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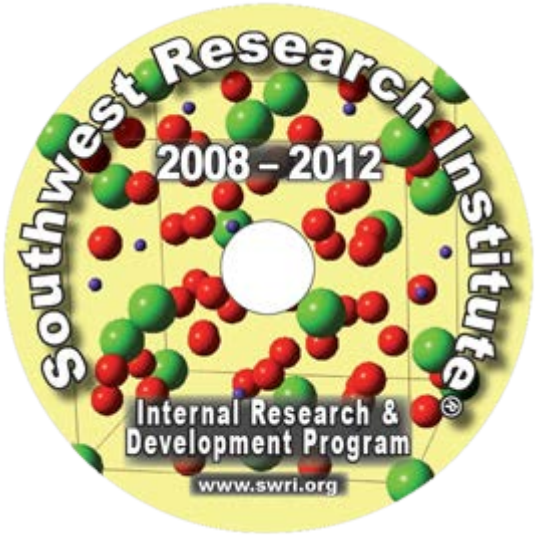
Internal Research and Development 2012



- 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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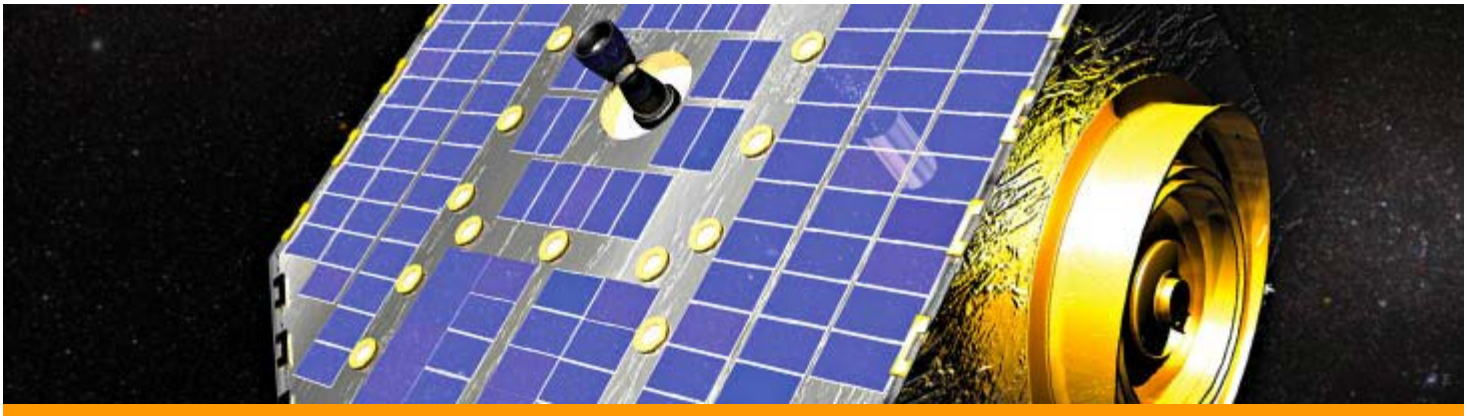
SwRI IR&D 2012 – Space Science



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- Capability Development and Demonstration for Next-Generation Suborbital Research, 15-R8115
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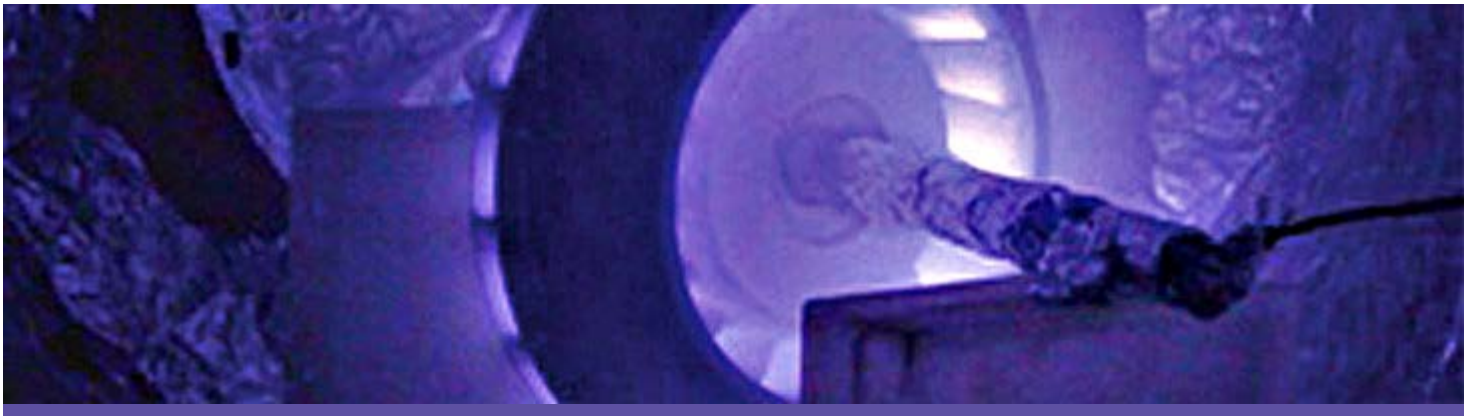
SwRI IR&D 2012 – Materials Research & Structural Mechanics



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- Analytical Methods and Concentrations of Exposure Biomarker Chemicals in Deciduous Teeth, Quick-Look, 01-R8235
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2012 IR&D Annual Report

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

Principal Investigators
Paul Wood
Carlos Quiroz
Allison Bertrand
Sue Baldor

Inclusive Dates: 04/01/11 – 09/30/12

Background — Two plug and play (PnP) protocol options for SpaceWire (SpW) exist – one defined by the U.S. Air Force Research Laboratory (AFRL) and one developed by the European Space Agency (ESA). The ESA Spacecraft Onboard Interface Services (SOIS) protocol aims to work within the framework of the SpaceWire standard, blending PnP structures into existing SpaceWire features and retaining protocol-level support for legacy devices. The AFRL space plug-and-play architecture (SPA) protocol is geared more towards agility and adaptability to provide generalized support for more kinds of devices and networks (including blended networks of SpaceWire and other protocols). This effort investigated whether a common interface could be developed by using a PnP adaptation layer to interact through both variants of plug and play and a simulated SpaceWire network attached storage (NAS) device as a challenge task. The project was extended to examine feasibility of performing OPNET Modeler simulation that integrated with a SPA implementation.

Approach — The approach was to build a lightweight implementation of various components of the system combined with existing hardware and software so that experiments could be conducted. Using SwRI experience in the first half of the project, researchers performed additional work in merging their understanding of an actual SPA implementation to perform experiments in a combined simulation of the SPA with OPNET. A test bed was assembled using available SwRI resources. The test bed consisted of a SpaceWire network with two routers and Linux computers. An adaptation layer for the PnP capability was defined and implemented. A SPA middleware implementation (Utah State University [USU]) was acquired from AFRL and ported to the physical system. Simulated producer, consumer, and NAS applications were written. The USU SPA was successfully operated using the test bed in both a raw mode and with the adaptation layer in place for the simulated applications. No ESA reference implementation was available; thus, a second SPA implementation was acquired from Broad Reach Engineering (with AFRL support). This implementation proved to be too different in its hardware and software interfaces to be practical to port to the test bed. Researchers analyzed the implementation and determined that, in principle, it should be usable with the adaptation layer. The project was extended to investigate the feasibility of combining an OPNET simulation with an actual SPA implementation. Researchers used the USU SPA V9.1 and verified that a simulation was feasible using OPNET co-simulation and a custom controller program external to OPNET. The external project provided an interconnect between the SPA executables and the OPNET internal model.

Accomplishments — This work showed that an adaptation layer was feasible to add to existing PnP implementations. The addition of the adaptation layer to the USU SPA implementation was straightforward and effective. Researchers built a lightweight NAS along with producer and consumer applications that were connected using the adaptation layer and the USU SPA. The adaptation layer impact on system performance was negligible. A second SPA implementation was analyzed. This implementation was not directly operable on the underlying hardware. It was concluded, however, that this version would have been compatible with the adaptation layer. Also, although no reference implementation of the ESA

approach existed, researchers concluded that the adaptation layer concept was workable for that environment as well. Finally, in the project extension, researchers showed feasibility that the SPA could be successfully integrated with OPNET Modeler. The ability to perform software-in-the-loop (SIL) simulation (for example, the SPA) is an enabling factor in performing very high fidelity simulations of SpW networks.

2012 IR&D Annual Report

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

Principal Investigators
S. Alan Stern
Daniel Durda

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: more frequent access to the space environment, lower launch cost compared to conventional sounding rockets, capability for human operator presence, better experiment affordability, 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.

SwRI staff members completed pressure suit testing and centrifuge evaluation in November 2011.

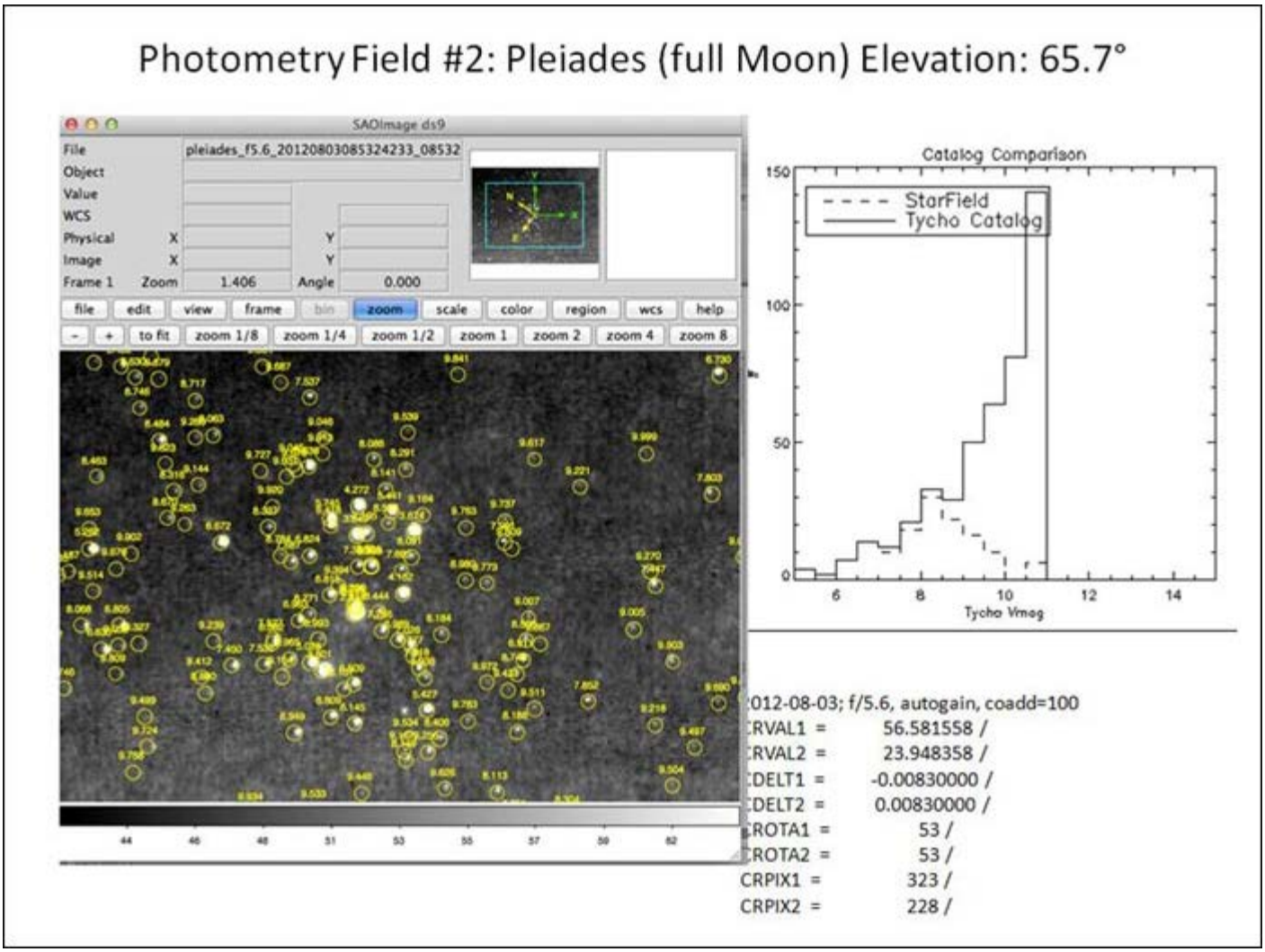
Therefore the overarching objective for this project is to put SwRI in the lead of the burgeoning suborbital research field using next-generation, manned vehicles by becoming one of the first, and quite possibly the first, organization to fly payloads with research payload specialists on these vehicles. This will open up SwRI to 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 providing payload specialists for next-generation suborbital work.

Accomplishments — Accomplishments on this IR this year include:

- SwRI staff completed pressure-suit familiarization training at the David Clark Company and staff undertook centrifuge training at NASTAR to test/evaluate the David Clark CHAPS pressure suit under launch g-loads.

Completed an upgrade and re-calibration of SWUIS experiment for flight.

- Initiated planning for high altitude (75,000 ft) flight training in F-104 and F-18 aircraft for later 2012.
- Negotiated early flight test phase spaceflights with XCOR.
- Completed FAA Class I medical to maintain expected suborbital flight medical qualification standards.
- Continued aerobatic jet aircraft training.
- Completed flight data requirements and collection plans for each suborbital experiment.
- Invited oral presentation on the SwRI Suborbital Program at AIAA annual meeting (Nashville, Tenn.).
- Oral presentations on the SwRI Suborbital Program and SwRI's three suborbital experiments at the Next-Generation Suborbital Researchers Conference (Palo Alto, Calif.).
- Invited oral presentation on the SwRI Suborbital Program at Spacefest IV (Tucson, Ariz.).
- Invited panel presentation and discussion on the SwRI Suborbital Program at Spaceup Houston 2012 Commercial Spaceflight event (Houston).



The SWUIS experiment was upgraded and re-calibrated during laboratory and field ops in 2012.

2012 IR&D Annual Report

An Optimized Ion Neutral Mass Spectrometer Design for the NASA/ESA Europa Jupiter System Mission (EJSM), 15-R8201

Principal Investigators
J. Hunter Waite
David T. Young
Timothy Brockwell
Keith Pickens
John Roberts
Greg Miller

Inclusive Dates: 01/01/11 – Current

Background — This project had two primary objectives: 1) determine the science traceability of a mass spectrometer for a mission to the Galilean satellites, and 2) develop a low-resource, mass spectrometer design based on the multi-bounce time-of-flight mass spectrometer that could carry out the proposed science objectives.

Table E-1. ANGIO Characteristics, Resources and Performance Summary		
System Characteristics		
Subsystem	Type	Specification
GIS - collimator	Anti-scattering baffle, ST172 coated, single use cover	FOV: 1π steradian in ram direction
GIS - cryotrap	Cryotrapping/direct inlet, neutral gas	Sensitivity boost: up to 2,000 counts s^{-1} per mol cm^{-3}
MS - closed source	Storage, electron ionization, redundant emitters	Ambient sensitivity: 0.02 counts s^{-1} per mol cm^{-3}
MS - ion optics	Multibounce time-of-flight	Resolution: 12,300 m/Δm FWHM for HDO
MS - detector	Electron multiplier	MCP, 3 plate z-stack, 5μm pore
Resources - Current Best Estimate (CBE), see §F.1.8 for margin		
Mass & Volume	Power (W)	Average Data Rate
7.52 kg, 0.0183 m^3	38.80 (Peak), 28.80 (Average), 2.00 (Standby), 1.50 (Survival)	55.12 kbps (peak), 12.33 kbps (average)
Performance		
Measurement	Requirement	Capability in 200 km Ganymede Orbit

Noble gas abundances wrt H_2 (major isotopes)	Mixing fractions >1 ppm	Determined in <300 s with cryotrapping (132 hours sampling time)
D/H in H_2O isotopic ratio	Ratios >10^{-6} ±25%	Determined in <60 s with cryotrapping (132 hours sampling time)
Organics, abundance wrt H_2	Masses to 300 u, >1 ppm	Determined in 63 min

Approach — The project was undertaken to place SwRI in a competitive position for the joint NASA/ESA EJSM. However, the scientific focus of the mission changed from Europa to Ganymede in the course of the study, due to the NASA science priorities set by the Planetary Decadal Study and SwRI's proposal, "A Neutral Gas Investigation of Origins (ANGIO)," was submitted to the NASA SALMON PEA K for participation in ESA's JUpiter ICy moons Explorer (JUICE) mission. The science objectives were derived from the Science Requirements document:

> **Objective 1 (Origins)**: Make definitive measurements to constrain the formation conditions of the Galilean satellites: D/H, $^{18}O/^{16}O$, $^{17}O/^{16}O$, $^{14}N/^{15}N$, and noble gases.
> **Objective 2 (Habitability)**: Measure the composition, distribution, and evolution of surface materials from sputtering processes, with emphasis on comparative habitability.
> **Objective 3 (Habitability)**: Investigate geological features that may be linked to ice shell or interior composition.
> **Objective 4 (Coupling and Interaction)**: Determine the spatial structures of the neutral atmospheres and neutral clouds.

