aquifers and to develop a universal or general model for the hydraulics of epikarst layers.

The hydraulic effect of epikarst on recharge is exhibited by the lag time between the occurrence of recharge events and times when the groundwater elevation and spring discharge respond to precipitation. Not accounting for the lag introduces large errors into groundwater flow models and renders water-resource management decisions inaccurate. Recharge lag time can be determined using hydraulic or water chemistry responses observed in groundwater or spring discharge. Lag times can vary from hours to months depending on the size of the recharge zone, the climatic season of interest (i.e., rainy or dry), the physical nature of the epikarst, and related hydraulic features of the aquifer. In general, larger recharge zones or catchment areas with a more extensive or better developed epikarst layer will have longer lag times. Lag times determined solely by a hydraulic response may be misleading, particularly if the response caused by a pressure pulse or piston flow in which case the response is not reflective of actual groundwater velocity. It is prudent to examine chemical and isotopic tracers, such as trace and major elements, temperature, alkalinity, specific conductance and isotopes, in addition to hydraulic responses to discern actual groundwater flow mechanisms and to parse out the source of the sampled water.

Approach — The technical objective of this project is to quantify the effect of epikarst on recharge of a karst aquifer. To accomplish this, the project will physically characterize features important to the hydraulic capacity of a prominent karst aquifer with a defined epikarst layer; characterize hydraulic inputs (i.e., spatial and temporal distribution of precipitation) and responses exhibited by the regional aquifer system (i.e., spring discharge quantity and chemistry, regional and perched groundwater elevation); and develop a mathematical or quantitative representation of the hydraulic effect of epikarst by relating input to output as a function of system properties. The Edwards-Trinity Aquifer in west-central Texas will serve as the study site. The Edwards-Trinity Aquifer is a large, regional-scale karst aquifer located sufficiently close

to San Antonio to facilitate field surveys and data acquisition. The first task will examine the hydrostratigraphy of the Edwards-Trinity Aquifer. This examination will include field surveys, water chemistry testing and analysis, hydraulic response data collection, and assessment of the geological structure. The second task will integrate all relevant data and assemble a coherent conceptual model of the hydraulic mechanisms of the epikarst. The importance of scale dependency to the hydraulic response needs to be recognized and fully incorporated into the conceptual model. The last task will develop a model or algorithm that accounts for these mechanisms in groundwater recharge and storage in karst aquifers.

Accomplishments — To date, research focused on evaluating the internal relationships of recharge, storage and discharge of the targeted study area in the western Edwards Aquifer and the southern Edwards-Trinity Aquifer. Correlations among 39 rain gauges, two index wells (i.e., J-17 and J-27), and two springs (i.e., Comal and San Marcos springs) were analyzed. Results from these analyses indicated low correlation (i.e., no greater than about 0.1) when the entire period of record of the rain gauge data was considered. These results were interpreted that correlations among recharge areas, well locations and spring discharge overlapped both temporally and spatially when taken for long time periods. Subsequent analyses have been undertaken to assess correlations for shorter time periods. Particular emphasis is taken to target a specific time period with a large precipitation event followed by a period of drought or limited precipitation. Such an analysis hopefully will allow assessment of correlations not obscured by multiple overlapping signals. The large rain events of late 2009 and early 2010 followed by prolonged minimal precipitation are targeted for this analysis.

Potential springs and discharge points for water sampling and water chemistry analysis were identified. Protocol for water sampling and target water chemistry parameters have been specified. Two multi-sample *in situ* samplers were purchased for project use. Each sampler is programmable and capable of collecting up to 24 water samples during specified sampling periods.

Conceptual models for the targeted focused-study areas have been formulated based on available information. Additional data and site-specific hydrogeological information have been compiled to augment and vet these models. Reservoir modeling packages MATLAB, STELLA, and VENSIM have been evaluated for precipitation/groundwater storage/spring discharge assessments. Input data collected during the project are being used in these reservoir modeling exercises. At this time, a simple reservoir model is conceptualized that has a fast and slow phase to recharge, an aquifer storage component and a spring discharge component. The timing of fast recharge, change in storage, and spring discharge is known. The timing of slow recharge and the relative fractions of fast and slow recharge are unknowns. Various candidate lumped-parameter, reservoir models are being assessed to understand the effect of epikarst delaying recharge (i.e., instigating the slow recharge component) into the reservoir system.

2011 IR&D Annual Report

A Novel Approach for Improved Axial Vibration Suppression of Multi-Stage Launch Vehicles, 18-R8108

Principal Investigators
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Benjamin White
Harold Doiron

Inclusive Dates: 10/01/09 – 04/01/11

Background — A record number of launch vehicles (rockets) are in development at this time. This includes the National Aeronautics and Space Administration (NASA) yet to be named Heavy Lift Vehicle, as well as the privately funded Antares, Falcon 1 and 9, and the New Shepard vehicles being developed by Orbital Sciences Corporation (OSC), Space-X and Blue Origin, respectively. Each vehicle is in a different state of development. The NASA vehicle is progressing at a very slow pace as NASA efforts are focused on new engine systems at this time and not on the vehicle itself. OSC progress on Antares continues to make the news with the most recent development being the successful test firing of several AJ 26 engines, which will be used to power the first stage. Space-X is breaking records with successful launches of both Falcon 1 and 9 in the past year, most recently demonstrating re-entry capability with the recovery of the Dragon spacecraft from orbit. Blue Origin continues in silence, releasing no new information to the press in the past several years.

At the same time, expertise in some of the more specialized areas of vehicle development is lacking in the industry as engineers from the previous development programs leave the workforce. In the area of coupled propulsion and structural dynamics, very few experts outside of major aerospace companies are available to serve the needs of the growing commercial launch vehicle industry. This provides SwRI a unique opportunity to expand involvement in the launch vehicle business by re-developing the skills and institutional knowledge required to provide the expert guidance and support each of these development programs will need in the coming years.

Approach — The focus of this research project is the application of a relatively common propulsion system component (pogo accumulator) to a new vibration issue. In typical use, pogo accumulators are designed to improve the frequency separation between structural and propulsion system modes so that pogo-type vibrations are prevented. In the case of a launch vehicle with a solid first stage and a liquid second stage, only the second stage would have such a device. However, as predicted to occur on Ares I (part of the cancelled NASA Constellation Program), significant longitudinal vibration problems can occur during first-stage flight, which is propelled by a Solid Rocket Motor (SRM) adopted from the Space Shuttle program. This research project was established to focus on this problem through the adaptation of the conventional pogo accumulator for both first- and second-stage vibration control. Although the Ares I program has been suspended, the work is still relevant, since other solid-fueled rockets could benefit from such a technology in the future.

Properly designing such a device requires precise control of the three main dynamic characteristics of an accumulator: inertance, compliance and resistance. While inertance and compliance are well understood and accurately represented by linear models, resistance is a highly non-linear parameter and remains a poorly understood parameter in the design of pogo accumulators. It is common to under-estimate the damping of a hole pattern, which can lead to an ineffective accumulator in the worst-case scenario. The premise of this research project is that the mismatch between theory and experiment is tied largely to the

presence of high turbulence in the mean flow passing by the accumulator. This highly turbulent flow generates flow disturbances at various frequencies, which pass into and out of the accumulators. This unaccounted-for dynamic flow occupies some of the available flow area through the resistance, effectively reducing the size of the flow area available to the system mode of interest. Therefore, as an initial step in developing this novel first-stage damper concept, this report also includes developing a validated flow resistance model that provides a much improved match between predicted and measured damping for typical pogo accumulator scenarios.

Accomplishments — The project approach resulted in multiple accomplishments. First, a validated flow resistance model for accumulator hole patterns in cross-flow now exists and can be used to design a specified flow resistance into any liquid feedline accumulator. This new capability is already being applied to a commercial launch vehicle program for one of SwRI's clients. Second, two potential design concepts for damping the SRM-induced oscillations for the Ares I launch vehicle were developed. Both designs result in a significant reduction in vibration, with one of the designs being much easier to implement in a real vehicle system. Although Ares I is no longer under development, the design continues as a viable concept for future solid-fueled rockets with liquid stages.