These science objectives were addressed with a low-resource multi-bounce time-of-flight mass spectrometer with the characteristics shown in the table below:

Accomplishments — Both primary project goals were met.

2012 IR&D Annual Report

Invitation to Conduct High-Resolution Optical Observations in Conjunction with the Global Network of State-of-the-Art Radar Facilities, 15-R8206

Principal Investigators
Marilia Samara
Robert Michell
Michael Muller

Inclusive Dates: 01/01/11 – 06/30/12

Background — This project comprises several observing campaigns at different incoherent scatter radar (ISR) facilities throughout the world, using recently acquired, high-tech imagers. The scientific focus was two-fold: a) the physics of meteor interactions with Earth's atmosphere and b) auroral structure and dynamics. The meteor data especially held many surprises, providing solid bases for further research.

Approach — Individual coordinated campaigns were successfully completed alongside the Jicamarca Radio Observatory (JRO) in Peru, the Southern Argentine Agile MEteor Radar (SAAMER) and the Arecibo Observatory in Puerto Rico, all targeting meteor physics. Observations also took place alongside the Sondrestrom ISR in Greenland and the Poker Flat Incoherent Scatter Radar (PFISR) in Alaska, targeting auroral structure and dynamics. The data collected during these campaigns and the collaborations with the researchers at the respective radar sites have been invaluable in constructing a unique meteor analysis approach as well as new insights to auroral signatures in radar data.

Accomplishments — There were two main accomplishments expected during this project and both were achieved. SwRI researchers established new collaborations with colleagues among far-reaching research areas beyond those they are currently engaged in. Equally importantly, unique, groundbreaking data sets were collected that are valuable, not only scientifically, but in demonstrating SwRI technological capabilities in future external proposals for further science and for acquiring additional imagers. Highlights include: a) Observations of Polar Cap Boundary Aurora (Sondrestrom): The types of auroral structures observed contained much more variation than expected. Such tall colorful auroral rays are not often observed at lower latitude locations within the auroral oval. b) Meteors (SAAMER): It was expected that the radar would see every meteor that would have been see given the large beam size and high power of the radar. However, a more complex relationship emerged, where researchers sometimes observed bright meteors optically that the radar did not see and sometimes the radar would observe strong returns that they did not see optically. These observations are the first of their kind with this type of radar. c) Meteors (Arecibo): This campaign also yielded unexpected results. SwRI researchers were able to detect far more common events than originally thought. In addition, both radars were operating (430 MHz and 46.8 MHz) and detected common events. These observations show that meteors with magnitudes down to about +10 can be detected that correspond to very low mass meteors (~100 µg).

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2012 IR&D Annual Report

Support for NASA Lunar Science Institute – Year 2, 15-R8225

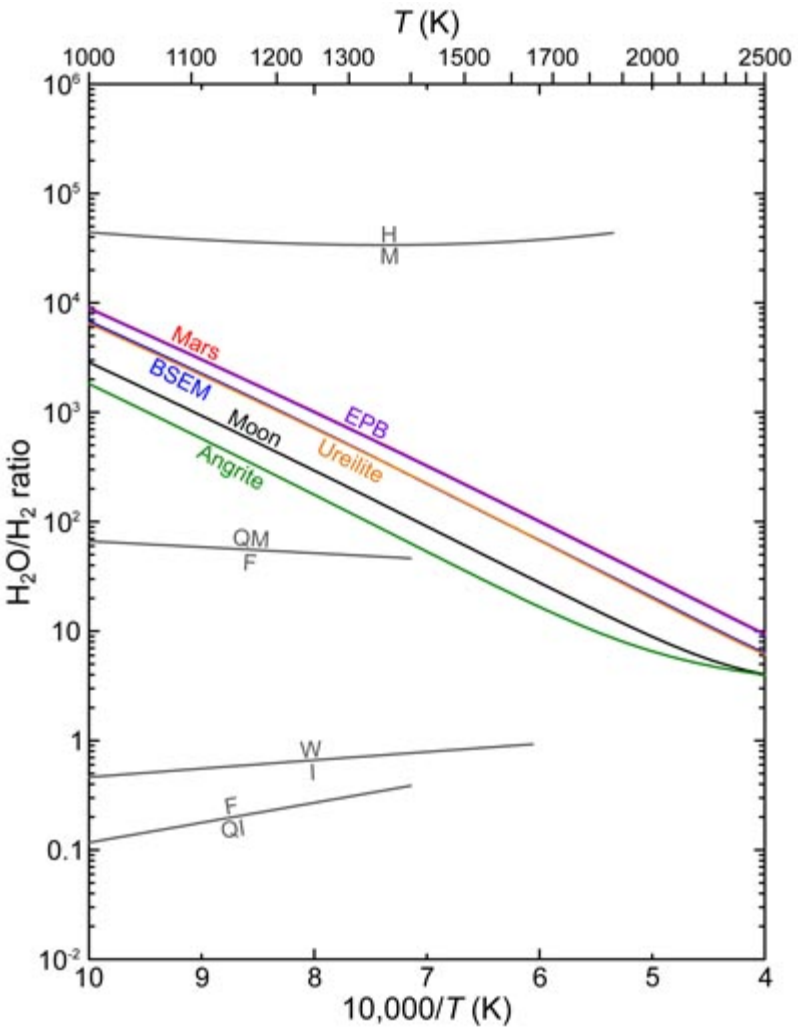
Principal Investigators
Robin M. Canup
J. Salmon
C. Visscher

Inclusive Dates: 10/01/11 – 10/01/12

Background — It is generally accepted the Earth's Moon accreted from a disk generated by the impact of a Mars-size object on the protoearth. However, predictions of existing models of the Moon's accumulation from such a disk are problematic because they (1) seem inconsistent with the likely state of disk material, (2) do not allow for compositional equilibration between the disk and the protoearth, which may be necessary, and (3) necessitate a fully molten Moon, potentially at odds with geological and geochemical constraints.

Approach — In Task 1, the project team is developing a more physically realistic model of the Moon's accretion after a giant impact. It was previously thought that the Moon's mantle was anhydrous. Recent water content estimates of lunar volcanic glasses, however, suggest that the Moon's mantle may contain up to several hundred parts-per-million water, comparable to the Earth's bulk water content (Saal et al. 2008). Numerical simulations of the giant impact predict disk temperatures of ˜ 2500 K to 5000 K, and imply tidal disruption of much of the disk material down to meter-sized droplets (Stewart 2000), which would lead to volatile degassing and potential water loss. At present it is not known to what extent a moon formed from an impact-generated disk can retain water. In Task 2, the project team is developing a model for water loss/retention from the protolunar disk.

Accomplishments — To better address the Moon's accretion, a hybrid numerical model was developed consisting of (1) a fluid disk to represent the material within the Roche limit (the distance below which accretion is prevented by tidal forces from the planet), and (2) an N-body code to track solid particles orbiting outside the



Equilibrium water-to-hydrogen ratio in the vapor phase, based upon calculated oxygen fugacities for different anhydrous silicate melts

(colored lines). Oxygen fugacity buffers are shown for comparison (gray lines); MH: magnetite-hematite, QFM: quartz-fayalite-magnetite, IW: iron-wüstite, QFI: quartz-fayalite-iron.

Roche limit. The Roche-interior disk spreads due to its viscosity, and can deliver material beyond the Roche limit, where it can accrete to form new moonlets. For the disk's viscosity, either an instability-driven viscosity (Ward and Cameron 1978) or a radiation-limited viscosity (Thompson and Stevenson 1988) is used, depending on the disk's properties. Collisions between orbiting particles are treated using the tidal accretion criteria of Canup and Esposito (1995). They also interact with the fluid disk at Lindblad resonances. Finally, the project team included the possibility of bodies scattered toward the planet and crossing the fluid disk to be captured. If such a capture happens, it is assumed that the body is tidally disrupted, and its mass and angular momentum are added to the fluid disk. This results in a three-step accretion process: (1) outer bodies rapidly collide and accrete, until only a few massive bodies remains, then (2) these massive bodies confine the inner disk within the Roche limit due to resonant interactions, and they in turn recede away, and (3) the fluid disk spreads back out to the Roche limit, new moonlets are spawned and collide with outer object to form the final Moon. Contrary to accretion timescales of a few months with prior pure N-body simulations, the slow spreading of the fluid disk leads to accretion timescales of hundreds of years in the SwRI model, which is comparable to the timescales necessary for the disk's composition to equilibrate with that of the Earth. These results have been accepted for publication in the *Astrophysical Journal* (Salmon and Canup, "Lunar Accretion from a Roche-interior Fluid Disk," 2012).

A modified version of a melt-vapor equilibrium code (MAGMA; Fegley and Cameron 1987) was used to determine the total vapor pressure and chemical speciation in the vapor phase for a number of different potential disk compositions, including bulk silicate Earth-Moon (BSEM), present-day Moon as inferred from lunar samples, and various meteorite classes. The BSEM composition has been adopted as a nominal initial composition and plausibly represents the silicate composition of the Earth-Moon system shortly after the giant impact (e.g., higher initial Na and K contents than in the present-day Moon because of subsequent escape of volatiles). The model results have also been used to calculate oxygen fugacity of the silicate vapor — a key parameter that influences the overall chemical behavior of the disk. Preliminary results suggest a highly oxidizing vapor phase dominated by Na, O, O_2, and SiO, which is largely independent of the adopted bulk composition. Assuming equilibrium between melt and vapor phases, the oxygen fugacity can be used to calculate the H_2O/H_2 in the gas phase, via the equilibrium reaction $H_2 + 0.5O_2 = H_2O$ (cf. Elkins-Tanton & Grove 2011). Results of this calculation are shown in the illustration. The resulting H_2O/H_2 ratios will be used to estimate the expected escape rates of water vapor from the protolunar disk.

2012 IR&D Annual Report

Tactical Aerobotic Launch System (TALS), 15-R8226

Principal Investigators
William D. Perry
David Lopez
Michael L. Fortenberry

Inclusive Dates: 04/18/11 – 02/29/12

Background — The process for inflating and launching typical LTA (lighter-than-air) systems presently requires a large paved or grassy area that is clear of obstructions, where the hull can be unpacked and laid out length-wise in preparation for inflation. This process often can take 12 or more people to accomplish. This process often must be conducted inside a very large hangar or outdoors under very low wind conditions because these hulls can be several hundred feet in length and made from very lightweight material. It often requires large handling equipment along with an experienced launch team to get it launched without damage. Most military applications would prefer to deploy LTA systems quickly from remote unimproved sites with minimum personnel in less than optimal meteorological ground conditions. Using current launch processes, that is presently not possible.

This project investigated a concept for rapidly launching LTA systems from a self-contained package that provides inflation, stabilization, protection and finally release. TALS could be operated by a small team or autonomously to launch a LTA system on command. SwRI has been conducting a spiral development of the HiSentinel stratospheric airships for several years. These prototype airships have been manually launched, a process requiring very low surface winds, and a large team to get the airship inflated and launched. SwRI's DOD clients have indicated a quick and easy way to deploy these LTA systems is needed. TALS could greatly improve the versatility and utility of the airship, and other LTA systems, allowing them to be used in a wider variety of tactical applications.

Approach — The TALS concept uses a single shipping container in which the LTA system is packed along with a supply of lifting gas (helium or hydrogen). The inflation subsystem includes batteries for power and a digital electronics system that controls the inflation and launch process. The TALS container will be transported to the launch site by truck or helicopter, where the container is secured to the ground, vehicle, or other structure. Once the container is secured, the LTA system can be launched or it can be left to be autonomously launched at a later time by either a timer or telecommand. After launch, the container housing the inflation system and launch controls can be recovered and refurbished for reuse.

Field testing of the 35-Percent Scale TALS Demonstrator

At the planned launch time, the integrated control system will determine if the wind velocity and direction are acceptable. If acceptable, the inflation and launch process will begin with the top of the container

opening to expose the protective tent that covers the folded LTA system. Guy lines attached to the tent with automated tensioning will provide stability during the inflation process. Inflation rate and total gas quantity will automatically be controlled. The hull will rise from the container as it is inflated inside a protective tent. When the predetermined amount of lifting gas has been injected, the gas flow will cease and the top of the tent will open, allowing the LTA vehicle to escape and ascend. Once released and ascending, the hull will unfold until it is fully extended.

Accomplishments — Phase 1: The team successfully conducted a feasibility study for the TALS concept. The study included four primary tasks:

- Performance Requirements for a full-scale TALS System
- Preliminary design for a full-scale TALS System
- Feasibility Analysis
- Detail design for a functional 35-percent scale model of TALS.

Based on the results of these tasks, it was determined that the proposed go/no-go criteria had been met and Phase 2 was authorized.

Phase 2: A functional 35-percent scale model of the TALS was fabricated and integrated. Subsystems for the TALS demonstrator were each independently tested in the laboratory. The completed TALS prototype was integrated, and functional tests were conducted. The illustration shows a TALS launch sequence during a field test of the demonstration prototype. Based on these tests, the team has shown the feasibility of the TALS concept.

2012 IR&D Annual Report

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 SwRI's 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 — This project demonstrated that the detectors are sensitive to UV light at levels ranging from 9 to 22 percent at 1,216 Å to 20 to 40 percent at 1,600 Å. These detectors met the initial criteria of 10 percent sensitivity in the vacuum UV for their use in future spaceflight instrument concepts. Indeed, the finding of ˜40 percent sensitivity at 1,600 Å greatly exceeded expectations for the potential suitability of these devices to SwRI's UV studies. Therefore, further development and UV-optimization of these devices is warranted.

2012 IR&D Annual Report

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

Principal Investigators
Ed Patrick
Ben Teolis
Greg Miller
F. Scott Anderson

Inclusive Dates: 07/01/11 – Current

Background — The discovery of pit craters on the lunar surface and of volatiles trapped at the lunar poles has created a renaissance in lunar science. The motivation for this project was the desire to develop a laboratory space environment simulation of the lunar polar regolith. The intended purpose of this laboratory system is not only to study the conditions at the lunar surface, but also to aid in the design of the "front-end" components for a landed lunar mass spectrometer. Any proposed instrument for a future lunar surface mission must have a high technical readiness level (TRL) and show a capacity for maximizing the science return from investigations of the volatiles trapped within the lunar regolith. These materials may not only reveal the ancient volatile history of the inner solar system, but they may also represent resources (e.g., water) critical to the future of lunar outposts and the prolonged presence of humans at the lunar surface.

Approach — A lunar regolith simulant known as JSC-1A was placed within a vacuum system and exposed to various volatiles and gases (H_2O, CO_2, N_2, Ar) while the system was monitored by a mass spectrometer. The JSC-1A simulant is a dark, finely-ground, powder-like, basaltic material. It was processed in air by a proprietary mechanical technique from basaltic ash at the foot of a thousand year-old extinct volcanic cone in Arizona. The capacity of the simulant for entrapping gases at various temperatures and gas exposure pressures are being monitored. Laser ablation, ion and mechanical techniques will be employed as means for producing suitable vapor plumes for monitoring evolved gas constituents by mass spectrometry. A preliminary design will be drafted for a landed mass spectrometer based on the results of this investigation for inclusion in future proposals targeting investigations of the lunar surface environment.