2011 IR&D Annual Report

High-Pressure Entrainment Measurement/Modeling, 18-R8156

Principal Investigator
Flavia Viana

Inclusive Dates: 06/07/10 – Current

Background — Wet gas scenarios are encountered during natural gas production, transmission and processing. The amount and distribution of liquid in the gas stream plays an important role in the selection and operation of flow measurement devices, the design of transmission lines, the design of gas processing and separation equipment, and corrosion occurrence and mitigation inside the pipe. In this last scenario, the distribution of the gas and liquid phases is very important, as it affects the contact of corrosion inhibitors with the pipe wall.

Several experimental projects have been conducted to investigate and characterize wet gas flows in pipes. Most of these studies are based on experimental data collected at low pressures (less than 100 psig). However, the pressure has a significant effect on the distribution and behavior of two-phase flow mixtures. In a mixture of natural gas and hydrocarbon liquid, the gas will dissolve in the liquid phase as the pressure is increased. The density of the gas increases with the pressure, which affects the separation of the gas and liquid phases as a consequence of a decreased density gradient. One of the motivations for this project is to fill the gap in the understanding of wet gas and rate of liquid droplet entrainment at high pressures.

Approach — The general approach of this project is to develop modeling and experimental tools for characterizing multiphase and wet gas flows in high-pressure environments. The main components of the project are tool development, high-pressure testing and modeling.

The goal of tool development is to design and fabricate two devices to be used in test programs at SwRI's Multiphase Flow Facility (MFF) to investigate and characterize multiphase flows. Given that the design pressure of the MFF is 3,600 psig, the design pressure of the two devices was selected to match that of the MFF, which imposes a significant challenge in the mechanical design of the tools. The first device consists of a non-intrusive, high-pressure optical system that would allow visualizing the structure of the multiphase flow stream through a pipe. The second device would be used to measure the amount of liquid entrained in the gas.

The purpose of the experimental project is to develop the experimental technique for undisturbed flow visualization and liquid entrainment measurement using the devices developed on the project, and to generate non-existing data on liquid entrainment at high pressure. Tests will be conducted at the MFF under various superficial gas velocities, liquid volume fractions and pressures. Methane gas and a hydrocarbon liquid will be used as the test fluids to simulate field-like conditions.

Modeling for this project involves reviewing existing models and correlations for predicting liquid entrainment in gas, developing new or

improved models or correlations that take into account the pressure of the system and validating the modeling tools using experimental data generated during the experimental program.

Accomplishments —

- An extensive review of potential methods for measuring liquid entrainment at high pressure was conducted. Optical, light diffraction and mechanical methods were considered and the readiness level of existing technology was evaluated. A sampling method was selected for development as the most feasible option.

Figure 1. Cutout view of iso-kinetic sampling system designed for measuring liquid entrainment at high pressure.

- An iso-kinetic sampling system was designed and is being fabricated for the testing. The sampling system can be used at pressures up to 3,600 psig and in pipe sizes up to six inches in diameter. Figure 1 shows a cutout view of the liquid entrainment measurement device.
- A high-pressure, flow-visualization device was designed and fabricated by a contractor. This device will allow visualizing the flow through a 3-inch pipe without introducing any perturbation on the flow and without affecting the flow pattern. The unit has already been received and is undergoing some preliminary testing to develop a flow visualization technique to be used during the high-pressure experiments.
- A customized test section has been designed for the experimental project. The setup to be installed at the MFF includes the injection of the liquid phase into a gas phase stream, a 60-foot-long flow development section to allow a fully developed flow pattern, a liquid entrainment measurement section using the isokinetic sampling system and a flow visualization section.
- A review of existing models and correlation for predicting liquid entrainment fraction has been completed, and the various models are being evaluated and compared with existing data.

2011 IR&D Annual Report

An Experimental Facility and Analytical Methodology for Determining Frequency-Dependent Force Coefficients of Foil Gas Bearings, 18-R8189

Principal Investigator
Aaron Rimpel

Inclusive Dates: 10/01/10 – Current

Background — Accurate knowledge of linearized stiffness and damping coefficients of bearings is a critical aspect in the successful design of high-performance turbomachinery. In recent years, improvements in foil gas bearing technology have led to their increasing application in the expanding oil-free turbomachinery market (current applications include air cycle machines, auxiliary power units, automotive turbochargers, micro gas turbines, refrigeration compressors, etc.). Foil gas bearings use a gas, such as the process gas of a compressor, as the lubricant that separates the rotor from the stationary bearing surfaces. Thus, the need for a separate lubrication circuit with seals, as required for traditional oil lubrication, is eliminated. Foil gas bearings are also not limited by precessing-inertia speed limits as with rolling element bearings, nor do they require expensive control systems as with active magnetic bearings. The relatively low damping of foil gas bearings, when compared to oil lubrication, is mitigated through the use of friction damping mechanisms in the compliant support structures within the bearing. Foil gas bearings of various types are the main focus of gas bearing research today, and they are also the most common gas bearings currently found in commercial applications. Despite the growing popularity of foil gas bearings, there is considerable uncertainty regarding their stiffness and damping coefficients.

Approach — The approach used for this project is experimental and analytical. An experimental test rig will be capable of measuring frequency-dependent stiffness and damping coefficients of foil gas bearings for journal speeds up to 60 krpm and for lubricating air supplied at ambient pressures up to 200 psig (although not in the scope of the current project, different gases and higher pressures up to 635 psig may be tested in future work). The analytical method will apply transient fluid-structure interaction (FSI) modeling techniques to simulate the gas film and structural components of the foil gas bearing via coupled computational fluid dynamics (CFD) and finite element analysis (FEA). The transient FSI method will allow modeling of the complex structures of foil gas bearings, and it will be general enough to be applied to a wide range of foil gas bearing geometries and extensible to other turbomachinery components such as seals.

Accomplishments — The design of the test rig was completed, and the construction is nearly complete. Commissioning of the main test rig subsystems (electric motor drive, bi-directional impulse turbine-driven exciter shaft, test enclosure/pressure vessel, instrumentation, etc.) is still in process. The algorithms necessary to extract frequency-dependent stiffness and damping coefficients from the measured data have been tested extensively and are ready for implementation. The transient method has been demonstrated on a simplified geometry (plain sleeve bearing, centered whirl) for which other established methods are typically applied due to the simplicity (steady-state intermediate reference frame simulation). Comparisons of the new and established methods show excellent agreement for the simple geometry. Parameter studies of transient time-step resolution and mesh density have been conducted to provide insight to optimal simulation settings. The next step is to apply the transient FSI method to foil gas bearing geometry, which will be compared to measured data.

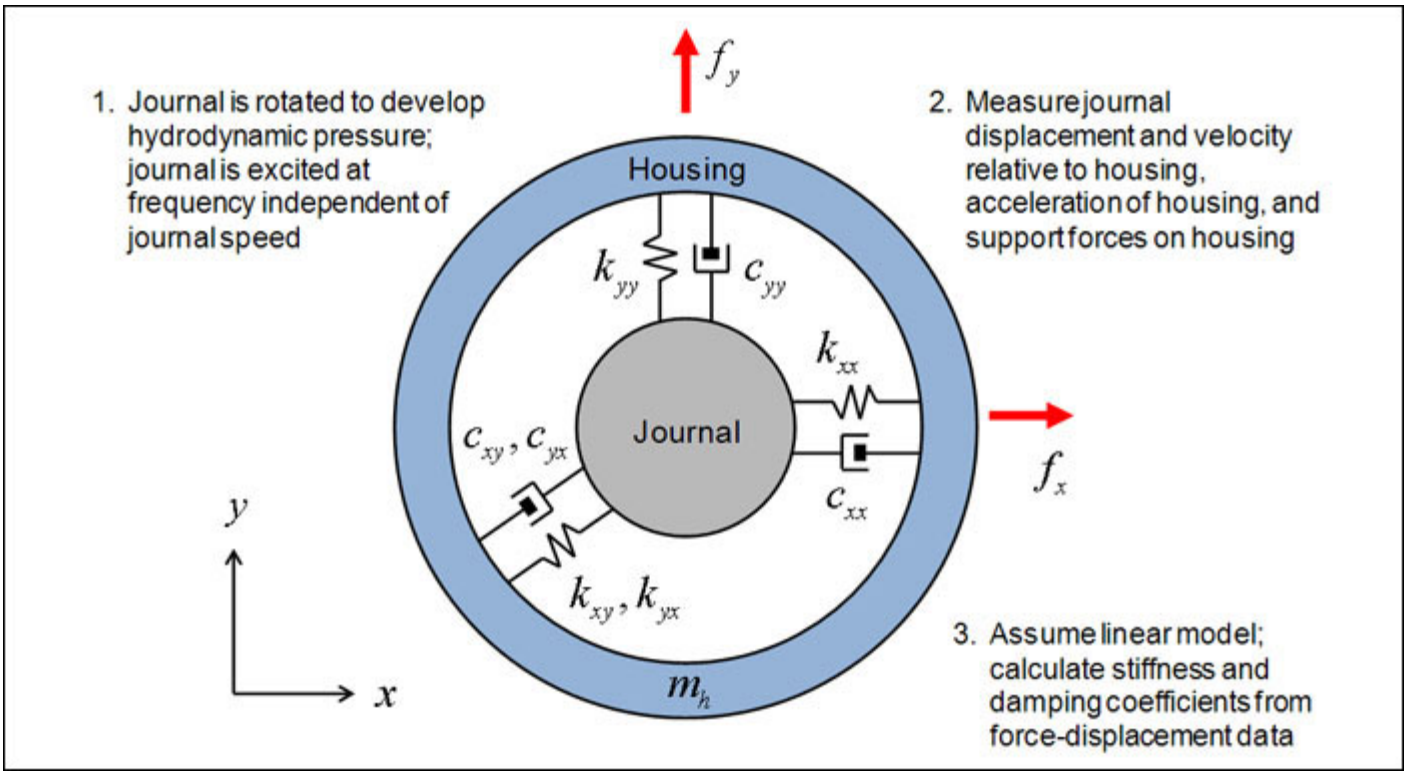

Figure 1. Model of a Bearing Using Linearized Stiffness and Damping Coefficients.

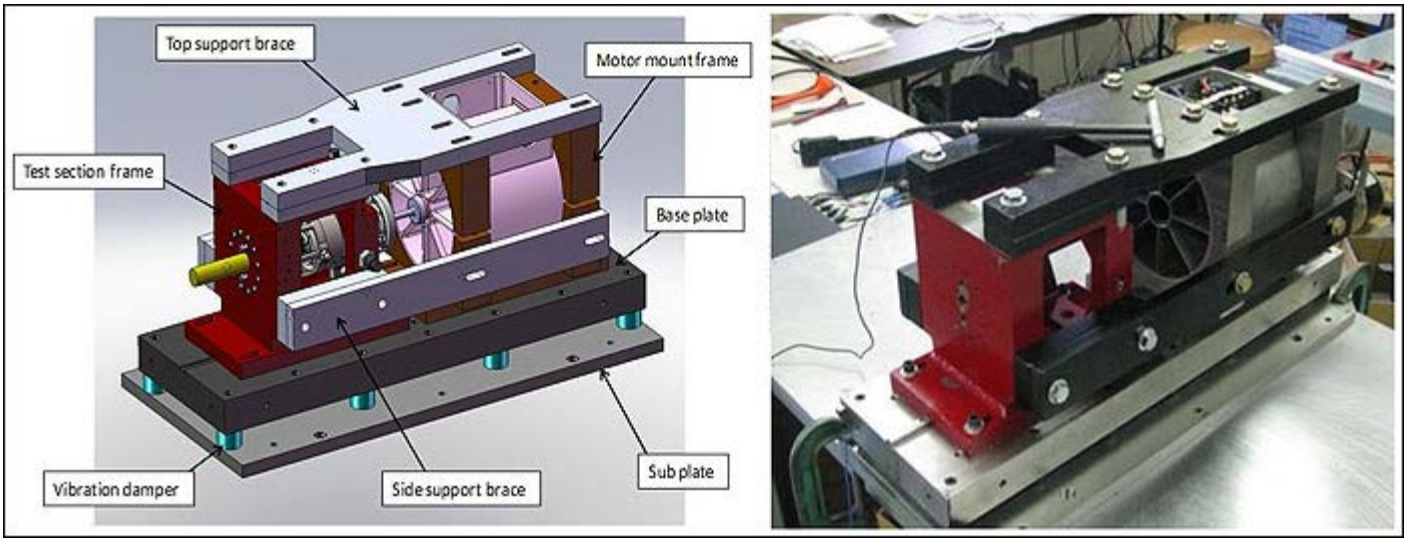

Figure 2. Solid Model of Test Rig and Photograph of Test Rig Undergoing Modal Tests.

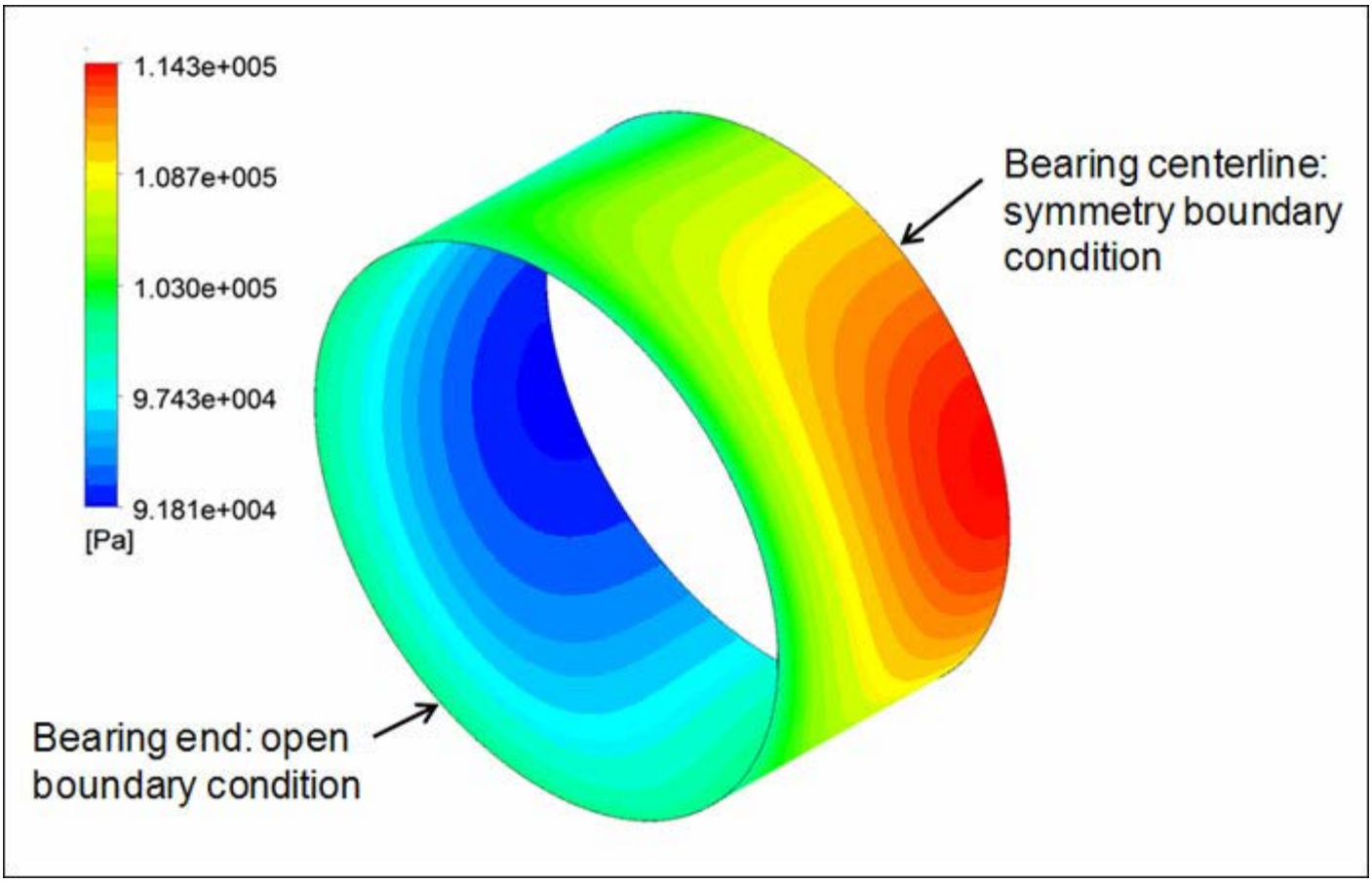

Figure 3. Example Static Pressure Contours from Intermediate Reference Frame CFD Simulation for Forward, Synchronous Whirl (Journal Excitation Frequency = Journal Spin Frequency).