Accomplishments — Though the introduction of the JSC-1A lunar soil simulant into an ultrahigh vacuum (UHV) system has been a problematic process owing to the large surface area of the material, preliminary data are intriguing and suggest multiple gas-trapping effects that may be analogous to, and appropriate for, future studies of the lunar surface environment. The mass spectrometric analysis of the JSC-1A simulant in vacuum is currently focused on four gas processes that may affect the evolution and behavior of the material under exposure to gases and volatiles: (1) the original entrained gases and volatiles within this refractory oxide-rich basalt as it reached the surface of the Earth, (2) exposure of this basaltic material to gases and volatiles when it was ejected and cooled during the volcanic eruption process, (3) exposure of this material to terrestrial gases and volatiles during long-term weathering processes in terrestrial air, and (4) the subsequent processing that crushed this material and exposed it to gases and volatiles in terrestrial air. SwRI researchers are currently studying the interaction of the simulant with various gases in order to separate terrestrial material effects from those anticipated in future studies of the lunar surface. SwRI researchers have also determined that minimal energy is necessary to produce gas plumes sufficient for analytical techniques (e.g., mass spectrometry) for detecting and analyzing volatiles in the JSC-1A lunar regolith simulant. The PREMISE project helped support the submission of a NASA

Research Opportunities in Space and Earth Sciences (ROSES) Lunar Advanced Science and Exploration Research (LASER) proposal by the same name ("PREMISE") that is currently pending. This project reduced program risks related to the handling of lunar regolith simulant in the laboratory and improved the technical maturity of the LASER proposal submission to NASA.

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2012 IR&D Annual Report

TiME Discovery Phase A Science Support: Producing an Atmospheric Engineering Model for Titan, 15-R8251

Principal Investigators
Hunter Waite
Jared Bell

Inclusive Dates: 08/19/11 – 12/31/11

Background — The Titan Mare Explorer (TiME) was the first mission proposed to land on an extraterrestrial sea. It represents a unique opportunity to explore Titan's methane cycle, a multi-phase planetary surface, and the limits of life. *In situ* exploration of a major sea is the essential next step for advancing our understanding of Titan and provides an unprecedented opportunity to engage the public in the excitement inherent in visiting a fascinating new environment on this alien world. TiME makes that possible — within the Discovery program and within the coming decade. The objective of this project was to generate a Titan atmospheric engineering model in support of the TiME. The model was used by NASA Langley engineers to design the descent and landing phases of the TiME mission and by NASA AMES engineers to simulate the aerodynamics of the spacecraft and heat shield. Previous Titan atmospheric engineering models were constructed to design the entry and landing of the ESA-Huygen's Titan lander (Yelle et al., 1997). However, the Cassini-Huygens mission has supplied a wealth of new data that must be incorporated into a new engineering model to support the TiME mission design. The model can serve as an engineering and science tool for the design of any future orbiter aerocapture or lander missions to Titan.

Approach — Titan's atmosphere has been extensively studied during the Cassini-Huygens Mission. The polar environment undergoes considerable seasonal variation and is distinct from the more quiescent equatorial environment experienced by the Huygens probe in 2005. The thermal structure of the upper atmosphere is affected by interaction of Titan's atmosphere with the plasma and energetic particles in Saturn's magnetosphere or in the solar wind. Titan's polar regions, and its hydrocarbon lakes in particular, are of interest for future exploration. Thus specific environmental models are required for polar exploration. Furthermore, the models developed to support the design of Huygens had to accommodate wide uncertainties, requiring large design margins. The extensive observations by the Cassini spacecraft (and indeed Huygens itself) provide a basis for narrowing these uncertainties, notably in composition.

Accomplishments — The empirically constrained neutral temperatures and densities presented here also have important implications for fundamental chemical modeling. Detailed chemical models, such as Krasnopolsky [2009, 2010], Wilson and Atreya [2004] among others, typically rely upon specified major neutral densities and temperatures. The empirical modeling presented here would provide much-needed constraints on these models, and thus lead to improved estimations of chemical products. This would, in turn, provide improved estimates for important science questions at Titan, such as (1) global production of aerosol haze particles, (2) estimates of the deposition of heavy hydrocarbons on the surface of Titan, and (3) better constraints for photoionization of the upper atmosphere. This paper describes a new model of Titan's atmospheric structure to guide both scientific studies and studies of entry and descent. Of particular interest is the proposed Titan Mare Explorer (TiME) mission in the period 2023–2025.

2012 IR&D Annual Report

Non-Intrusive Gas Temperature Measurement for Stratospheric Applications, 15-R8262

Principal Investigator
Michael L. Fortenberry

Inclusive Dates: 10/01/12 – Current

Background — Finding a non-intrusive technique for determining gas temperature in the stratosphere is of particular interest to the stratospheric lighter-than-air and the meteorological communities. Air is of obvious interest for meteorological interests, and helium is of interest for lighter-than-air (LTA) applications such as balloons and airships. The low-pressure environment of the stratosphere makes it difficult to measure gas temperature accurately, whether the gas is atmospheric air or an internal lifting gas (i.e. helium) for lighter-than-air (LTA) craft. This is due mainly to changes in the relative contribution of convection, radiation and conduction to the thermal balance of objects or gases as altitude increases and atmospheric pressure decreases. At the low pressures found in the stratospheric environment, radiation and conduction play a much more significant role in the thermal balance than they do at higher pressures. For the stratospheric LTA community, determining the internal gas temperature of helium in a balloon or airship (especially if the gas envelope is pressurized) is critical to accurate balloon analysis and in-flight projections for long missions. While obtaining localized (i.e., point) measurements of helium temperature is useful, the ability to obtain average gas temperature measurements over large distances provides a better global picture because of the overall size of the vehicles ranging from a volume of 250,000 cubic feet up to 40,000,000 cubic feet.

Approach — The approach used in this project is to characterize a non-intrusive gas temperature measurement technique suitable for stratospheric LTA applications. The two techniques to be investigated, thermistor array and acoustic, are drastically different in operational principle and each technique could be useful in an operational environment if they provide accurate measurements.

Accomplishments — This is an on-going project that should be complete early in 2013. An acoustic methodology is undergoing test currently. Testing and analysis of data should be finalized by early 2013.

2012 IR&D Annual Report

MASPeX Detector Development, 15-R8288

Principal Investigators
Hunter Waite
John Roberts
Keith Pickens
Gregory Miller

Inclusive Dates: 02/06/12 – Current

Background — The purpose of this project is to develop a new microchannel plate (MCP) based, high-dynamic range detector to be incorporated on SwRI's multi-bounce high-resolution time-of-flight mass spectrometer (MBTOF). The detector development is in support of the NASA-funded MASPEX and the MBTOF instrument as well as other potential flight programs that require a ruggedized high dynamic range TOF detector. The MASPEX technology development program is developing key technologies necessary to increase the readiness of the instrument suite to TRL 6 by demonstrating the entire system performance in the target environment. The detector will be designed to meet both the performance and environmental requirements for a MASPEX-based space flight mission profile. This includes the ability to subject the detector to the equivalent launch loads, and bake the detector to ensure a contamination free environment within the mass spectrometer. The MASPEX detector incorporates two stages of amplification to meet the science requirements for measurement of ion ratios that require high dynamic range. The first stage of amplification and its collector are used to measure species at high abundance, while the second stage of amplification and its dedicated collector are used to measure the low abundance species. The second stage of amplification is protected from damage due to excessive ion currents by a blanking grid that is activated when the signal exceeds a current value. Significant overlap between the two stages ensures that the signal falls within the linear response range.

Approach — Once the detector is fabricated, SwRI will perform a baseline optical performance test for the detector using the existing MBTOF-III instrument as a test platform. The performance envelope of the detector will be established and recorded, and its dynamic range performance will be verified against the minimum performance requirement. The detector will then be subjected to vibration testing and temperature cycling. The detector will be instrumented and observed during testing to watch for visible or detectable anomalies that take place during testing. Upon completion of environmental testing, the detector will again be installed into the MBTOF-III instrument for performance measurement. The performance level will be compared to the baseline performance level to verify that the detector's performance has not degraded or otherwise changed significantly from the baseline.

Accomplishments — The mechanical design of the ruggedized detector has been made. The material properties of the ceramics used in the construction have been selected that meet or exceed the requirements for baking out the detector at high temperature to ensure cleanliness. All materials have been selected for low outgassing requirements. A finite element model has been made to model the loads expected on the detector. The microchannel plate requirement documents have been written for use in the fabrication of the microchannel plates used in the detector.

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2012 IR&D Annual Report

Scientific Design Studies for a Polarizing Heliospheric Imager, 15-R8309

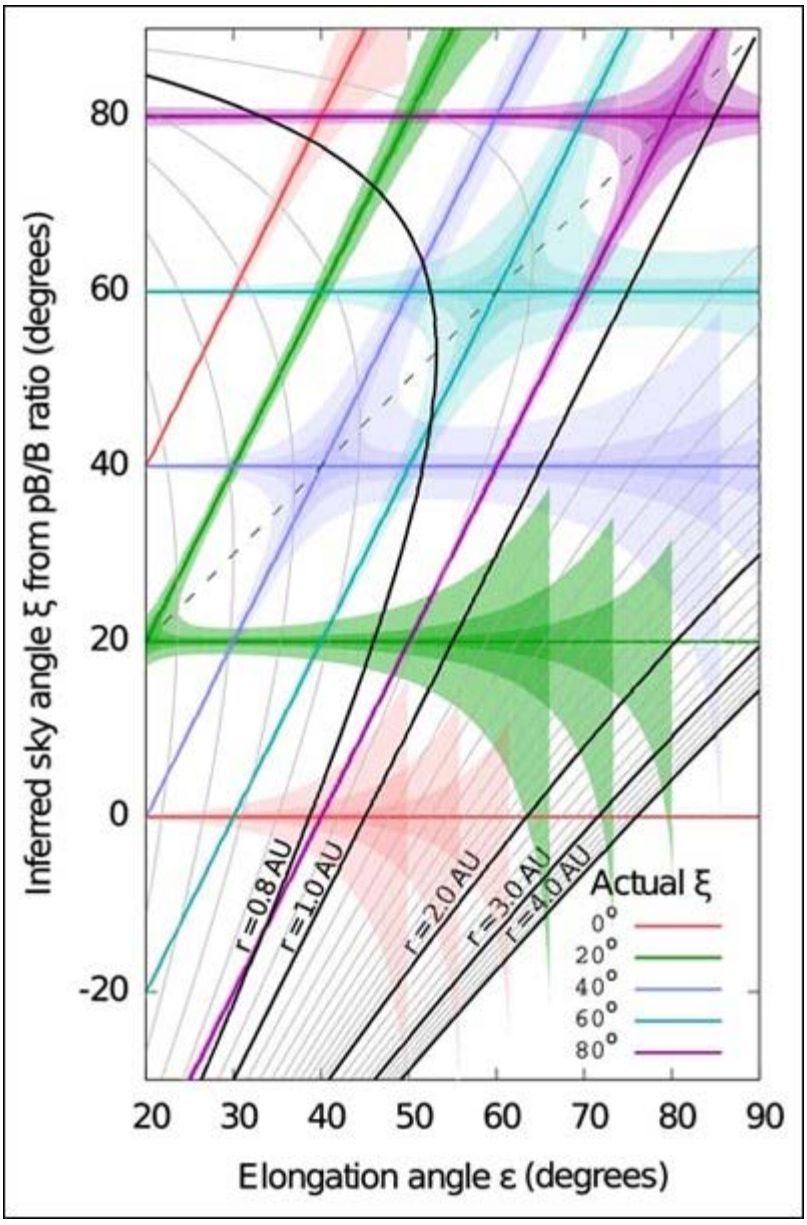
Principal Investigators
Craig DeForest
Tim Howard

Inclusive Dates: 04/30/12 – 8/30/12

Background — SwRI researchers are advancing the technology of "heliospheric imaging" of tenuous clouds of free electrons and ions in interplanetary space. The clouds, while visible, are extremely faint compared to other objects in the night sky. The technology will aid understanding of the solar wind and coronal mass ejections (CMEs), two phenomena that link activity in the Sun's atmosphere with the Earth and other planets. The clouds are visible because sunlight scatters off of individual free electrons in interplanetary space. The physics of the scatter gives rise to a polarization signal, which can potentially be exploited to measure the 3-D location of features in the solar wind. This concept had never been fully developed, and is a key step to building a next-generation heliospheric imaging instrument.

Approach — SwRI researchers developed an analytic theory of small feature polarization given the known physics of Thomson scattering (the process that renders plasma clouds visible), and a simulation framework to demonstrate the effect on realistic images of a simulated CME. A numerical inversion scheme was also developed to extract 3-D location of propagating CMEs, and it was demonstrated using data from the simulation framework.

Accomplishments — The development goals were met and the results were published in two papers submitted to the



This illustration shows that 3-D imaging of solar wind and CMES is possible.

Astrophysical Journal. SwRI researchers were able to demonstrate that 3-D imaging of solar wind features and CMEs is feasible, given an instrument with similar imaging quality to existing instruments and also polarization capability. The illustration shows the fundamental result, indicating inferred location of 15 modeled small features as they propagate away from the Sun. For example, the green shape represents a feature leaving the Sun 20° from the plane of the sky, as it crosses various "elongations" (angles from the Sun). The feature is inferred to be traveling along its correct trajectory (horizontal sheaf of curves) or along a physically unfeasible "ghost trajectory" that can be ruled out by dynamics considerations (angled green line). Each shape in the sheaf represents a different feature brightness in the instrument focal plane. Similar plots in the companion paper show the feasibility of similar analysis for large features.

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2012 IR&D Annual Report

Analysis and Testing of Ceramic Column Grid Array Component for Space Applications, 15-R8315

Principal Investigators
James Noll
Kelly Smith

Inclusive Dates: 05/25/12 – 09/25/12

Background — High-connection density, large lead-count ceramic column grid array (CCGA) packaged components bring new and improved capabilities to electronic systems for space applications. Prior SwRI efforts have qualified specific CCGAs for spaceflight use, but these devices had at most 624 leads with 1.27 mm pitch spacing. This project tested SwRI's capability to install a 1,752 lead, 1.00 mm pitch CCGA on a printed wiring assembly (PWA), and have those connections survive typical vibration and thermal loading for a space application.

Approach — Analysis of the environmental loading was performed to predict joint stresses for various CCGA installation locations and different stiffener designs. A test board emulating the mechanical and thermal properties of the predicted next version of the IRB (engineering model and flight model) was designed and fabricated. Two test CCGAs were installed in two different locations. One location minimized solder joint stresses, and the other provided the greatest flexibility for connections routing. The test board was subjected to environmental testing, including vibration and thermal cycling, to validate the analysis and manufacturing process.

Accomplishments — Analysis of the vibration-induced solder joint stresses predicted the CCGA could be installed safely near the board center with a reinforcing cross stiffener attached to the PWA. The assembled PWA passed vibration and thermal testing as predicted by analysis. Both installation locations passed testing. The CCGA was installed successfully, demonstrating the capability to meet the more challenging requirements of this larger CCGA: greatly increased column count, finer positioning requirements, and larger overall footprint. The quantity of solder paste required for successful installation was determined. The thermal profile needed to form the solder fillets was developed. This research effort uncovered a need for improved pick and place tooling to handle large CCGA installation. Mitigating this manufacturing risk has given SwRI a stronger technical position for proposed builds of IRB and DARPA System F6 flight components.

2012 IR&D Annual Report

Capability Development for Modeling Small Icy Satellites in the Solar System, 15-R8319

Principal Investigators
Daniel Boice
Raymond Goldstein

Inclusive Dates: 06/20/12 – 10/20/12

Background — Data from the Cassini spacecraft have transformed our view of the Saturnian system, including its icy satellite, Enceladus. The surprise discovery was the observation of plumes of material being emitted from a region near the south pole of Enceladus, later identified as composed primarily of water with entrained grains, likely of ice and dust. Similarities to activity of comets abound. Almost two-dozen flybys of Enceladus have provided a host of measurements of neutral and ion composition and dynamics in its surrounding environment. Moreover, a detailed understanding of how gas in the plumes and plasma in the environment surrounding Enceladus interact is lacking. SwRI's experience with modeling chemistry in cometary atmospheres allows for a unique quantitative approach to address key issues regarding the plumes of Enceladus and its surroundings.

Approach — Researchers analyzed the available composition data obtained by the Cassini Plasma Spectrometer (CAPS) during the fifth Enceladus flyby (E5) with a chemical dynamics model originally developed for comets in order to understand the processes that produce the observed ion composition. The combination of this unique dataset together with a novel modeling approach originally developed for chemistry in comets has been used to address key outstanding issues regarding this icy satellite. The sophisticated chemical model presents a powerful new tool with which to understand the complexity of the ion-neutral, gas-plasma interactions and to contribute significantly to understanding Enceladus and its surrounding environment.