Radio Frequency (RF) Detection of Small Arms Fire, 10-R8173

Principal Investigators
Thomas C. Untermeyer
Gregory C. Willden
Carl E. Weiss
Andrew R. Cormier
Chuong D. Khuc

Inclusive Dates: 07/01/10 – 12/31/11

Background — For defense purposes, the military has an interest in detecting weapons as soon as possible after their firing or launching from as far away as possible. Optical, Infrared (IR), and acoustic systems exist today that can detect the firing of a variety of weapons. However, these detection methods do not work as well in obscured environmental conditions caused by clouds, fog or rain. Acoustic systems also provide much slower response time and limited range. Since the 1950s, the open literature has reported the possible generation of radio frequency (RF) emissions caused by the launching of a variety of weapons. Passive RF detection of weapon launches could provide a benefit over optical, IR, and acoustic systems by providing fast detection through obscured environments over extended ranges.

Approach — Using lessons learned during previous testing, including developing sensors used to collect RF data from a variety of weapons, researchers attempted to reliably and consistently detect the RF signals caused by the firing of automatic weapons at a distance of more than one-quarter mile (400 meters) and to understand the phenomenology associated with the cause of the RF signals.

Accomplishments — The team developed a test plan and assembled the appropriate antennas and test equipment to collect RF and video data at the SwRI outdoor ballistics range and inside one of SwRI's RF shielded enclosures during the firing of a small arms weapon. Although the team did capture RF signals during this testing, the signals did not occur every time. Also the signals did not provide an adequate signature to differentiate them from other external transmitters.

Modeling and Applications of RF and Optical Negative Index of Refraction Materials, 14-R8050

Principal Investigator
Diana Strickland

Inclusive Dates: 04/01/09 – 09/01/11

Background — Negative index of refraction materials (NIMs) are engineered materials that are designed to bend electromagnetic radiation "backwards" (in the direction opposite to the conventional Snell's Law). This is often accomplished by arranging and shaping metallic structures that are much smaller than a wavelength within a host dielectric. In this project, SwRI researchers used periodic arrays of printed copper structures on host dielectrics, either circuit board or air. NIM structures are useful in creating novel lenses, antennas and filters.

This project focused on developing the capability to create the NIM models. To ensure a design cycle could be completed, researchers also built and tested two applications, a novel ground plane for antennas and a filter.

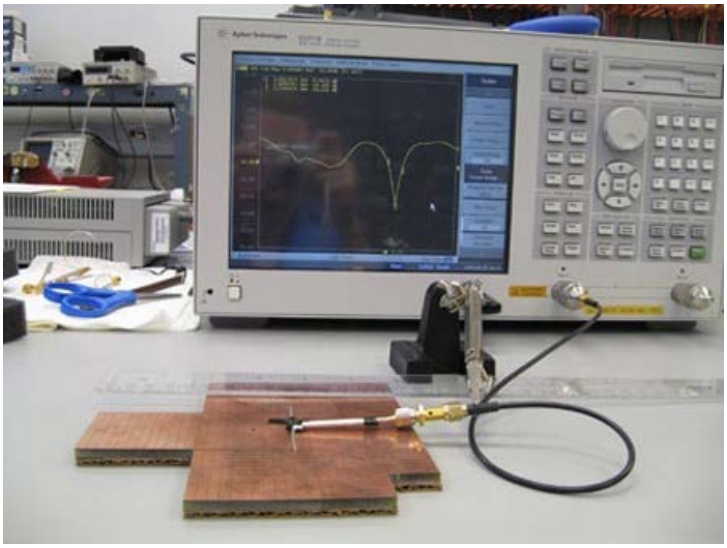

Figure 1. A dipole antenna in direct contact with a novel ground plane. The impressive return loss in this low profile system would be impossible using a conventional ground plane.

Approach — For several types of metal structures (split rings, mushroom structures, rod arrays and hole arrays), published data was used to validate computational models for entire periodic arrays, as well as the individual repeated units within arrays. Researchers also built and tested a dipole antenna with a NIM ground plane. Finally, working planar NIMS inspired filters were fabricated on conventional circuit board and on flexible substrates that validated the computational models.

Accomplishments — Researchers validated computational models of the listed structures, but also found analytic models to be useful in understanding complex behavior. Researchers developed analytic models where no conventional mixing rules apply. This work was presented as a poster, "Modeling Small Arrays of Spirals with Strong Interactions," at the *Fourth International Congress on Advanced Electromagnetic Materials in Microwaves and Optics* at Karlsruhe, Germany, and published in its peer-reviewed proceedings.

Researchers found that the NIM ground plane, pictured in Figure 1, could be used as copper "mushroom" structures printed on circuit board in complete contact with a dipole antenna and still achieve increased directivity and a strong impedance match. This means the antenna and ground plane system have an unusually low profile. The performance of the antenna was also found to be sensitive to position and orientation of the antenna with respect to the ground plane.

A compact version of a printed NIM filter is shown in Figure 2. Reserachers fabricated and

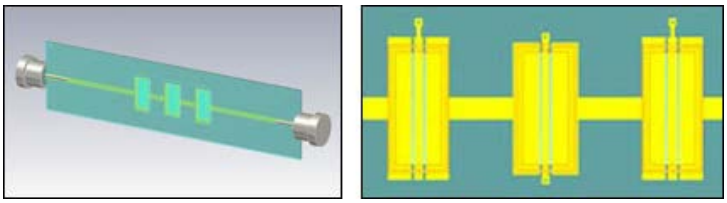

Figure 2. A distributed band pass filter using NIMs (negative index of refraction materials) design elements. Left: A filter circuit with three elements printed on circuit board. Right: A magnified view of the three filter elements. This filter is about an eighth of a wavelength long, yet it performs well.

tested several types of these filters on both conventional circuit board and flexible substrates. The filter is not sensitive to temperature-like surface acoustic wave (SAW) filters. It has solid performance characteristics, yet it covers less than an eighth of a wavelength in its longest dimension. The filter may be arbitrarily small at the expense of losses.

This project explored methods of modeling NIMs and two applications. Most of the modeling conducted was computational by plan. However, researchers developed and published a new analytic model. The antenna ground planes and filters investigated performed well.

2011 IR&D Annual Report

Dual Wavelength Injection-Locked Pulsed Ring Laser with Improved Noise Immunity, 18-R8168

Principal Investigators
Thomas Moore
F. Scott Anderson
Joseph Mitchell

Inclusive Dates: 07/01/10 – Current

Background — Interest in developing tunable laser systems that have the capability to produce two wavelengths of light simultaneously has intensified over the past several years. The motivation for developing dual-wavelength laser systems includes differential absorption lidar (DIAL), non-linear frequency mixing, pump-probe detection and resonance ionization. Recently, work on developing a portable Laser Desorption Resonance Ionization Mass Spectrometer (LDRIMS) instrument, by SwRI space researchers, has led to a need for several specialized laser systems. The LDRIMS instrument will be used to perform geochronology and geochemistry measurements based on the ratios of certain rubidium (Rb) and strontium (Sr) isotopes. The resonance ionization technique selectively ionizes specific atoms or molecules by exciting them with specific wavelengths of laser light simultaneously, identifying specific isotopes. The LDRIMS system, as it exists today, requires seven laser systems that require a large amount of space and power. Developing a tunable laser, with the capability to deliver two wavelengths simultaneously, will significantly reduce the space and power requirements, avoid timing jitter issues among multiple systems, and decrease the burden of maintaining multiple laser systems.

Approach — SwRI has developed a unique laser system that has the capability of producing two wavelengths simultaneously, generating Fourier transform limited output, and providing stable output with immunity from mechanical vibration throughout the acoustic range. The system has the potential to reduce the number of lasers systems needed by the LDRIMS system by approximately half, and provides the capability to be ruggedized in a small portable package. To achieve these objectives, a Ti:sapphire ring laser design with a total path length of 50 cm is used to form a traveling wave oscillator. The traveling wave provides the capability to utilize the entire length of the Ti:sapphire laser crystal while eliminating standing modes. The ability to independently tune the two wavelengths of the laser system is provided by two independent seed lasers that are injected into the cavity via the output coupling mirror and propagate within the ring laser cavity. Enhanced noise immunity and the ability to achieve Fourier-transform limited laser output on every pulse is accomplished with the use of an electro-optic crystal and a Ramp-Hold-Fire cavity control technique, which mode matches the amplifier cavity with the seed laser. The laser system and techniques under development represent a substantial step forward in dual wavelength and pulsed laser design.

Accomplishments — SwRI has successfully developed a dual wavelength ring laser system that is immune to noise throughout the acoustic range, see Figure 1. Single- and dual-wavelength seeded output, at the Fourier-transform limited output, has been demonstrated, as illustrated in Figures 2 and 3. The ability to drive the 780 nm (D2) and 776 nm transitions in Rubidium 87 has also been demonstrated, as shown in Figure 4. In addition, the capability to simultaneously produce multiple, discrete laser output is possible, as illustrated in Figure 5. The results of this work were recently presented at the Frontiers in Optics 2011 conference and the SPIE Photonics West 2012 conference. Work is complete and papers have been presented.

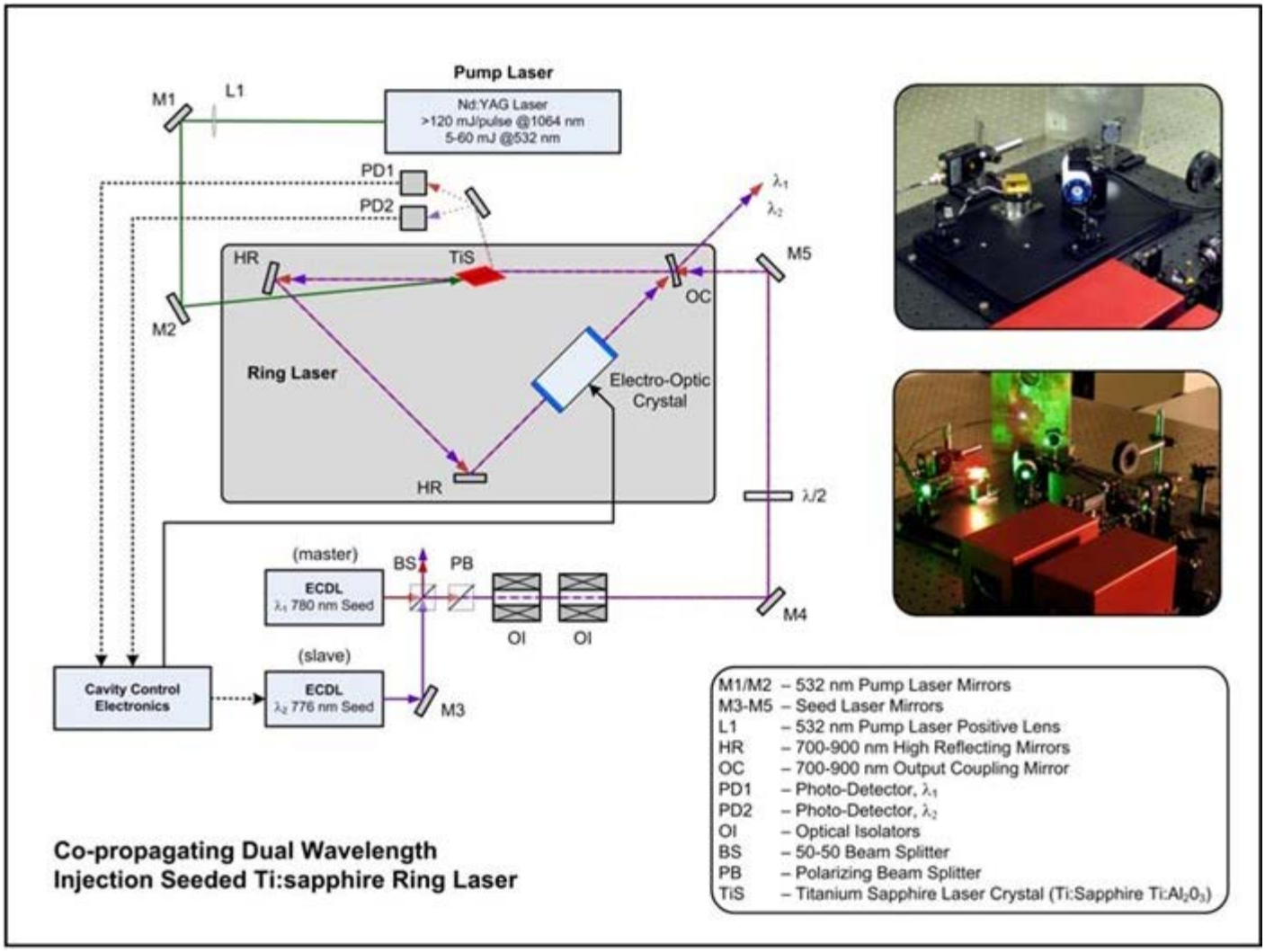

Figure 1. Ti:Sapphire Ring Laser System.

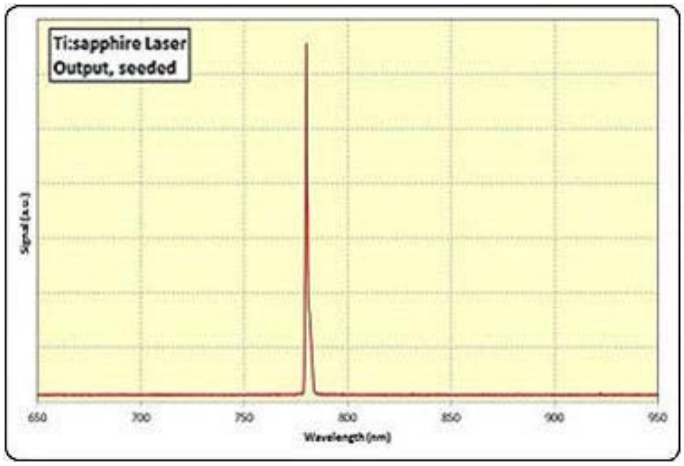

Figure 2. Single-Seeded Ti:Sapphire Laser Output.

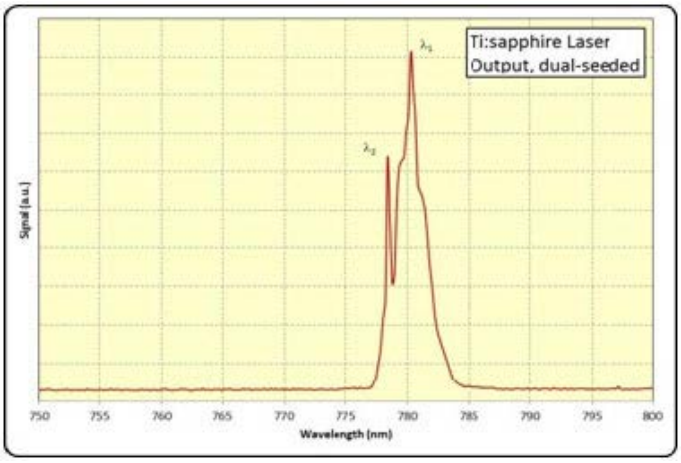

Figure 3. Dual-Seeded Ti:Sapphire Laser Output.

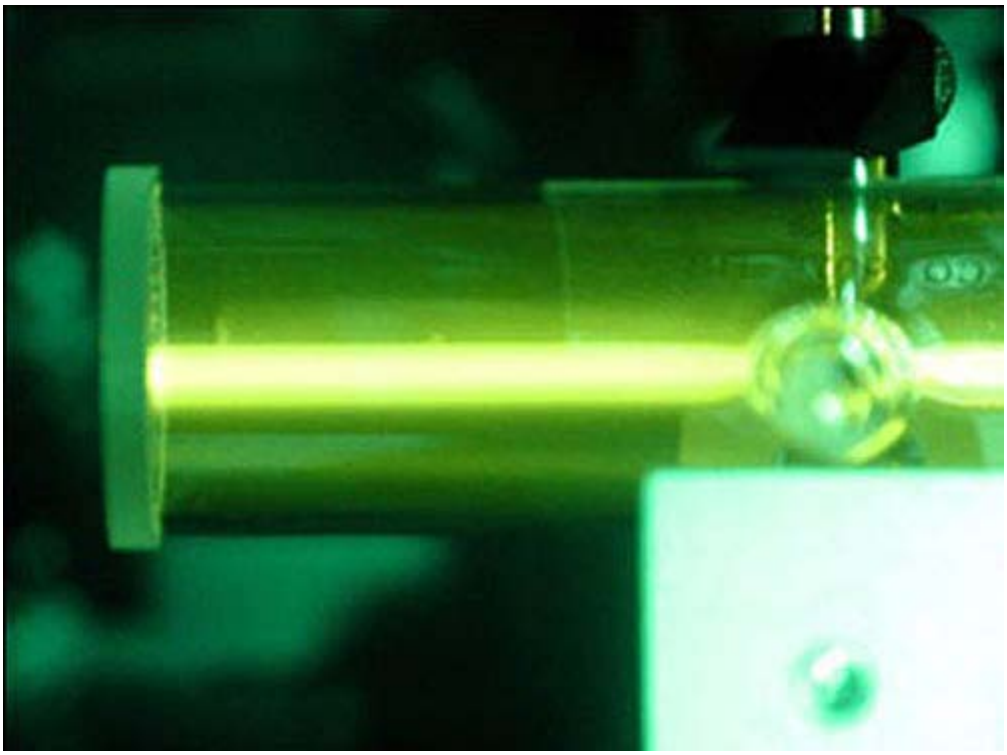

Figure 4. Rb^{87} D2 Resonance Transition.