Accomplishments — Researchers made comparisons between their new model results and the CAPS data analysis. The model has been enhanced by the inclusion of energetic electrons that surround Enceladus in the E-ring of Saturn as described by Cravens et al. (2011). These hot electrons interact primarily with the plume species via electron impact reactions. Additional electron impact reactions were added to the chemical network of the code to properly account for them. They produce another source of water group ions and further dissociate the neutral water, resulting in the formation of more H_2O^+, OH^+, and O^+ at the expense of H_3O^+. This results in the improved agreement of the current model with the preliminary model without the hot E-ring elections (Boice and Goldstein 2010). Results are encouraging even though there is work to be done concerning OH^+ and O^+. This will make an intriguing issue to be addressed in a proposal submitted to NASA for future work.

2012 IR&D Annual Report

Capability Development for Extreme Ultraviolet Imaging and Calibration, 15-R8322

Principal Investigators
Michael W. Davis
G. Randall Gladstone
Jerry Goldstein
Thomas G. Greathouse
Kurt D. Retherford
Gregory S. Winters
Bill R. Sandel

Inclusive Dates: 07/01/12 – Current

Background — SwRI has a nearly 20-year history of designing, integrating, testing, and launching ultraviolet spectrographs. Beginning with the EUVS rocket in 1993 and continuing through four iterations of the Alice line of spectrographs, SwRI's UV spectrographs have successfully returned data from comets, asteroids, the Moon, planets and even stars. However, virtually all of these observations were made in the far ultraviolet (FUV) range, longer than 100 nm. The next step is to expand SwRI's capabilities to even shorter UV wavelengths.

Approach — The objective of this project is to develop the capability to build and calibrate instrumentation that operates solely in EUV wavelengths. SwRI plans to design an improved version of the IMAGE-EUV imager that upon selection by NASA will be built and calibrated at SwRI. Along with a notional design, SwRI plans to reduce some of the technical risks in building and testing an EUV imager, in preparation for the next appropriate NASA mission opportunity. Finally, SwRI will perform a calibration of an existing detector system at EUV wavelengths, going through all of the steps that would be performed in a real flight EUV instrument calibration. By the conclusion of this project, SwRI will be positioned to be the leader in EUV instrument design and calibration.

Accomplishments — SwRI has a baseline imager design that increases the field of view 43 percent while increasing collecting area by 20 percent over the previously built imager. SwRI researchers have found a multilayer mirror coating that doubles reflectivity over the previously built imager, along with a vendor experienced with said coating. Filters were procured to proceed with laboratory testing.

2012 IR&D Annual Report

Capability Development for Modeling Small Icy Bodies in the Solar System, 15-R8323

Principal Investigators
Daniel Boice
W. Huebner
J. Mukherjee
J. Benkhoff (ESA)
H. Kawakita (Kyoto Sangyo University)
C. Western (University of Bristol)
Chris McKay (NASA)

Inclusive Dates: 07/01/12 – Current

Background — In 2011, the bright comet Lovejoy made a very close encounter with the Sun, providing a rare opportunity to study the physical properties of sungrazing comets and their coupling to the near-solar environment. Multiple spacecraft observed its perihelion passage at a variety of wavelengths with spatial resolution. There is much to be learned from this and other sungrazers; however, no comprehensive model exists to aid in the interpretation of these observations. Phosphorus is a key element in all known forms of life, and phosphorus-bearing compounds have been observed in space. It is ubiquitous in meteorites, and it has been detected as part of the dust component in comets, but searches for P-bearing species in the ice phase in comets have been unsuccessful.

Approach — The goal of this project is to adapt SwRI's general-purpose simulation code of the physical and chemical processes in comets to study the sungrazing Comet Lovejoy and the phosphorous chemistry of comets with implications to astrobiology. The innovative model that results will combine SwRI's codes with two codes supplied by collaborators, extending and enhancing SwRI's existing capabilities. No computer model currently exists that is capable of addressing the key physical processes and conditions that are thought to be relevant in sungrazing comets in a self-consistent manner as well as likely phorphorous chemistry in comets. Software will be developed that facilitates the comparison of model predictions with ground-based spectral observations needed to reap the full benefits of the model and foster collaborations with observers. The resulting Universal Virual Spectrometer (UNIVERS) software will be used to address key science issues.

Accomplishments — During the first quarter, researchers have: 1) Started developing the SwRI comet model for sungrazing comets by including thermodynamic data for cometary dust that undergoes sublimation in the extreme thermal environment experienced by a sungrazer and considered secondary ionization and dissociation processes by energetic photoelectrons; 2) Created the web interface for UNIVERS on a Linux-based server. Sample model output has been used to successfully test the web interface and different aperture sizes have been implemented for developing the instrument modules; and 3) Began discussions with Prof. Kawakita at the annual DPS meeting (October 15–19) and Dr. Benkhoff (ESA/ESTEC) who visited SwRI during October 23–26. The big astronomy news this quarter was the surprising discovery of a new sungrazing comet, C/2012 S1 (ISON) that will heighten interest in this work.

2012 IR&D Annual Report

An Advanced UV Spectrograph Concept for the JUICE Ganymede Orbiter Mission, 15-R8324

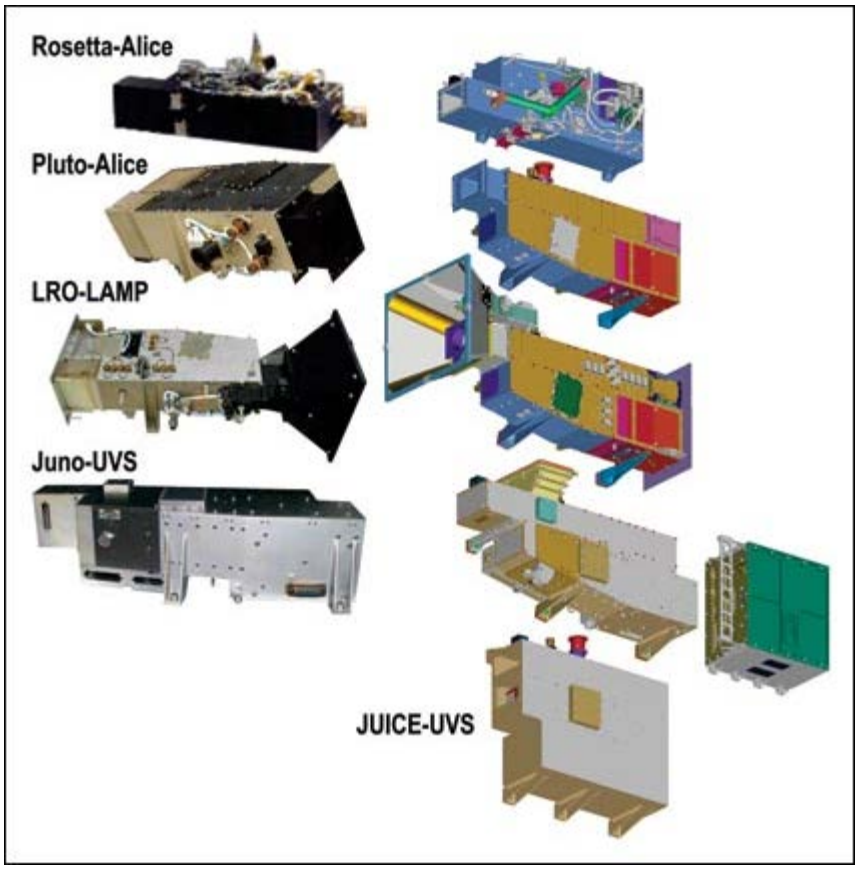
Principal Investigators
Kurt D. Retherford
G. Randy Gladstone
Mike W. Davis
Steve Persyn
Tommy K. Greathouse
John R. Spencer
Andrew J. Steffl
S. Alan Stern
Greg Dirks
John Eterno
Kristian Persson
Brandon Walther
David White
John Trevino
Greg Winters
Maarten Versteeg
Melissa A. McGrath (NASA/MSFC)
Paul D. Feldman (JHU)

Inclusive Dates: 07/01/12 – Current

Background — SwRI's preliminary concept study for an advanced UV spectrograph (UVS) tailored for the European Space Agency's (ESA) Jupiter Icy Moons Exploration (JUICE) mission has recently supported an SwRI proposal to NASA's Stand-Alone Mission of Opportunity 2 (SALMON-2) call for contributed JUICE instruments. The JUICE mission launches in 2022 and arrives at Jupiter in 2030, where it conducts a few dozen flybys of Ganymede, Callisto, and Europa and then finally enters orbit around Ganymede. A UVS instrument is in the straw-man payload, since it performs many useful observations of the intriguing atmospheres, aurora, airglow, and surfaces of the Galilean satellites, Jupiter, and gas clouds and plasma tori located in the Jovian magnetosphere. These UV spectral imaging observations address many (>2/3 rds) of the key science objectives of the JUICE mission.

Approach — Instrument pre-Phase A concept work included conducting several UVS instrument trade studies. With the recent Juno-UVS instrument already on its way to Jupiter, SwRI researchers baselined this heritage spectrograph for their concept and refined its mechanical design for radiation shielding and mass optimization. To devise methods for improving scientific performance when operating in Jupiter's harsh

radiation environment, SwRI conducted beam-line experiments with shielding mass models at MIT's High Voltage Research Laboratory. Optical ray-trace design studies informed the trade-offs between including in the design a front-end scan mirror, an additional microchannel plate and/or photodiode detectors for extended bandpass coverage, and various aperture sizes for bright source imaging and occultation measurements. A formal technical risk-reduction review (TRR) was held by the SwRI team and was very productive.



Spectrographs designed by SwRI for previous space missions are the basis for the JUICE-UVS.

Accomplishments — SwRI's proposal titled, "JUICE-UVS: An Ultraviolet Spectrograph for the JUICE Mission," was submitted on September 24. The preparatory work completed several UVS instrument trade studies that results in a low technical risk program and provides excellent advantages for the JUICE payload competition. SwRI expects to learn the results of the award process in late December 2012, or no later than February 2013.

2012 IR&D Annual Report

Design, Modeling and Fabrication of Metamaterials, 14-R8008

Principal Investigators
Michael Miller
Jeremy Pruitt
Diana Strickland
Jerry Helffrich
Leigh Griffith

Inclusive Dates: 12/01/08 – 05/01/12

Background — Metamaterials are engineered materials consisting of arranged components, usually metallic and dielectric, designed to exhibit specific and often unusual electromagnetic properties not found in natural materials. The components typically consist of inclusions, structures much smaller than a wavelength, placed within a host background (e.g., polymer, ceramic, or air). Surface plasmons 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 some metamaterials at infrared frequencies and above.

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, small and novel radio frequency components and antennas, high-sensitivity chemical sensors, and optical cloaking among many others. In this project, SwRI developed 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 staff employed metamaterials to reduce the size of electrically small antennas while maintaining an impedance match to their power source. Additionally, metamaterial surfaces were used to improve the performance of antennas by reducing lossy surface waves and also to improve gain, directivity and element isolation in arrays. SwRI staff also postulated the fundamental question and subsequently demonstrated that surface plasmons could be elicited from metamaterials at infrared frequencies to affect the binding of adsorbed molecules when the frequency of the surface plasmon is matched to molecular vibrations, the molecule's resonance conditions. This demonstration paves the way to engineered repulsion or chemical transformation of adsorbed molecules.

Approach — To determine whether metamaterials improved electrically small antennas and whether they were practical to implement, a novel, electrically small patch antenna incorporating metamaterials as the key component was selected from the literature for a feasibility study. SwRI staff designed, built and tested this metamaterial antenna at several frequencies and compared its performance to conventional, electrically small antennas. Additionally, the effects of various metamaterial surfaces were tested 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 surface plasmons 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 EM 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.

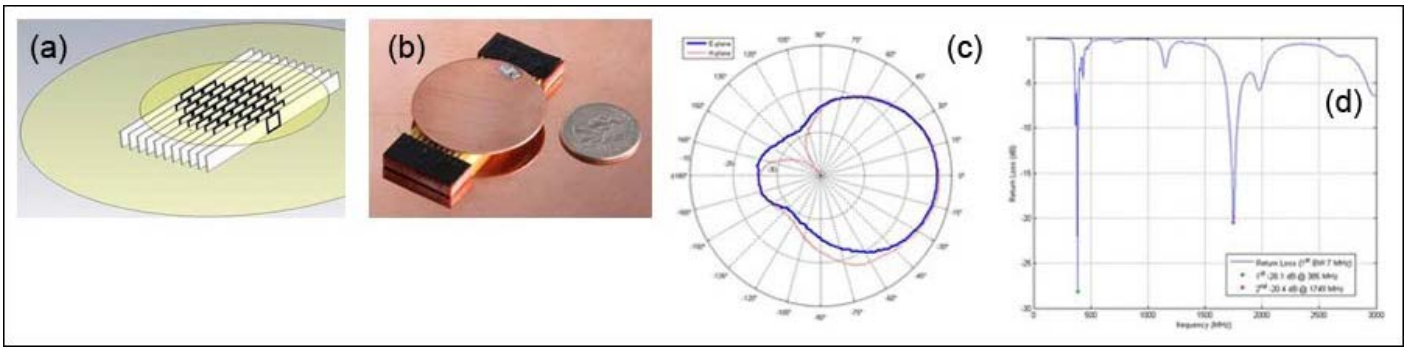


Figure 1. A copper patch antenna with metamaterial between the ground plane and patch. a) A drawing with transparent patch, exposing a view of aligned spiral rings that compose the metamaterial. b) A top view of the fabricated antenna. c) Radiation pattern measurements. d) Return loss measurements.

Accomplishments — SwRI researchers found that antenna resonance could be tuned independently of antenna dimensions (Fig. 1). 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 as seen in Fig. 1, an array of barium strontium titanate cubes, and Sievenpiper 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 metamaterials. These metamaterials were printed on the same substrate as the antenna with conventional circuit board manufacturing methods.

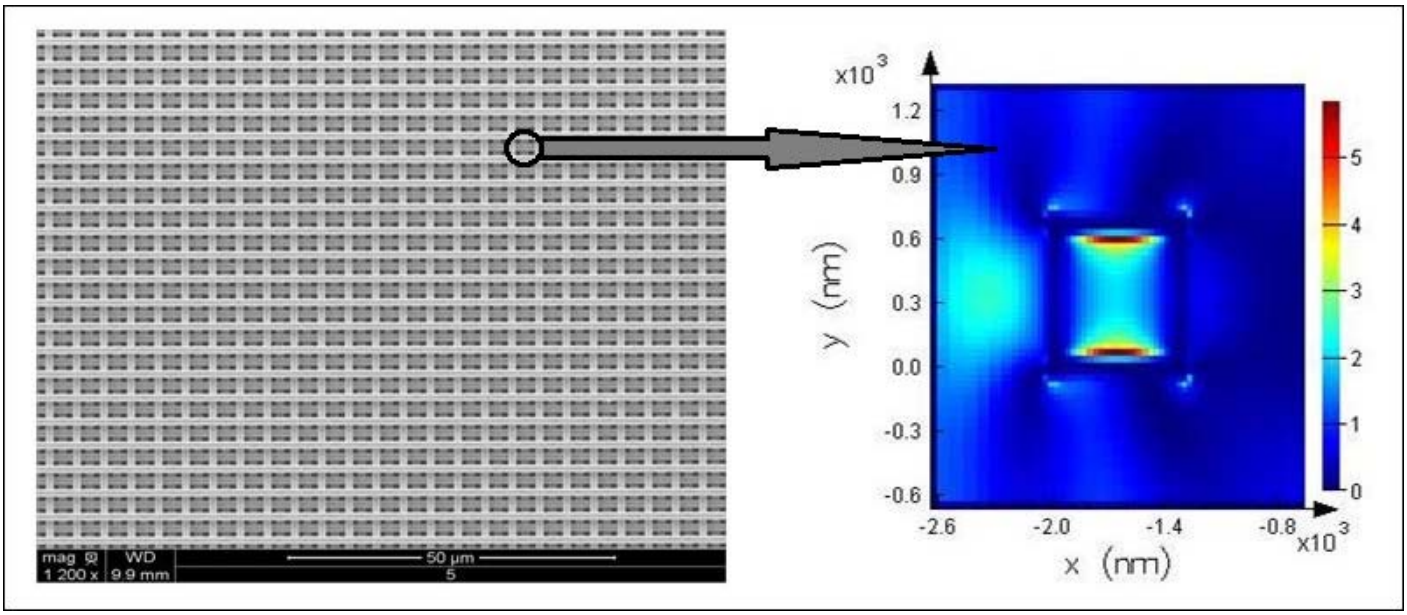


Figure 2. A 3-D "log pile" structure designed to support surface plasmons at 60 THz. a) Scanning electron micrograph of a log pile sample. b) Simulation of surface plasmon generation in a log pile unit cell.