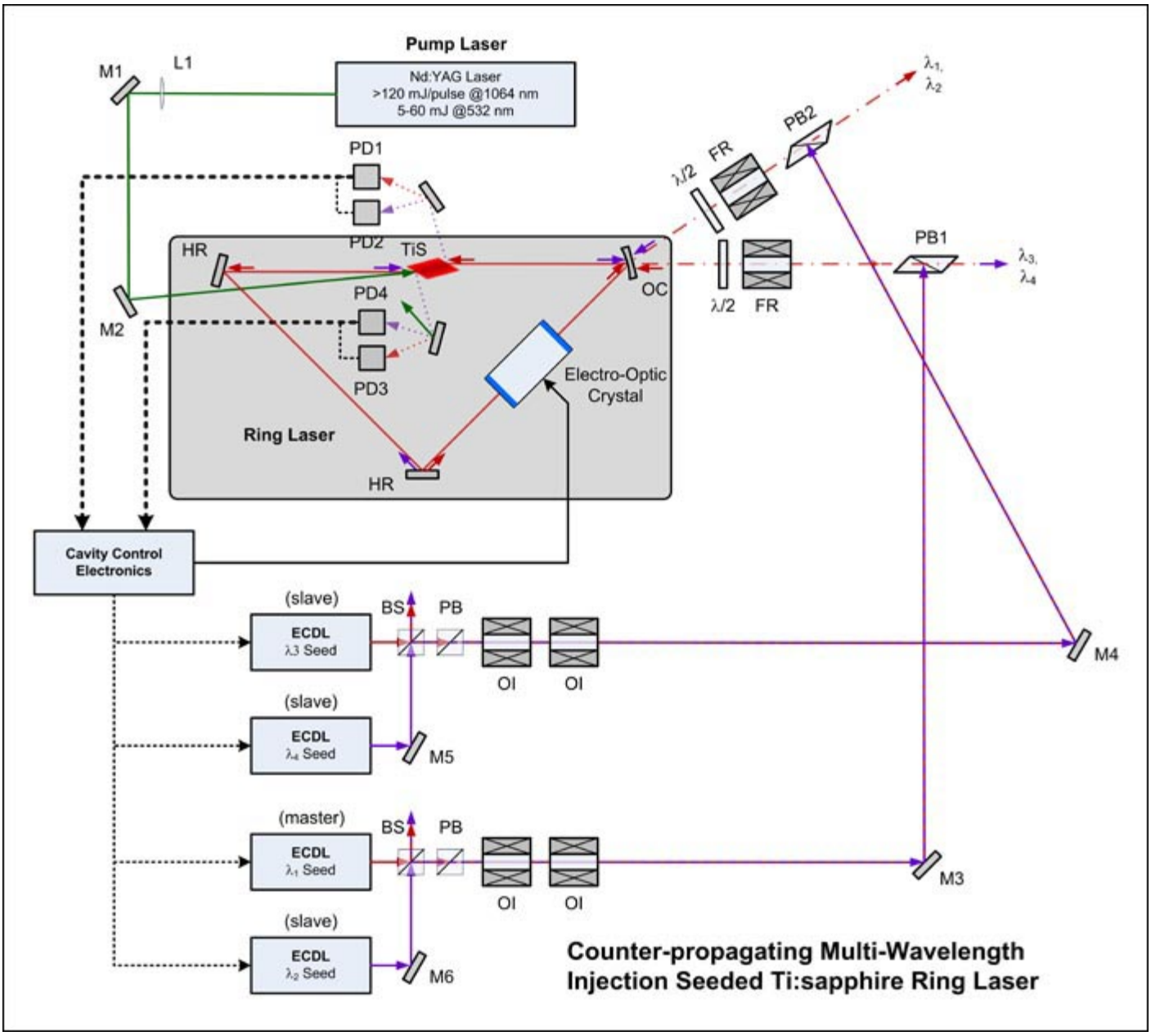

Figure 5. Multi-Seeded Ti:Sapphire Ring Laser System.

2011 IR&D Annual Report

Determination of Thermal Properties for Structural Fire Modeling Using a Genetic Algorithm, 01-R8103

Principal Investigator
J. Marshall Sharp

Inclusive Dates: 09/28/09 – 04/01/11

Background — In all fields of engineering, substantial efforts have been put forth to develop models or other systems to predict performance in response to an external input. As technology advances, these models have grown in size and complexity. However, in all cases, the accuracy of the models is limited by the quality of the input data and the underlying assumptions. Structural fire modeling is no different. In the past decade, significant efforts have been placed on measuring fire events in order to improve fire models for predicting both structural and thermal response of a structure exposed to the fire. One area that has not received a lot of attention in recent years is the characterization of thermophysical properties of materials. These properties are inherently difficult to measure due to the temperature-dependent nature of the properties. Other significant factors are: 1) the broad range of values that can be expected for fire-resistant materials (i.e., materials with very low thermal conductivity are difficult to accurately measure) and 2) the dynamic nature of the combustion event and the potential for reactions to occur as the materials are heated by the fire (in some cases, materials may ignite and contribute to the fire or facilitate moisture migration away from the heat source).

Approach — In this project, SwRI personnel investigated a technique to determine these thermophysical properties by analyzing bench-scale fire test data using a parameter estimation technique known as genetic algorithm optimization. Through this technique a full set of thermophysical properties (density, specific heat capacity, and thermal conductivity) is compiled as a function of temperature. The approach will be compared to model predictions of full-scale fire resistance test performance of assemblies comprising the materials. Additionally, a second technique called genetic programming will be evaluated to determine its effectiveness on predicting the response of materials exposed to fires.

Accomplishments — Small-scale testing was conducted on several materials. Testing included thermo-gravimetric analysis (TGA), differential scanning calorimetry (DSC), modified cone calorimetry, and micro-flow combustion calorimetry. Furnace testing was conducted to compare the thermal model with actual experimental results. During this period of performance, successful fits of mass and mass loss rate were achieved using a model based on the Arrhenius function. The kinetic parameters associated with the Arrhenius function were optimized using a genetic algorithm to create the mass loss rate model. The mass curve was then reconstructed by integrating the mass loss rate with respect to time. The predicted and calculated mass loss rate and mass of type "X" gypsum wallboard are shown in Figure 1. One set of Arrhenius parameters was able to accurately predict mass and mass loss rate curves from TGA data at three different heating rates (5, 10, and 20 °C/min). The mass curves were then used to calculate density as a function of temperature. Next, the DSC data was used to estimate the apparent specific heat capacity of the material. Given the specific heat capacity and density, the final parameter, thermal conductivity, can be estimated using heat transfer data from a bench scale fire test such as the cone calorimeter test method.

A genetic algorithm was used to optimize a linear piecewise fit of thermal conductivity as a function of temperature. The predicted and calculated temperature response of Type "X" gypsum wallboard is shown in Figure 2. The transient 1-D heat transfer equation was used to model heat transfer through a slab of material. The midpoint temperature was compared and used as part of the fitness calculation for the

genetic algorithm during thermal conductivity optimization.

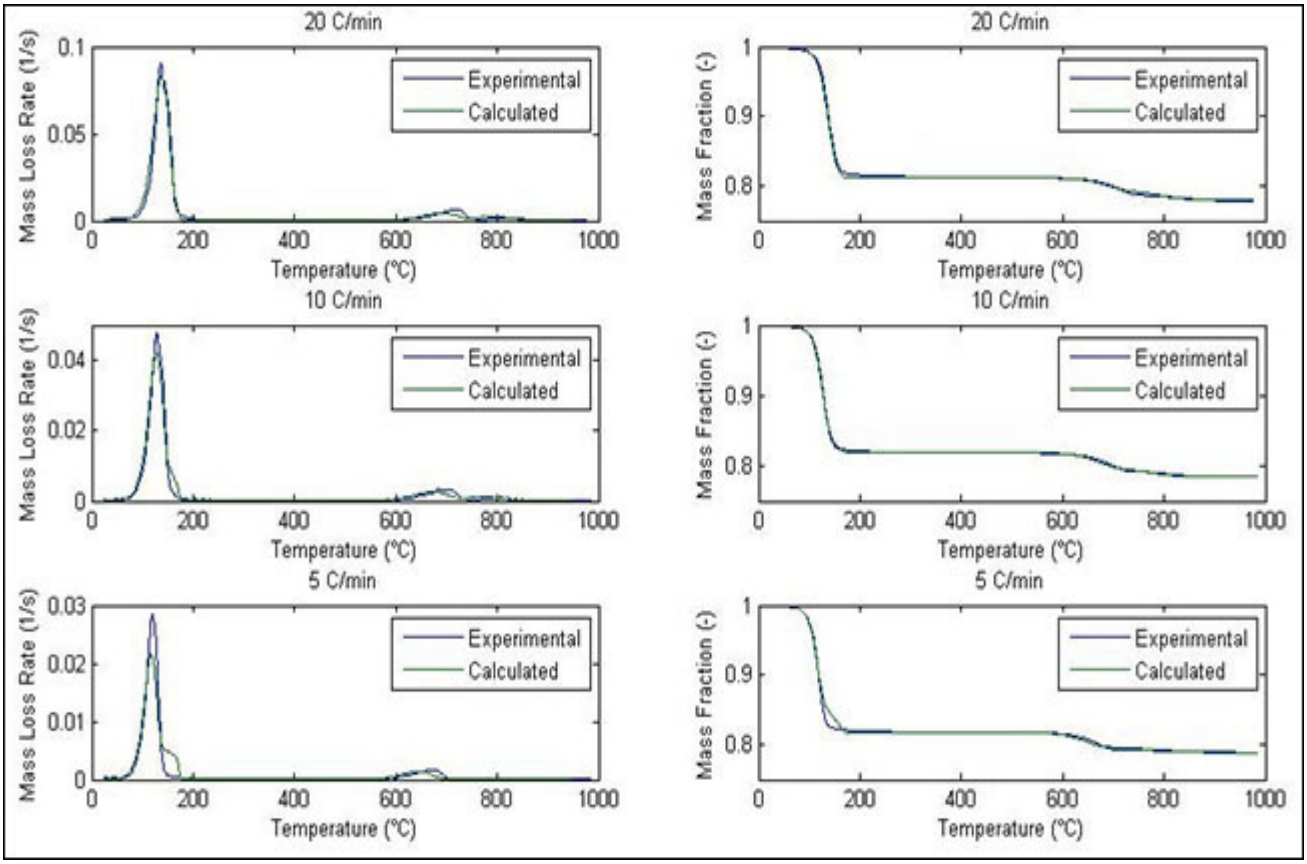

Figure 1. Mass and Mass Loss Rate of Type "X" Gypsum Wallboard as a Function of Temperature for Varying Heating Rates

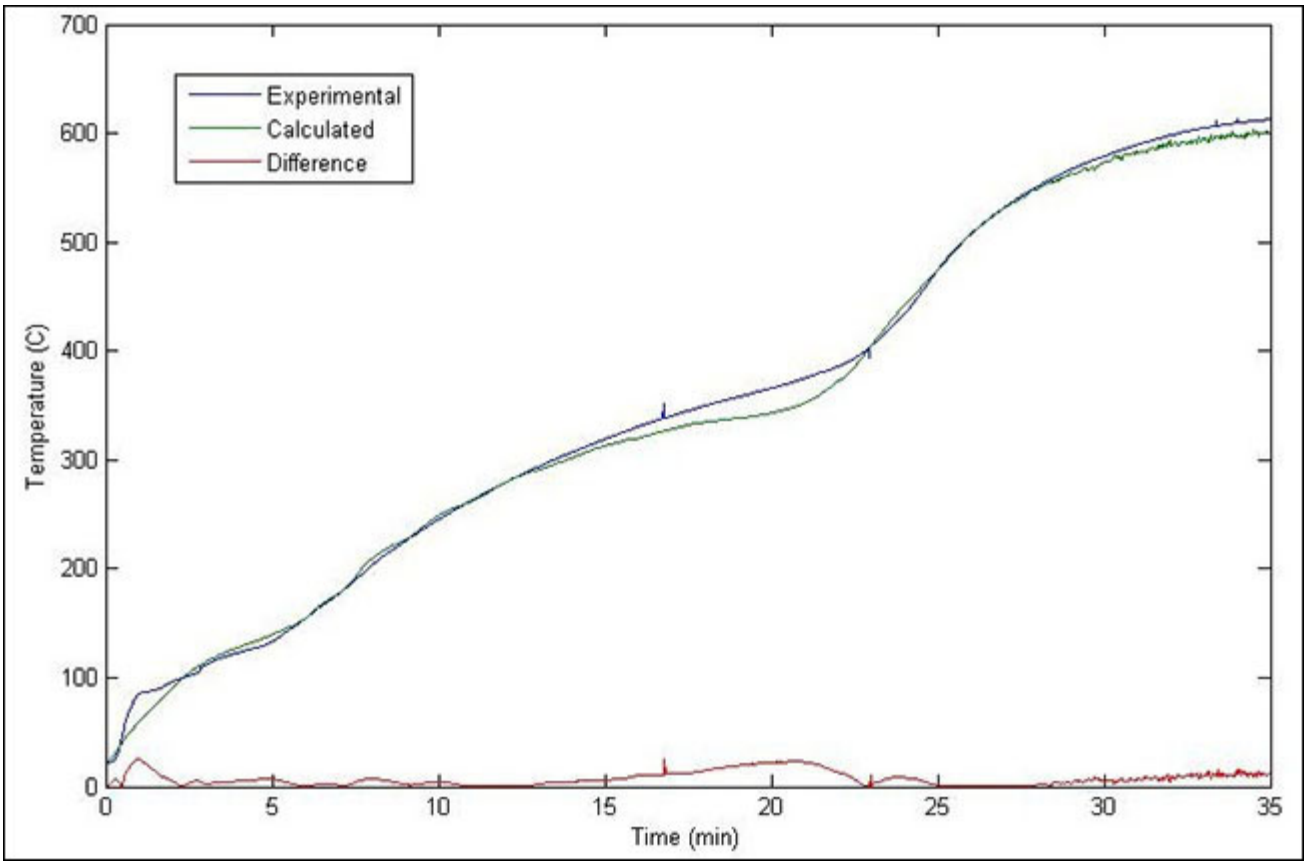

Figure 2. Midpoint Temperature of Type "X" Gypsum Wallboard during Modified Cone Calorimeter Testing

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Analytical Methods and Concentrations of Exposure Biomarker Chemicals in Deciduous Teeth, 01-R8235

Principal Investigators
David E. Camann
Alice Y. Yau

Inclusive Dates: 06/27/11 – 10/27/11

Background — Recent prospective cohort studies suggest that chemical exposures in the prenatal period and first year after birth have a greater adverse affect on a child's neurodevelopment, IQ and behavior. However, no methods currently exist to objectively measure exposures that a child received before birth and during specific intervals in early life to most medications, environmental chemicals and nutrients. The chemical and its metabolite measured in urine generally reflects exposure within 24 hours, while levels in hair reflects exposure in recent months and concentration in blood cannot be related to any specific past time point. A biomarker technique that documents exposure at a specific time during early development would greatly facilitate epidemiologic case-control studies of childhood diseases/conditions such as autism, attention deficit hyperactivity disorder, asthma, leukemia and obesity.