SwRI staff demonstrated via systematic computations that free-standing (3-D) wire grids of cubic symmetry could be tailored to evince surface plasmons with infrared frequencies. It was further shown that the oscillating EM field of these plasmons directly coupled 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, 2-D devices consisting of simple, pad-like periodic structures surrounded by nanowires, as well as 3-D "log pile" devices (as seen in Fig. 2), were designed to evince surface plasmon modes in the infrared near 60 THz. Under a Cooperative Research and Development Agreement with Sandia National Laboratories in Albuquerque, N.M., these devices were successfully fabricated and were evaluated using the LTDMS technique to measure the coupling strength between surface plasmons and adsorbed molecules, such as carbon monoxide. 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.

2012 IR&D Annual Report

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

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

Inclusive Dates: 01/01/10 – 12/31/11

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, researchers proposed to design and build a high-fidelity shock tube apparatus.

Approach — The goal was 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 that was developed is unique in that it includes an adjustable length high-pressure gas reservoir section allowing for independently tailoring 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 significant hardware changes. This approach had not been attempted before and required a significant research and design effort.

SwRI-designed shock tube system.

Accomplishments — A new shock tube system was designed and fabricated, see photo above. The system consists of four primary components: the 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. Through testing, the system has been validated to achieve shock pressures up to 10 psi, and durations up to 10 milliseconds. Much higher shock pressures can be achieved by reducing the diameter of the test section and increasing driver fill pressure. 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 installed. The system consists of a control console with various pressure readouts and controls that actuate the high speed valves used to fill and fire the shock tube.

SOUTHWEST RESEARCH INSTITUTE®

2012 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:

1. 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.
2. 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.
3. Determine the changes in knee mechanics resulting from known OA risk factors.

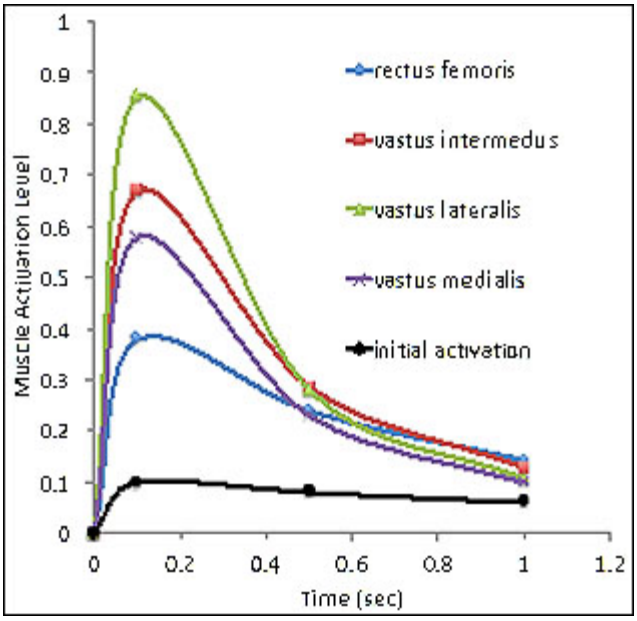


Figure 1. Initial and final muscle activations. The optimally determined muscle activations required to perform a leg extension compared to the initial muscle activations.

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.

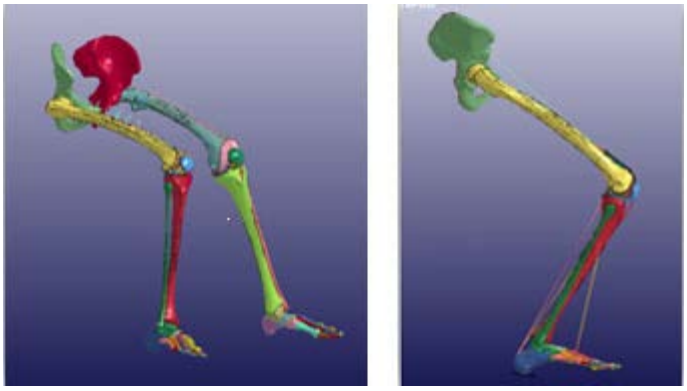


Figure 2. The lower limb dynamic finite element model (left) was used to simulate a standing squat (right). Active time varying muscle forces were applied using a Hill-type muscle model for the quadriceps muscles (vastus lateralis, vastus medialis, rectus femoris, and vastus intermedius), tibialis anterior,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

SOUTHWEST RESEARCH INSTITUTE®

2012 IR&D Annual Report

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

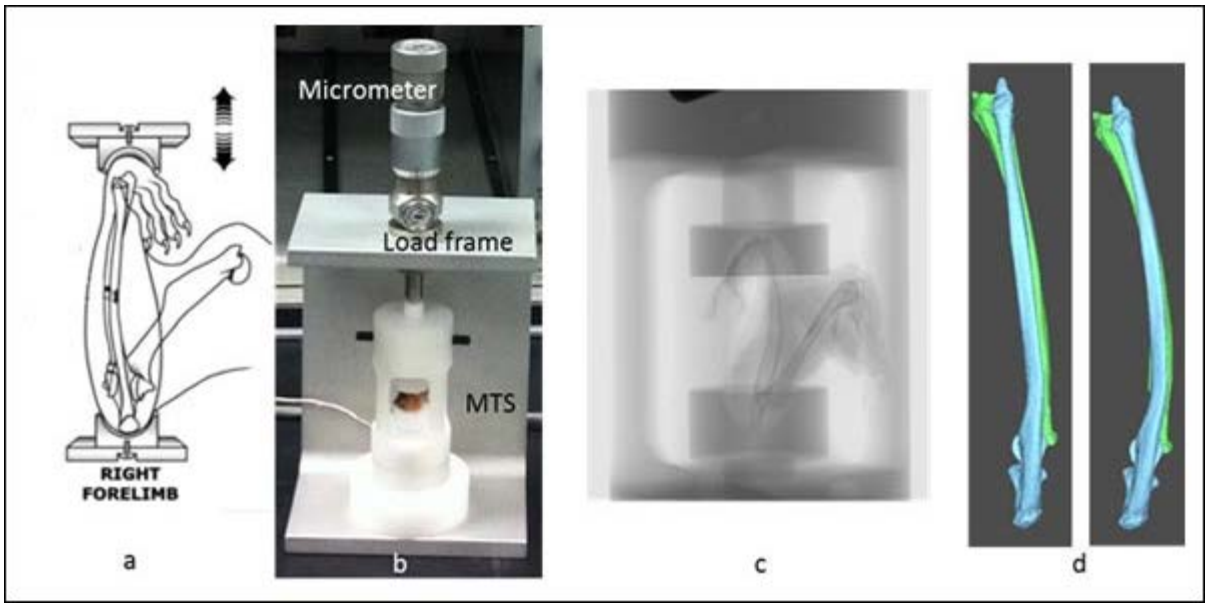
Principal Investigators
David S. Riha
John M. McFarland
Todd L. Bredbenner
Daniel P. Nicolella
Barron J. Bichon
Don Moravits

Inclusive Dates: 07/01/10 – 07/02/12

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 humans or animals. Valid model predictions become increasingly important as the cost, reliability, and experimental complexity for 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 were 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.



Finite element models were developed to simulate the in vivo mouse forearm compression model (a). The mouse forearm was loaded in the material testing stage (b). One x-ray slice from the micro-CT shows the loaded arm within the cupped platens (c). The micro-CT images were reconstructed to determine the undeformed and deformed shape of the ulna for the loading protocol (d).

Accomplishments — Variance decomposition methods as described by Saltelli et al.[1] 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 development and validation for the mouse ulna in the *in vivo* forearm compressive loading model protocol was performed following ASME V&V 10 Guide. A V&V plan was developed and followed. The plan identified the modeling assumptions, calibration and validation experiments, and validation metrics and is a useful tool to communicate assumptions and uncertainties about both the models and experiments. Model V&V is typically used for models of complex systems that seldom have standard test protocols for validation experiments. Based on experience working other validation projects and this research in particular, the uniqueness of validation experiments leads to potential errors in the experiments and additional unknown uncertainties. In many cases, the experiments are not successful, leaving little information for the model validation. The uniqueness of validation experiments have the potential to impact schedule and cost budgets and should be carefully planned and executed. In addition, regular communication between the model developers and those performing the experiments is essential to successful model validation. The early model predictions can be used to assist in designing the experiments, and the model developers need a thorough understanding of the uncertainties in the experiments. Several challenges were experienced during this research such as completing all experiments for the calibration and validation due to new experimental protocols, equipment availability, and specimen availability, which are all real-world issues for model validation. Overall, this research effort developed new tools and methods to support model validation efforts and provided valuable experience in the relationship between experiments and model development. One main outcome was the development of sensitivities that identify the contribution of both aleatory and epistemic uncertainties. This information can be used to guide the allocation of resources to improve models and/or to perform additional experiments. These variance based sensitivities methods were implemented in the NESSUS® software through CENTAUR™ and are now available to support future V&V efforts. Experience was also gained

about the complexity and challenges to obtain quality experimental data for calibration and validation of complex systems. While a rigorously validated model of the mouse ulna was not achieved, there is more confidence in the model predictions based on the qualitative comparisons of the model and measurements and information about how to improve the model to better match reality.

Saltelli, A., S. Tarantola, F. Campolongo and M. Ratto. Sensitivity Analysis in Practice: A Guide to Assessing Scientific Models, Wiley, New York, NY, 2004.

2012 IR&D Annual Report

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

Principal Investigator
Florent Bocher

Inclusive Dates: 01/01/12 – Current

Background — Existing nuclear reactor fleets in the United States are fast approaching the end of their operating license period. The Nuclear Regulatory Commission (NRC) and utilities are in the process of extending the 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 since 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 over 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. The objective of the project is to combine electrochemical and fracture mechanics techniques in high-temperature and high-pressure solution to identify the impact of passive film properties on SCC initiation.

Approach — The approach for this project was:

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 — This project was a partial success. A high pressure and temperature flowing test setup to perform electrochemical testing under realistic conditions was successfully assembled. Electrochemical measurements were successfully performed at high pressure and temperature.

The electrochemical data could be related to the semiconductor properties of the surface oxide film. However, it was not possible to link those data to mechanical properties because no crack initiation was observed over the relatively short test duration (one month). Samples were statically loaded and successfully instrumented in order to make potential drop measurements under high temperature and pressure conditions. Mott-Schottky and potentiodynamic scans have been successfully correlated at ambient pressure and temperature when assessing the oxide film properties of 316 stainless steels. Furthermore, the effect of polarization on mechanical failure was measured using SSRT at ambient temperature. The oxide film properties were measured using both Mott-Schottky and potentiodynamic scans. As with high temperature testing, no cracking was initiated. In both cases, the oxide film displayed n-type semiconductor properties.

2012 IR&D Annual Report

Corrosion Measurements in Fuel Systems, 18-R8203

Principal Investigators
James F. Dante
Gary B. Bessee

Inclusive Dates: 01/01/12 – Current

Background — Corrosion in fuel systems has become a widespread problem in recent years for underground storage tank manufacturers and operators as well as engine and engine part manufacturers. Some of these issues appear to be related to the introduction of ultralow sulfur diesel fuel (ULSD). One of the difficulties in studying metals corrosion in fuel systems is the low conductivity of the fuel, which makes conventional electrochemical techniques to measure *in situ*, real-time corrosion rates virtually impossible. Another 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. Moreover, no confirmed root cause has been established to explain the corrosion failures observed in the field. The objectives of the proposed project are to 1) validate a method for measuring corrosion rates in fuel systems, 2) investigate the effect of dew point, water content and fuel chemistry on the corrosivity of ULSD, and 3) determine the conditions and parameters that lead to phase separation in ethanol/gasoline blends.

Approach — The proposed research project addresses the measurement issues by employing a multi-electrode array sensor (MAS) to measure corrosion rates in fuels. The MAS are able to measure corrosion rates in thin electrolyte layers, such as the ones forming in fuel. 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 the MAS technology.

Accomplishments — Corrosion currents in a surrogate fuel with varying amounts of "aggressive" ethanol were measured using the MAS. Data indicated a significant increase in corrosion current with increasing ethanol concentration. Low-sulfur diesel (LSD) and ultra-low sulfur diesel (ULSD), both filtered and unfiltered, were also investigated. A small amount of tap water, DI water, or artificial contamination water (ACW) was mixed with the fuel during corrosion testing. Although corrosion is a function of the ionic contamination, probe data in diesel fuel indicate that corrosion currents are very small in systems with small amounts of contamination in the water phase. For example, no corrosion was observed in the presence of DI water while higher currents were observed in ACW. Further, no difference in corrosion behavior could be observed between LSD and ULSD fuels regardless of the composition of the added water phase. Comparatively higher current and anodic charge transfer were measured in filtered fuel in the presence of tap water. When using ACW, the filtering process did not affect the results due to the dominant effect of the low pH of the ACW. The average water content of both LSD and ULSD has been measured and was found to be very similar up to 50°C. Above 50°C, ULSD contained 50 to 100 ppm (20 to 25 percent) extra water. Thermodynamic modeling was performed using OLI focusing on ethanol and *tert*-amyl methyl ether (TAME) as oxygenate, and toluene, hexane and pentane as hydrocarbon. The

results were integrated into the OLI Analyzer Studio software and will be used to predict ethanol drop out from the blend.

2012 IR&D Annual Report

Evaluation and Development of Alternative Coatings to Reduce and/or Eliminate Bridging Oxidation, 18-R8239

Principal Investigators
Kent Coulter
Craig Engel

Inclusive Dates: 07/01/11 – 06/30/12

Background — The primary objective of this project was to evaluate and develop alternative coatings to avoid or minimize bridging oxidation. This project addressed bridging oxidation found in the nuclear industry affecting boiling water reactor (BWR) safety relief valves (SRVs.) Bridging oxidation is defined as when two mating parts, under a compressive load, at elevated temperatures, for long periods of time, bridge together due to an oxidation growth, requiring additional force to separate. The SRV's main function is to release in the event of an over-pressure scenario. Failure to open can cause a catastrophic failure.

Approach — By developing a simulated BWR environment to create bridging oxidation and by creating standardized mechanical testing procedures, one can quantify bridging oxidation to compare the materials currently used to alternative coatings that will reduce or negate the effects of bridging oxidation. The technical approach for this project was to design and develop test coupons and a mechanical test fixture that would quantify the apparent "adhesion" associated with the oxidation growth between the pilot disc and seat and then to assess the performance of different coatings and configurations in an attempt to minimize the effects of the bridging oxide in the overall performance of the SRV when in service.

Accomplishments — This project met three technical challenges:

1. successfully demonstrated the ability to generate bridging oxidation bonding,
2. successfully measured the forces required to separate the adhesion created by the bridging oxidation bonding,
3. successfully developed an alternative coating, CrSiCN, that when applied to the mating surfaces of test coupons, no bridging oxidation bonding occurred.

The CrSiCN coating is a candidate for marketing as a true oxidation-resistant coating, viable for application in the BWR nuclear environment. From a business standpoint, the ability to generate, quantify, and eliminate bridging oxidation bonding has set up the next phase of work, which is to qualify the improved process on BWR SRVs in the field. The results from this project have been presented to the Tennessee Valley Authority, a user of BWR SRVs, of which SwRI has been invited to present the results at its industry working group meeting in January 2013. In addition SwRI has submitted, and has been accepted to present the results at the annual 2013 TMS Meeting in March.