Approach — Each deciduous (baby) tooth can accumulate medications, environmental chemicals and nutrients from the bloodstream during its formation period. Each tooth has a specific period from initial formation through crown completion. This period can span from the 14th week *in utero* to age 1.5 months for upper central incisors and from the 19th week *in utero* to age 11 months for upper second molars. SwRI's approach is to develop methods to prepare and analyze exfoliated deciduous teeth for potential exposure biomarker chemicals, medications and nutrients, and to determine whether the level of a chemical or its metabolite in a tooth correlates with previously measured perinatal exposure, and could thus serve as a reliable biomarker of that exposure. A sample of pulled and shed deciduous teeth was chosen from 21 children in the general population to determine the detection frequency and the distribution of concentrations of the potential exposure biomarker chemicals.

Accomplishments — Tooth preparation, extraction, and analytical methods were developed for a broad spectrum of chemicals, medications and nutrients. Acetaminophen, anandamide, arachidonylglycerol, specific and non-specific metabolites of chlorpyrifos and diazinon, and monoethylhexyl phthalate were analyzed by tandem liquid chromatography/mass spectrometry and polyunsaturated fatty acids and pesticides by gas chromatography/mass spectrometry. The metal mercury was analyzed by cold vapor atomic absorption. Concentrations of most of these chemicals were determined in 35 deciduous molars. SwRI is teaming with The University of Texas Health Science Center at San Antonio in a grant application to NIH to measure these chemicals in 400 deciduous teeth as part of a study to investigate autism risk using tooth measurements to assess early life exposure.

2011 IR&D Annual Report

siRNA and miRNA Cell Delivery Utilizing a Novel Nanoplatelet Platform, 01-R9736

Principal Investigators
Larry A. Cabell
Kent E. Coulter
Vicky Z. Poenitzsch
Joel J. Kampa
Lucy M. Kimmel
Ranjan Perera

Inclusive Dates: 07/01/07 – 12/01/10

Background — Chromosomal mutations often convert normal differentiated cells to undifferentiated, highly adaptive, stem cells that can re-differentiate into cancer tissues such as melanoma. These adaptive tissues often escape first-pass chemotherapies and become resistant to the first-pass chemotherapeutic agent in recurring tumors. New therapeutics such as siRNA (small interfering) and miRNA (micro interfering) are being synthesized to re-regulate intracell metabolic pathways that cancer cells depend on for their unregulated growth, immortality, metastatic invasion and other hallmarks exhibited by the specific cancer phenotype. Since siRNAs and miRNAs are unstable in the *in vivo* environment, they must be stabilized by nanoencapsulation in particles (100 to 200 nm) that avoid the immune system and travel through the tissue from the site of application into the region of the tumor where they are incorporated into the cytoplasm (endocytosed) and release the siRNA in a controlled fashion. Proper endocytosis requires narrow particle size distribution and a defined morphology that is limited by co-participation methods. These characteristics offer substantial impediments to introduction of these new therapies into the drug pipeline that is administered by the FDA. Thus, a new nanoparticle delivery system must be designed to be biocompatible, non-immunogenic and bioresorbable at the cytoplasm of the target cell where it will release its drug cargo in a controlled fashion (in this case siRNA and miRNA targeted for melanoma pathways). In addition, the delivery particle must be monodisperse in size and shape to ensure proper endocytosis. Finally, this delivery system must be amendable to cGMP manufacturing requirements.

Approach — The primary goal of this project is to develop a revolutionary generic drug delivery platform that employs physical deposition of drug, inorganic encapsulating and coating multilayers on nanopatterned substrates produced by photolithography. Functional, fluorescently labeled siRNA and later miRNA will be alternating current (AC) nanoelectrosprayed on an amorphous, magnetron-sputtered calcium phosphate (magnesium or fluorine-doped) layer. After sandwiching the drug layer with another calcium phosphate-based layer, the film will be fractured along the nanoembossed pattern on the substrate into 200 nm lateral dimension nanoplatelets that will be incorporated into a vehicle dispersion and functionalized by polyethylene glycol. Nanoplatelets will be characterized with respect to particle size, charge, surface area, solution aggregation properties and any perturbations in the double strand siRNA or miRNA structure induced by processing to optimize the manufacturing process. The endocytosis of the labeled siRNA loaded nanoplatelets into HeLa cells will be mapped as a function of time by a Nikon Eclipse TE2000E inverted microscope equipped for multicolor fluorescence imaging and siRNA transfection efficiency determined. Once the initial stages of the platelet production are completed, miRNA (specifically directed against the production of critical proteins used by melanoma cell lines) will be encapsulated in nanoplatelets and characterized and evaluated against well characterized melanoma cell line pathways using array mRNA expression analysis and other molecular biology techniques.

Accomplishments — E-beam deposition of a first bioresorbable calcium phosphate (CaP) layer on specially manufactured nanopatterned substrate was accomplished. This material was then subjected to AC electrospray deposition of a siRNA (silencing interfering RNA) second layer on the first CaP layer. A second e-beam deposition process of a CaP layer to seal in the siRNAs was also accomplished. This three-layer film was then fractured along the nanopattern. The nanoplatelets were unstable to dissolution and recrystallization in suspension with the surface treatments employed. In addition, there was incomplete evidence that the test electrosprayed siRNA was stable on the CaP surface (possible base hydrolysis). Finally, there was difficulty in fracturing the films along the nanopattern to generate the desired narrow particle distribution. The instability of the nanoplatelets, the difficulty in the fracturing process and in the nanoplatelet recovery from the fracturing process were believed to be the synergistic product of a state-of-the-art nanopatterned substrate that could not be produced to desired specifications to produce 200nm particles and particle solvent process requirements to free and isolate nanoplatelets. At this time of this project, a finer mask to produce the nanopatterned substrate could not be produced. Therefore a better understanding of the solvent requirements to fracture a coated nanopatterned substrate and recover particles without CaP crystal growth or recrystallization was undertaken. Solvent requirements to fracture a multi-coated nanopatterned CaP substrate and recover particles without CaP crystal growth or recrystallization was not accomplished by the end of this project. CaP solvent requirement investigations did produce a repeatable co-precipitation solution process to produce CaP-encapsulated isRNA and miRNA 100-200-nm particles.

2011 IR&D Annual Report

Development of Calcium Phosphate Nanoparticles and Their Use as Vaccine Adjuvants, 01-R9831

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Inclusive Dates: 07/01/08 – 04/01/11

Background — With the recent threat of bioterrorism, stabilization of antigens or enzymes used in protective vaccines or treatments for potential bioterrorist agents can be an effective method to protect both emergency response teams and the general population. Nanoparticles show several advantages over microparticles when used in immobilization/stabilization applications because of large surface area, and the ability to provide functionalized surfaces for multiple adsorption or attachment sites. The stabilization and controlled release of vaccines by nanoprecipitation could result in new vaccines or drugs. Anthrax protective antigen (rPA) was chosen as a vehicle to demonstrate the stabilization potential of the nanoprecipitation technique. Potential benefits of a successful outcome of this project would be a more stable rPA formulation for use in vaccine development. This project expanded on SwRI nanobased drug development and delivery endeavors. An additional benefit was establishing a collaborative relationship with USAMRID.

Approach — CaP (calcium phosphate) was chosen as a means of delivery for the rPA because it has the proven ability to function as an adjuvant (an adjuvant is needed for an effective immune response to subunit vaccines) and is safer and less controversial than adjuvants currently used in marketed vaccines. CaP nanoparticles were prepared by precipitation prompted by the addition of a calcium precursor solution to a phosphate precursor solution in the presence of one or more charged polymers, which provide stability to the suspension (CaP nanoparticles tend to aggregate very rapidly).

The functional activity of the CaP-rPA complex was developed with a cytotoxicity bioassay performed on a macrophage cell line. The stability of the prepared nanoparticles was determined by exposure to varying environmental conditions of elevated and reduced storage temperature. The stability of the complex was compared to the currently available vaccine formulation and to rPA alone; the complex's activity was confirmed using the cytotoxicity assay. An animal study (mice) was designed to examine the impact of adjuvanation with calcium phosphate-based nano-particles.

Accomplishments — A variety of nanoparticles has been prepared investigating the use of additives and varying formation conditions. The cell-based cytotoxicity assay capability has been added and used on generated particles. Methods for the nanoparticle isolation have been developed that allow the collection, washing and re-suspension of the material. rPA is currently in use for particle preparation; particles have been successfully prepared, washed and lyophilized. A stability study has shown that the generated particles loaded with rPA are more stable than the rPA itself at elevated temperatures. The animal study showed that the particles were non-immunogenic, although they were active in the cell based assay.