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2012 IR&D Annual Report

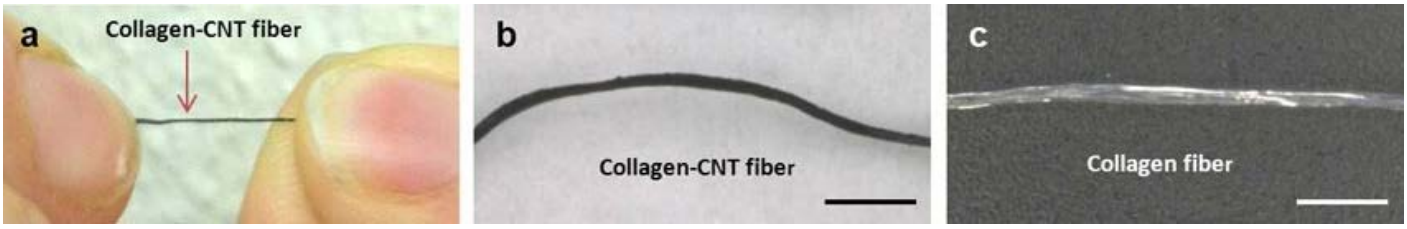
Novel Scaffolds for Tendon/Ligament Regeneration and Tissue Engineering Applications, SwRI-UTSA Connect Project, 18-R8253

Principal Investigators
Vasiliki Z. Poenitzsch
XingGuo Cheng
Rena Bizios (The University of Texas at San Antonio)

Inclusive Dates: 09/01/11 – 08/31/12

Background — This research is motivated by major clinical needs for tendon/ligament repair and by the current lack of innovative biomaterials for such applications. To date, material approaches in this field have not been successful because they lacked satisfactory biocompatibility, did not promote cell functions pertinent to new tissue formation and, most importantly, did not have the mechanical properties required for successful performance under the mechanical loading conditions that are characteristic to tendons and ligaments. This project investigated novel synthetic composite scaffolds containing aligned collagen and CNTs. Collagen is a naturally occurring, biocompatible and biodegradable material that is widely used as a tissue engineering and regenerative medicine matrix. CNTs are unique structures with remarkable mechanical properties. Combining of these two components has the potential to provide biomimetic, bioresorable, and mechanically competent composites for tendon/ligament repair.

Approach — The research was a multidisciplinary experimental study with two distinct, but complementary, components, one of which was accomplished at SwRI and the other at The University of Texas at San Antonio (UTSA). Specifically, SwRI personnel took the lead on fabrication and characterization of the novel constructs, and UTSA personnel concentrated on the *in vitro* assessment studies using cultured cell models. The overall objective of the research project was to design, fabricate, and establish the efficacy of novel scaffolds for tendon/ligament repair and regeneration. The two specific aims were to (1) fabricate unique collagen-CNT composite macrostructures with improved biochemical and biomechanical properties, and then (2) evaluate their efficacy for biomedical applications (such as tendon/ligament repair) by establishing their cytocompatibility *in vitro* using cultured adult mesenchymal stem cell (MSCs) models and investigating select cell functions pertinent to new tissue formation.



(a) A photograph of a collagen-CNT fiber. (b) Optical microscope image of collagen-CNT fiber and (c) collagen control (lacking CNTs) fiber. Scale bar is 1 cm for both images.

Accomplishments — SwRI has quantitatively demonstrated that aligned collagen-CNT fibers with improved mechanical properties can be fabricated. SwRI developed processes and procedures for the fabrication, and characterized the structure and mechanical performance of novel collagen-CNT based fibers. The collagen-CNT fibers have shown to contain a high loading and high degree of alignment of CNTs. Consequently, they have shown to be electrically conducting and to have 15 x increase in modulus

and a 3 x improvement in strength as compared to aligned collagen fibers. Cellular experiments examining cytocompatibility as well as select MSC functions pertinent to new tendon/ligament formation are currently under way at UTSA. While this project focused on tendon/ligament repair, the real benefit of the project was establishing a capability for fabrication of aligned CNT-based wires that has application in the rapidly expanding field of nanotechnology.

2012 IR&D Annual Report

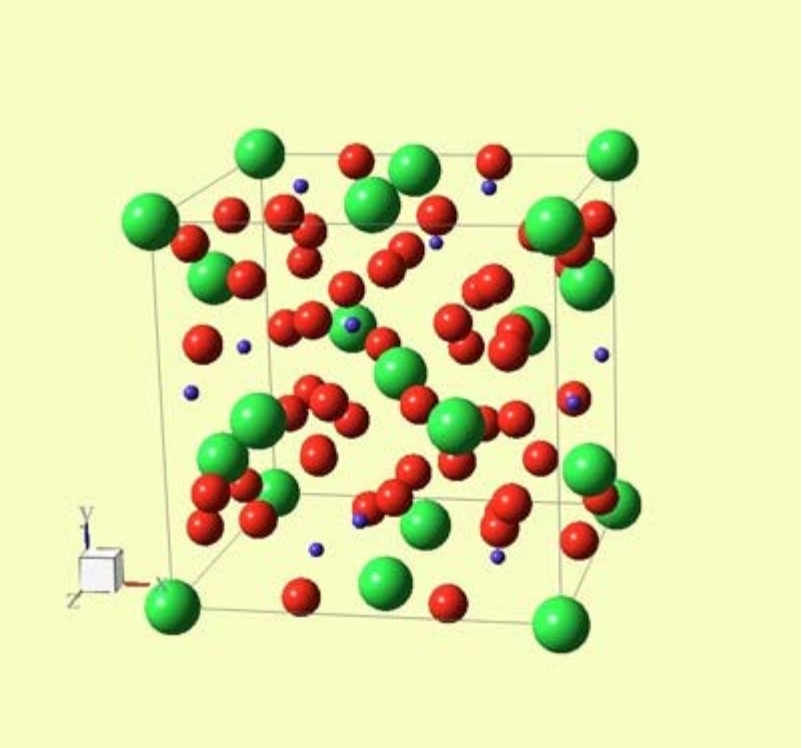
Development of Novel Silicon Clathrates for Energy Harvesting and Storage, 18-R8279

Principal Investigators
Kwai S. Chan
Michael A. Miller

Inclusive Dates: 01/01/12 – Current

Background — Solid-state thermoelectric devices (TEDs) exhibit many attractive features for electrical power generation compared to traditional fuel-combustion systems, which include extraordinary long life, no moving parts, no emissions, and high reliability. To this end, the Type I and II clathrates of silicon and germanium alloys are attractive thermoelectric (TE) materials because they can be engineered to exhibit high thermal power, high electrical conductivity, and low thermal conductivity by scattering phonons without interrupting electron conduction. Despite these attributes, the figure of merit of current silicon clathrates is still below that of existing TE materials based on rare-Earth elements and needs further improvements for industrial applications.

Approach — The objectives of this research project are to: (1) develop novel silicon clathrates by substituting clathrate framework and guest atoms with small-sized atoms, (2) characterize the thermoelectric properties, (3) develop a first-principles computational approach for modeling the effects of small-atom interactions, and (4) design and demonstrate a multilayered TED using the novel TE material. An innovative direct synthesis method and a traditional arc-melting method are used to synthesize Type I metal-silicon clathrates with small-atom substitution on the Si framework and guest-atom insertion within the cage structure. The thermoelectric properties of metal-silicon clathrate compounds in bulk and layer forms will be characterized with and without compressive stress. A computational methodology will be used to develop an understanding of the effects of small-atom substitution and encapsulation within the cage structure on the thermoelectric properties, and to design the desired multilayer architecture for optimum thermoelectric properties.



Unit cell of a Type I silicon-based clathrate with large guest atoms and small substituted framework atoms designed via first-principles computation.

Accomplishments — A first-principles computational approach was used to design new silicon-based clathrates with small atoms, as shown in the illustration, as either guest or substitute framework atoms.

The energy of formation of Type I clathrate compounds have been computed as a function of lattice parameter for various atom insertions or substitutions from a list of candidate elements. These energy calculations were used to identify Type I silicon-based clathrates that are amenable for synthesis and potentially good TE characteristics. Synthesis of selected silicon clathrate compounds is in progress. Preliminary results indicate that some of the compounds can be synthesized, but the yield and purity need further improvements.

2012 IR&D Annual Report

Fretting and Flow Assisted Corrosion Effects on Nitinol Stents for Biomedical Use, 18-R8282

Principal Investigators
Elizabeth Trillo
James F. Dante
Xingguo Cheng

Inclusive Dates: 01/01/12 – Current

Background — Nickel-titanium alloys, also referred to as nitinol, have been used for many years as a biomedical stent material to repair damaged vessels. Although there have been marked improvements in the design of stents and nitinol processing, the number of stent failures has remained high (1.7 percent to 32 percent). Failure of a stent is considered to be a fracture of the stent support system and/or corrosion on the stent that results in nickel-ion release, which is toxic to the body. A common procedure is to overlap stents in order to accommodate a longer damaged vessel length. This introduces a fretting scenario. A combination of fretting along with flow-assisted corrosion, pulsatile effects, as well as pH of the local wound site, are potential performance issues in the *in vivo* condition that have not been accounted for in the literature. The proposed research looks to understand these combined effects on nitinol stents. The project has three major objectives:

1. Determine the effect of fretting on the corrosion behavior of nitinol stent material under biological fluid flow and under different pH conditions,
2. Compare the effects of pulsing flow conditions, stagnant conditions, fretting and its relation to corrosion resistance of nitinol stent material, and
3. Assess the biocompatibility of nitinol stents using endothelium cells after fretting/flow testing.

Approach — The proposed research project set out to construct a test apparatus to simulate the combined effects of fretting and flow conditions in simulated biological solutions. The corrosion potential during fretting and flow are to be recorded for up to three months. Lower pH solution tests shall be performed to determine how the corrosion behavior will change when the material is near inflamed tissue or crevice areas. Also, pulsatile testing will be performed at rates that allow a comparison between resting and high heart-rate condition. After testing, the stent surface morphology will be examined by micro-CT, scanning electron microscopy (SEM), and auger spectroscopy. Cyclic polarization testing will be performed to determine general and localized corrosion effects. Nickel-ion concentration measurements will be obtained from the test fluid during the exposure. In addition, biocompatibility testing will be performed to see if there is cell adhesion and proliferation on the nitinol stents after exposure.

Accomplishments — A four-channel flow apparatus was constructed and baseline testing (flow testing only) has been completed. For the flow tests, the open circuit potential was monitored for 14 days, 30 days, 60 days and 90 days with phosphate buffered saline (PBS) solution flowing at a rate of 250 mL per min. In all four test cells, the open circuit starts very low and then increases to a value of approximately 90 mV after approximately 4 to 5 days. There were also small perturbations in the open circuit potential during testing for all four test cells. During this time the potential showed a sudden drop. These could indicate a potential breech in the surface oxide where corrosion may have occurred. Subsequent micro-CT and SEM performed on the sample surfaces, however, did not show any major surface degradation due to the flow on the samples. Haemocytolysis testing was performed on the stents after flow testing. Haemocytolysis refers to the destruction/ dissolution of red blood cells (RBCs). It was determined that flow

testing has no negative effects on haemocytolysis. In addition, metabolic assay and cell culture testing using human umbilical vein endothelial cells were performed on the stents after flow testing. All stents exhibited excellent cytobiocompatibility. Cells were able to attach and proliferate on each stent quite well.

2012 IR&D Annual Report

Characterization of Baboon Knee Articular Cartilage Mechanical Properties, 18-R8285

Principal Investigators
Todd Bredbenner
Daniel Nicolella

Inclusive Dates: 01/06/12 – 05/06/12

Background — Osteoarthritis (OA) is the most common form of arthritis and the major cause of activity limitation and physical disability in older people. The National Institutes of Health (NIH) has recognized the public health significance of OA and has issued a new Program Announcement (PA) aimed at encouraging and accelerating the characterization of new and underutilized models of osteoarthritis. A researcher from the Texas Biomedical Research Institute (TxBiomed) has been actively performing preliminary internal research at TxBiomed to characterize the incidence and severity of knee OA in baboons. In preparation for a collaborative response to this PA and in order to expand SwRI's musculoskeletal research in the key growth area of OA, SwRI researchers sought to characterize the mechanical behavior of baboon knee cartilage from a small subset of animals with emphasis on the investigation of age, sex, and OA status effects.

Approach — The objectives of this study were:

1. Evaluate whether the mechanical properties of baboon cartilage follow similar trends with age and sex as humans.
2. Evaluate whether the presence of affected cartilage leads to degradation in cartilage mechanical properties.

Accomplishments — Despite the small sample sizes used in this project, statistical differences were demonstrated between cartilage specimens obtained from young and old baboons in both strength and the strain at peak stress. It is well documented that cartilage mechanical properties demonstrate decline with age in humans, and SwRI's demonstration that baboon cartilage properties behaves in a similar fashion, further justifies the use of the baboon as a model for the human osteoarthritic condition, in addition to the physiological similarities between species. These results, along with other data previously collected at TxBiomed (in collaboration with SwRI), allow the pursuit of targeted funding opportunities within NIH and with commercial pharmaceutical and imaging clients. SwRI researchers believe that their preliminary data will allow for significant, externally funded collaborative research that can be applied to pre-clinical drug development, genetic analysis of OA susceptibility, and assessment of osteoarthritis risk, incidence, and progression from clinical MRI data.

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2012 IR&D Annual Report

Large-Area Synthesis of Graphene for Electronic Devices, 18-R8303

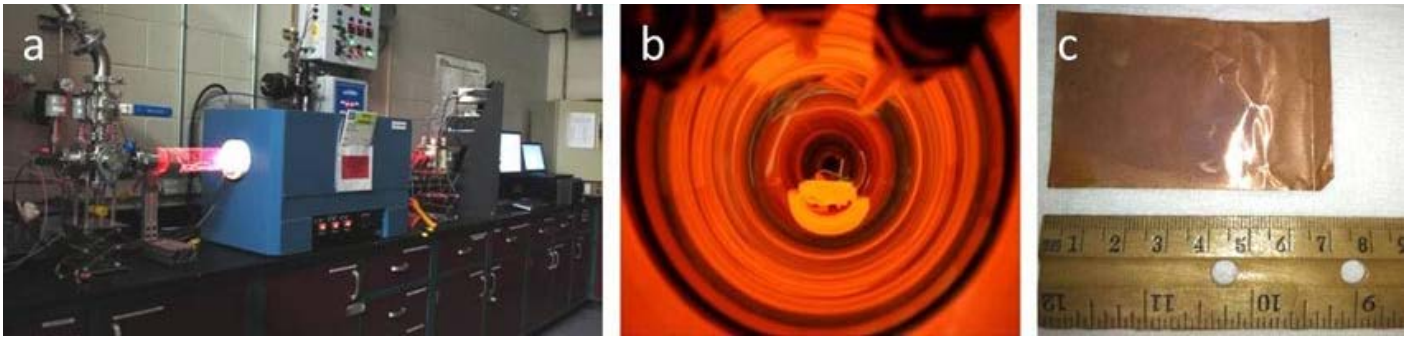
Principal Investigators
Vasiliki Z. Poenitzsch
Thomas Booker
John Harrison

Inclusive Dates: 04/01/12 – 04/01/13

Background — At present, graphene is one of the hottest topics in condensed-matter physics and materials science. Graphene is a monolayer thick planar sheet of sp2-bonded carbon atoms packed in a two-dimensional (2D) honeycomb lattice. The unique structure of graphene yields extraordinary thermal, mechanical, and electrical properties. In 2004, Novoselov and Geim first isolated graphene by cleaving graphite with adhesive tape. Research on graphene has since been a fast developing field, with exciting properties being confirmed and new concepts and applications appearing at an incredible rate. Potential applications include field effect transistors, interconnects, sensors, conducting films, clean energy devices, and conductive reinforced composites. Due to the promising and versatile properties of graphene, Novoselov and Geim were awarded the 2010 Nobel Prize in Physics. Despite intense interest and remarkably rapid progress in the field of graphene-related research, there is still a long way to go for the widespread implementation of graphene. It is primarily due to the difficulty of reliably producing high-quality samples, especially in a scalable fashion. This project seeks to help close the chasm between graphene manufacturability and its application. Development of graphene deposition technologies will enable SwRI to provide applied research and development on graphene to a range of clients.

Approach — The primary objective is to establish graphene deposition technologies at SwRI. The immediate aims of this project are:

1. Establish an in-house graphene thermal chemical vapor deposition (CVD) deposition processing technology.
2. Develop and characterize a novel graphene plasma-enhanced CVD (PECVD) deposition processing technology.
3. Fabricate electronic microdevices with SwRI produced graphene films and investigate their electronic application specific performance.



Photographs (a,b) of new thermal CVD chamber running process experiments for producing graphene films and of (c) as-grown film on Cu foil from a graphene deposition process experiment.

Accomplishments — During the first half of this project, SwRI has successfully completed the design

and fabrication of a new thermal CVD chamber and begun a design of experiments in which parameters are systematically varied in graphene deposition processes. The graphene samples have been characterized using scanning electron micrsocopy (SEM), Raman spectroscopy, and scanning tunneling microscopy (STM). SwRI has established a transfer method for transferring as-grown graphene films on copper substrates to oxidized silicon wafers substrates. Additionally, SwRI has designed and is currently fabricating a novel PECVD graphene deposition system.

2012 IR&D Annual Report

Develop Method for Hydriding Fuel Cladding and Characterize Influence of Hydriding on Mechanical Behavior, 20-R8269

Principal Investigators
Xihua He
Yi-Ming Pan
Kwai Chan

Inclusive Dates: 11/01/11 – Current

Background — Zirconium-based cladding material exposed to coolant water during nuclear reactor operations could absorb hydrogen ranging from less than 100 to up to 600 ppm, depending on temperature, fuel burnup, and material type. During extended dry storage, cladding plays an important role in safely handling, storing, and transferring spent nuclear fuel. As the cladding cools during extended storage, the hydrogen inside the cladding may precipitate as hydrides; furthermore, both existing and newly formed hydrides may reorient. Depending on size, distribution, and orientation, these hydrides may lead to premature fracture as a result of hydride embrittlement or delayed hydride cracking. Because the United States is actively considering extended dry storage as an alternative approach to managing the spent nuclear fuel and has an increase amount of high burnup fuel as a result of changes in plant-operating conditions, there is a strong need for relevant data. The objectives of this project are to develop methods and identify parameters controlling hydride formation at various hydrogen concentrations, identify conditions when hydrides reorient under stress, and characterize the influence of hydrides and their orientation on mechanical properties.

Approach — The primary objectives of this project are being achieved through the following four tasks:

- Develop method and parameters to prepare specimens with various hydrogen concentration levels.
- Identify conditions when hydrides reorient under stress.
- Conduct mechanical tests to characterize the influence of hydriding on cladding mechanical behavior.
- Provide required periodic reports and develop journal and conference papers.

Accomplishments — Significant progress has been made in the following areas.

Methods of hydriding Zircaloy-2: Four methods have been used to hydride the material: (i) electrochemical method—cathodic charging followed by diffusion annealing; (ii) hydrogen charging in a tubular reactor with continuous flow of a mixture of hydrogen-Argon gas; (iii) hydriding in pure hydrogen in a pressurized vessel at 300°C for 12 hours; and (iv) hydriding in supercritical water at 350°C in a pressurized vessel. Figure 1 shows the cross section of one specimen charged with hydrogen, where the hydrides were highlighted after etching.

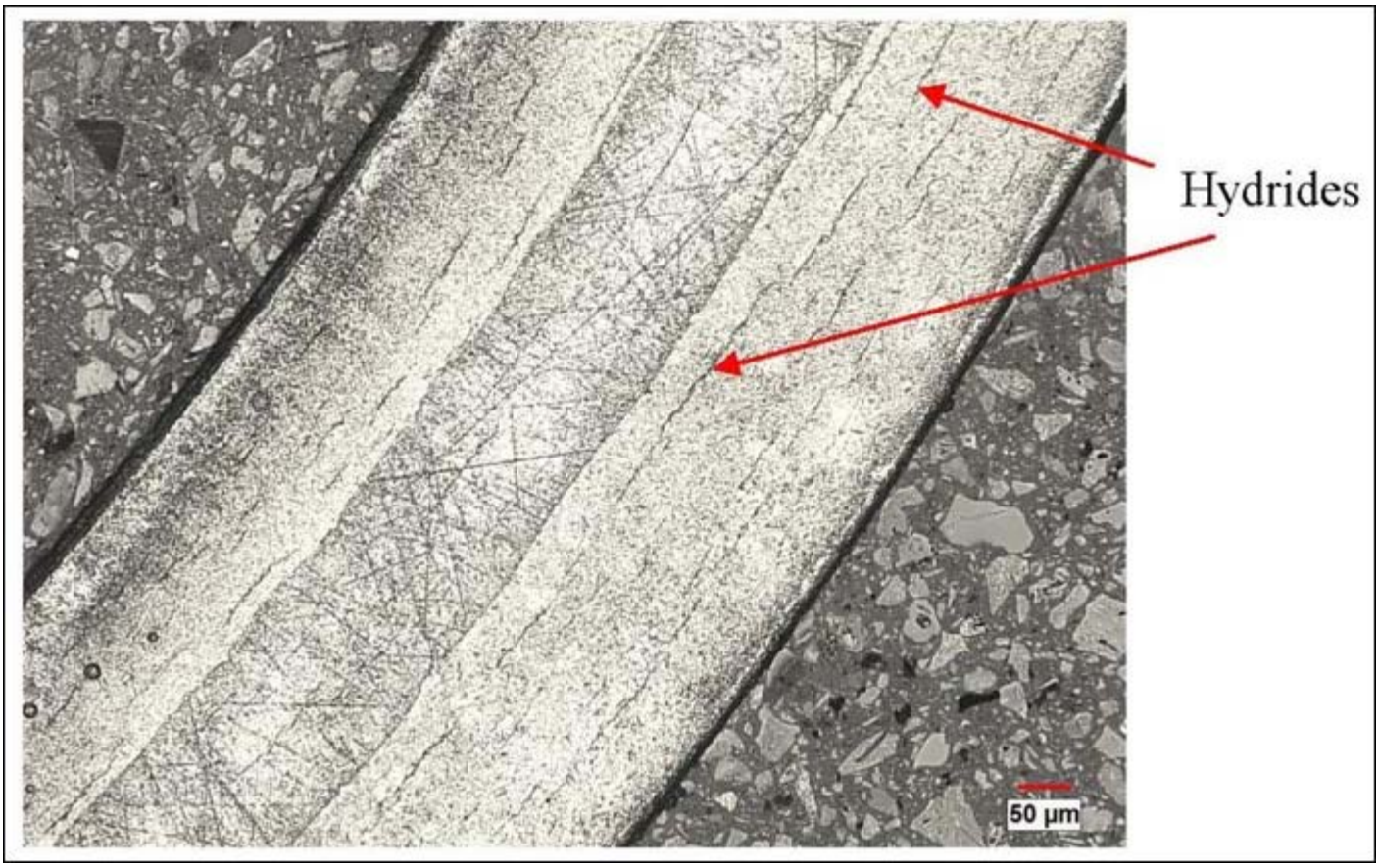


Figure 1. Cross section of Zircaloy-2 cathodically charged with Hydrogen and annealed at 400°C for 2 hours.

Hydride reorientation: A hydride reorientation test was conducted on a hydrogen-charged tensile specimen using an in situ loading stage inside a scanning electron microscope (SEM). Before loading, reference photographs of the hydrides were obtained at several magnifications ranging from 500X to 3,000X. The hydride microstructure viewed at 3,000X magnification shows that the hydrides, which appear as needle-shaped features, are parallel to the axial direction of the tensile specimen and the loading direction.

Mechanical properties of the hydrided Zircaloy-2: Fracture testing was conducted on hydride reoriented three-point bend specimens at 200°C in the SEM. Direct observations indicated that the reoriented hydrides, which ranged from ~1 to 22 µm in lengths, were more prone to fracture at larger sizes (>10 µm) compared to smaller sizes (<0.5 µm). The reoriented hydrides reduced fracture resistance through a void nucleation, growth, and coalescence process at the crack tip, as shown in Figure 2. The resulting crack resistance curves for Zircaloy-2, with reoriented hydrides, decreased from 38 $MPa(m)^{1/2}$ to 21 $MPa(m)^{1/2}$, with increasing hydrogen contents from 51 wt. ppm to 1,265 wt. ppm, as shown in Figure 3.

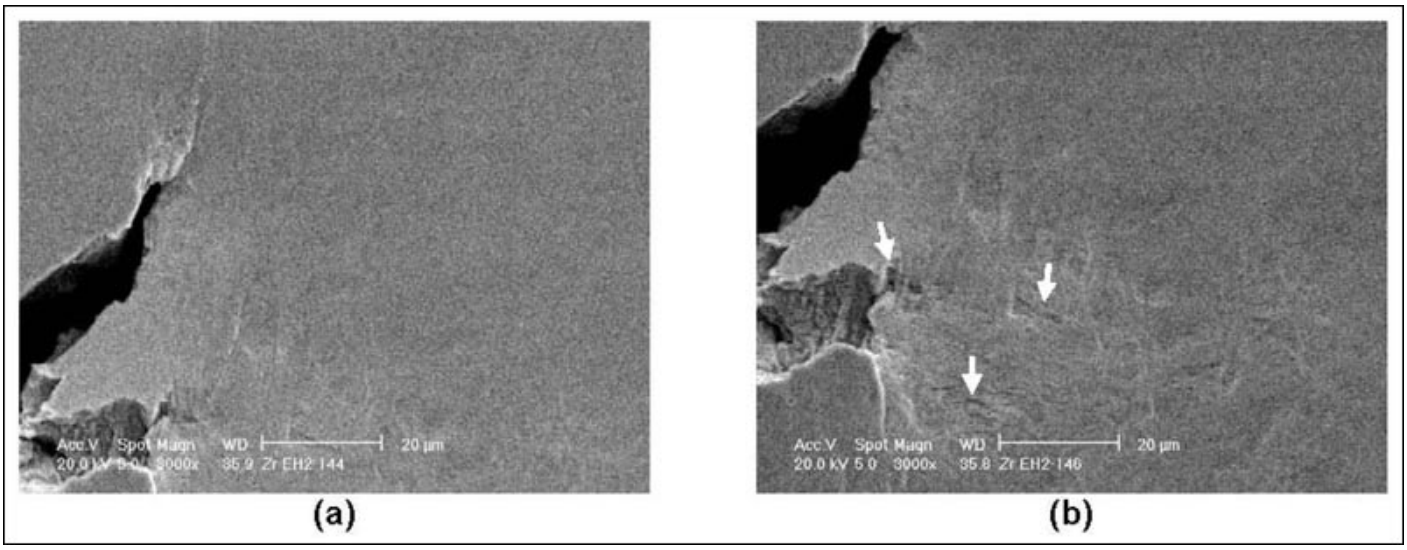


Figure 2. Crack tip fracture process in one specimen after hydride orientation: (a) K = 20.6 MPa(m)$^{1/2}$ and (b) K = 24.7 MPa(m)$^{1/2}$, showing hydride fracture ahead of the crack tip to form voids that link with the main crack tip.

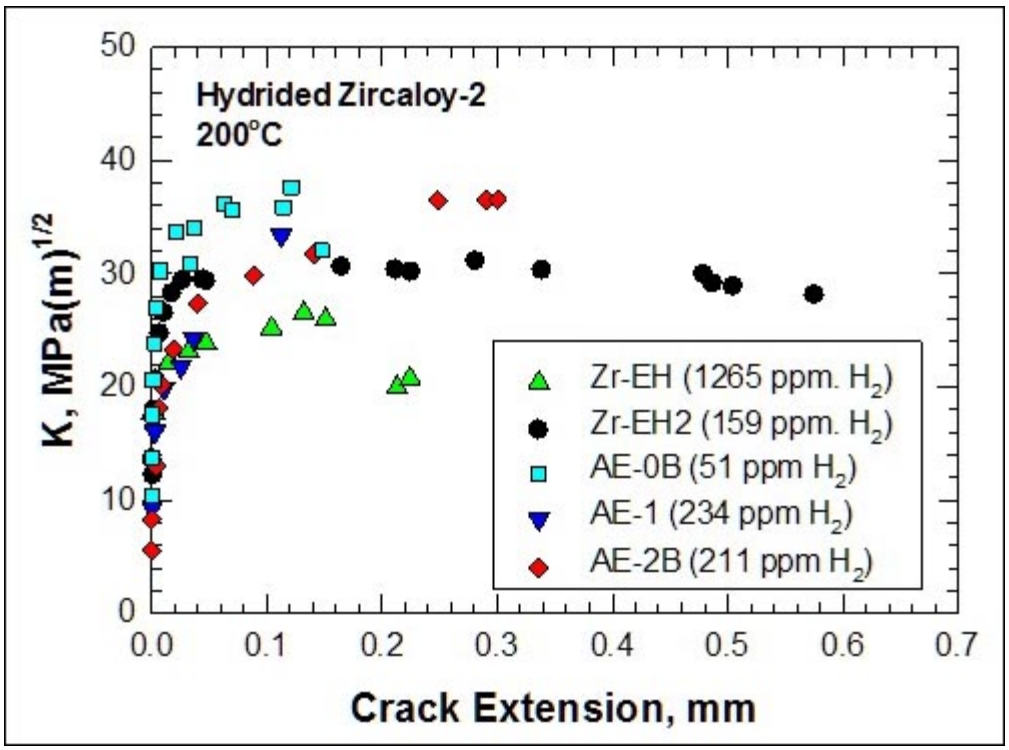


Figure 3. A comparison of KR curves of one hydrided Zircalloy-2 specimen tested at 200°C after hydride reorientation and corrected for the forked crack geometry.

2012 IR&D Annual Report

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

Principal Investigator
Jenifer Wheeler

Inclusive Dates: 01/03/11 – 11/23/12

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 mobile learning applications have focused on the delivery of training content and courses. 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 2D animation or 3D 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 consisted of the following phases:

1. Develop and analyze selection criteria for a MAR learning application based on human performance and learning theories.
2. Design a task for study that is tailored to the MAR selection criteria. That is, based on the criteria, design a task that is optimally suited for a MAR application.
3. Implement two different mobile learning solutions (i.e. 3D simulation and MAR) that are each intended to teach or support the task created.
4. Collect and analyze data from three different groups of participants, each using a different mobile learning application (and a control group), 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 — The project team developed a criteria model for selecting MAR as a learning delivery tool based on skill type, task characteristics, and task execution variables. This model was used in selecting the Soma cube puzzle as a study task. MAR and 3D applications were developed to teach and provide practice for the assembly of the Soma cube. A study was conducted to compare participants' ability to assemble the Soma cube after learning and practicing with the MAR application, the 3D application, or no mobile application (control group). Results suggest that the MAR group was able to assemble the cube more quickly than the other groups.

2012 IR&D Annual Report

Temporally Coherent Communications, 10-R8194

Principal Investigators
Travis R. Thompson
Michael S. Moore
Denise Varner
Kase Saylor
Jeremy Price
Mike Koets
Roger Chiodo

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 randomized 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, the project team was also able to obtain hands-on experience with CSAC devices that positioned them 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: experiments were conducted on actual CSAC development boards and a waveform was developed 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, and transmit frequency, power, and time patterns over time, based on *a priori* arranged pseudo-random sequences. 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. A custom dual-mixer, time-difference measuring system was designed and developed 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 special "sounding" messages between the pairs of radios. The proposed solution operated with very low power by executing a time-synchronized, pre-planned media access scheme. To functionally validate the research claims that the coherent waveform was feasible, the 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 for various potential application areas and customers. Numerous experiments with CSAC development boards were conducted, and a model of the clock drift over time and across temperature was developed. 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. There are many promising leads, and the team has been awarded a Small Business Innovative Research (SBIR) directly related to the work done on this project.

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2012 IR&D Annual Report

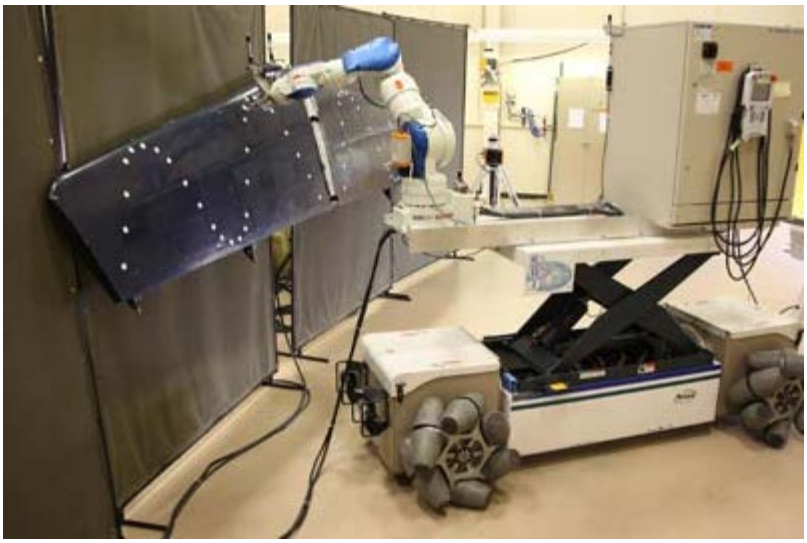
Metrology Referenced ROving Accurate Manipulator Phase 2 (MR ROAM 2), 10-R8205

Principal Investigators
Glynn Bartlett
Paul Hvass

Inclusive Dates: 01/01/11 – 12/31/12

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 utilizing 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 envelopes.

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 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.



Integrated MR ROAM 2 System

Accomplishments — The three individual systems (robot, mobile platform and localization) were

integrated. This integration included mechanical, electrical and software components. Calibration of the system and different control algorithms were tested to evaluate performance. The system maintained a standard deviation of less than one-quarter inch in the travel direction, and less than one-eighth inch in the other two directions. Maximum errors were only greater than one-half inch in the travel direction. The use of wheel encoders or inertial measurement unit would maintain maximum errors within one-half inch.

2012 IR&D Annual Report

3D Imaging for Behavior Classification, 10-R8221

Principal Investigator
Chris Lewis

Inclusive Dates: 04/01/11 – 10/01/12

Background — This research developed an automated behavior recognition capability, which uses a very low-cost, 3D color sensor for observing the motion of people. The system uses a variety of state-of-the-art machine learning techniques to estimate which of the trained behaviors is being performed. Several training tools were also developed which allow the system to be easily customized for a variety of applications. A novel feature derived from raw motion measurements was developed and shown to discriminate well between exercise behaviors. This feature, called a Motron, is constructed from natural cluster centers in data vectors containing position and velocity measurements of the subject. A new clustering algorithm was also developed and shown to be useful for both analysis and for accurately modeling sampled data.

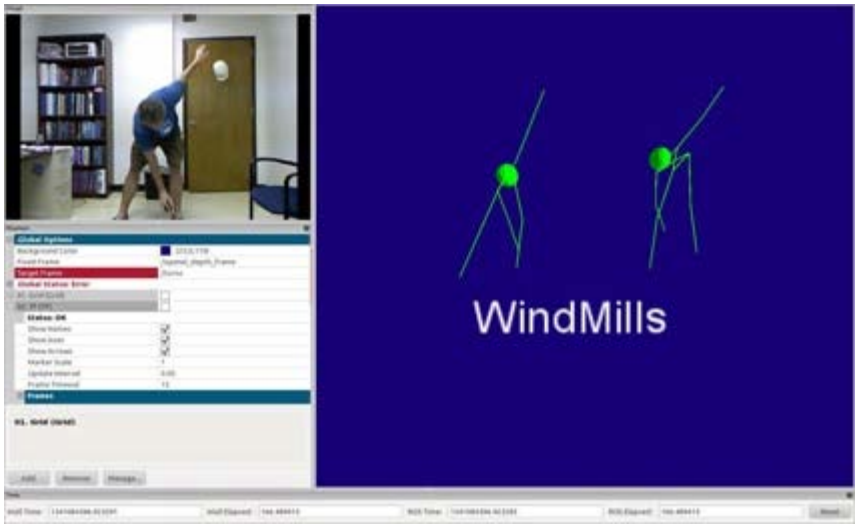


Figure 1: A real-time behavior recognition system is trained to recognize motions. This system relies on natural clusters in the complex motion measurement data. A novel cluster analysis algorithm, having wide applicability, finds these natural clusters in high-dimensional data.

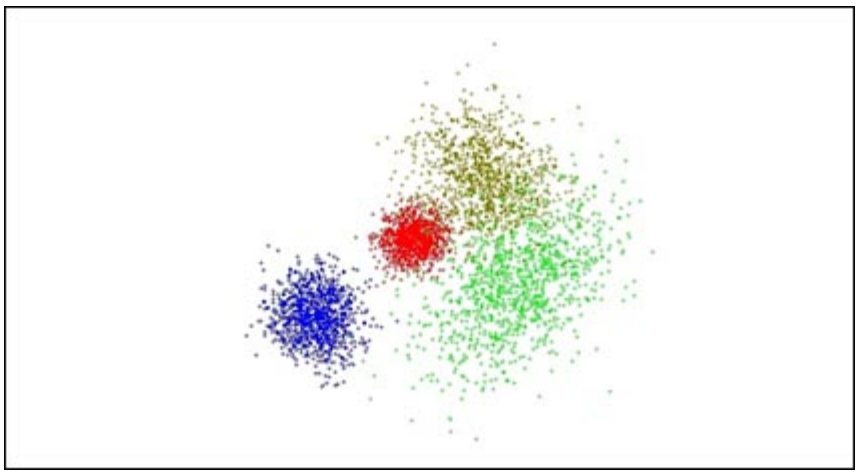


Figure 2: The image shows a two-dimensional slice of clusters found in twelve-dimensional data having significant overlapping distributions.

Approach — The techniques were implemented under ROS (Robot Operating System), which is an open architecture, publish-subscribe system that integrates drivers for common sensors and machine learning tools into a convenient development environment. ROS nodes were developed for training classifiers, analyzing clusters in data and estimating behaviors in real time.

Accomplishments — A novel motion descriptor, called a Motron, was developed that is formed from natural clusters in pose measurements. Histograms of observed Motrons over a time window were shown to be both salient and computationally inexpensive features for classifying behaviors in real time. In

addition, a novel cluster analysis algorithm was developed which automatically determines both the number of clusters and models for those clusters in arbitrary high-dimensional data.

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2012 IR&D Annual Report

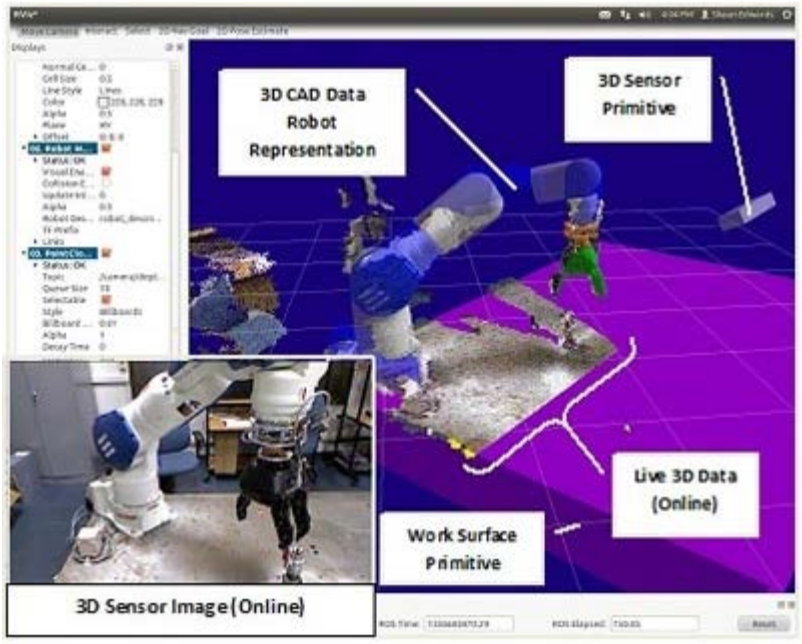
A Senior Staff Renewal IR&D Project at Willow Garage, 10-R8224

Principal Investigator
Shaun Edwards

Inclusive Dates: 05/16/11 – 04/01/12

Background — The "Robot Operating System" software, better known as ROS, is an open-source program 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 not feasible or cost prohibitive. SwRI has already utilized ROS for several industrial and advanced manufacturing projects. 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 worked closely with ROS developers at Willow Garage to develop an open source ROS-Industrial software stack (software suite) to support the use of ROS for industrial applications. The software provides a standardized interface to a variety of robot controllers, thus enabling robot agnostic ROS software. The initial version of software developed under this project, which includes robot drivers, documentation, and applications demonstrations, was released in March 2012.



ROS-Industrial has the ability to visualize a robot cell, including fusion of 3D CAD data, shape primitives and sensor data. This figure shows the various data sources used in the advanced pick and place demo application.

Accomplishments — The project has completed the following milestones:

- Developed a proof-of-concept code demonstrating remote control of an industrial robot via the ROS software.
- Developed a platform independent messaging structure that allows ROS to interface with a variety of industrial robotic platforms.
- Demonstrated a dynamic pick and place application that utilizes ROS perception and path-planning capabilities (see video below).
- Formalized ROS-Industrial as a continuing open source software development program that leverages community contributions from SwRI and other industrial software developers.
- Initiated ROS-Industrial Consortium to provide industry direction and support for the ROS-Industrial software.

ROS-Industrial video.

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2012 IR&D Annual Report

Special Purpose IP Routing, 10-R8243

Principal Investigators
Myron Moodie
Todd Newton
Ben Abbott
Patrick Noonan

Inclusive Dates: 07/01/11 – Current

Background — Network solutions permeate all domains, from our homes to cars, and from industry 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 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 only used 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. For example, Cisco has no business interest in providing specialized product markets smaller than 100s of millions of dollars.

Approach — The objective 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 and then built standard and modified router implementations based on several of these packages. The virtual router architecture was then augmented through the use of distributed physical network interfaces under the control of a central control node. A combination of open source software capabilities not originally designed for routing applications was leveraged to enhance the scalability and flexibility of the virtual router approach. The team has established a laboratory environment by implementing multiple virtual router nodes using a combination of SwRI network lab resources. These nodes are currently being modified and replicated as

needed to execute the challenge problems. Testing against the challenge problems is under way to determine the performance improvement possibilities of the virtual router architecture.

2012 IR&D Annual Report

Secure Mobile Applications for Corporate Travelers, 10-R8244

Principal Investigators
Sean C. Mitchem
Sandra G. Dykes
John G. Whipple

Inclusive Dates: 07/11/11 – 10/11/12

Background — Southwest Research Institute and its clients are seeing a surge in employee use of personal mobile devices for company business. Smartphones and tablets raise new security issues because they are often owned by employees and contain a mixture of personal and company information. The prevalence of this trend is illustrated by a new term coined to describe it: BYOD, for bring your own device. Small mobile devices are more likely to be lost or stolen, exposing sensitive company and client data. Malware risks are amplified because mobile devices connect to the Internet directly rather than from behind corporate firewalls and intrusion protection systems. Safeguarding mobile devices will require developing innovative security technologies that address these new usage patterns and device characteristics.

Approach — This project addressed multiple aspects of mobile device security, with a focus on the following areas:

1. Malware threats to mobile devices
2. Secure coding methodologies for mobile applications
3. Data protection and user authentication utilizing device sensors
4. Mobile device management systems trade space analysis
5. Mobile applications for corporate travelers

This approach combined web research, literature reviews, interviews with commercial companies, in-house testing of mobile device management systems, developing internal mobile apps for research and testing purposes, and experimentation, depending on the task being accomplished.

Accomplishments — The project produced two white papers: "Malware Threats for Mobile Devices" and "Secure Coding for Mobile App Development." The first is a general assessment of malware-related threats to mobile devices and secure protection provided by the iOS and Android® operating systems. The second white paper targets software developers and was intended to provide a primer on best practices for writing secure mobile applications. The research on mobile device management systems leveraged the information from these white papers to assess current solutions. This study produced a technology trade report that describes options and provides recommendations for enterprise organizations. Additionally, the project team produced the article entitled, "Mobile Applications Security: Safeguarding Data in a Mobile Device World," published in the March/April 2012 edition of *CrossTalk, The Journal of Defense Software Engineering*.

Aspects of this research required developing real applications to test understanding and validate new approaches. The team developed these as deployable apps, useful to SwRI employees while on travel. The mobile traveler apps were developed for iOS and Android and consist of Mobile SwRI WebID, SwRI Traveler, and Group Text Emergency Notification. The most innovative result of this project is in the area of sensor-based authentication. The motivation was to make authentication easier for users without reducing data protection — effectively balancing risk and usability. Sensors on mobile devices provide measurements of device orientation, touch pressure, touch size, and other data. In sensor-based

authentication, the project team used machine-learning methods to train a detector on sensor data. The model can then be applied to verify a user's identity and detect imposters.

Data was collected from 15 volunteers who entered practiced text (e.g., a password) and free-form text. In both cases, the average classification accuracies were more than 99 percent. These results are striking for a preliminary study and indicate that the approach should be pursued further. In a related approach called state-based authentication, sensor data was combined with system state to determine the required level of authentication. System state determines how easily sensitive areas of memory can be accessed. Sensors determine whether an attacker may be in possession of the device. For example, sensors can detect whether the device has been laid down since the last password entry. If sensor data guarantees that the owner has maintained possession, then no password is necessary. If not, device state is used to determine whether the user must enter a strong password or simple PIN.

In summary, this project has provided a deep understanding of the security issues unique to mobile devices. The white papers and reports will be made available to all SwRI divisions, improving the Institute's knowledge and capabilities in this area. Research results for user authentication will provide a foundation for pursuing externally funded research.

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2012 IR&D Annual Report

GPS-denied Localization System, 10-R8248

Principal Investigators
Kristopher C. Kozak
Christopher L. Lewis
Marc C. Alban
Samuel E. Slocum
Michael O. Blanton

Inclusive Dates: 09/06/11 – Current

Background — Global Positioning System (GPS) receivers provide a low-cost localization and navigation solution to a wide variety of commercial and military systems. As safety-critical systems come to rely on GPS (and other satellite-based localization systems), concerns have mounted due to its well-known vulnerabilities. GPS has limited accuracy and requires an unobstructed line-of-sight to multiple satellites. Its signals are subject to interference, multi-path, jamming and spoofing. While GPS has become more essential and ubiquitous, few practical alternatives have emerged. The fragility of GPS can be considered one of the limiting factors in the adoption of some cutting-edge technologies such as self-driven automobiles. The objective of this project is to develop a camera-based system that provides real-time localization measurements and can serve as a reliable supplement or alternative to GPS.

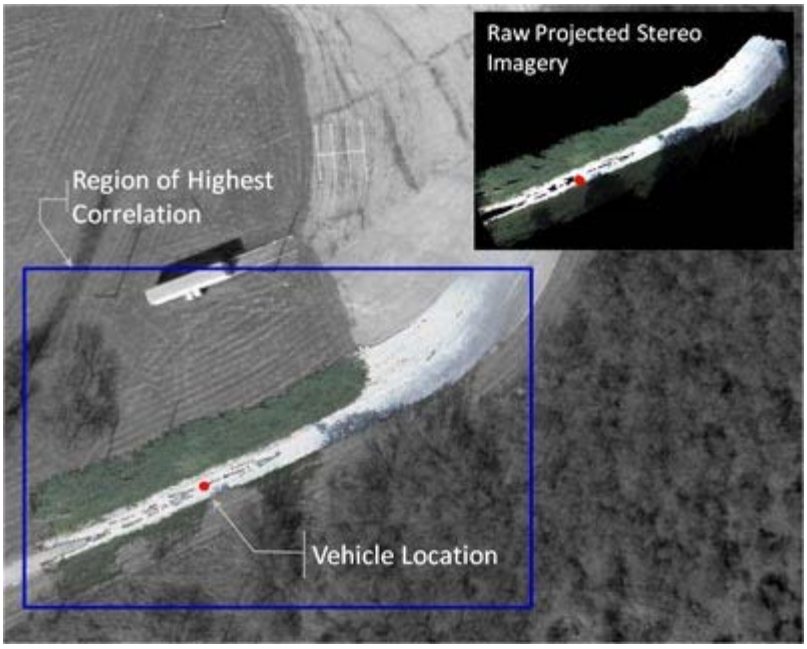

Figure 1: Features of opportunity in ground images are matched by appearance subject to geometric constraints to identify overlapping frames and determine vehicle location.

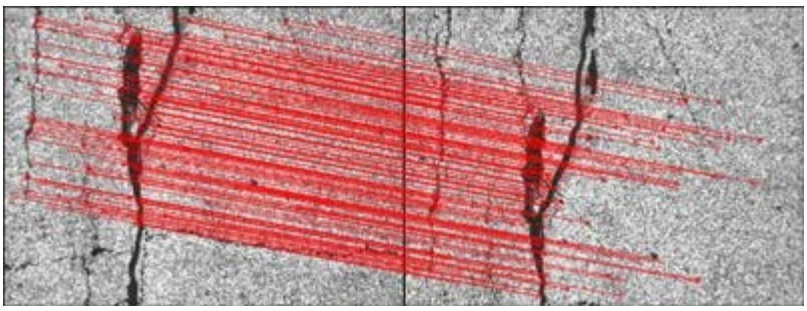

Figure 2: Stereo imagery acquired on a ground vehicle can be used to determine location relative to a georegistered aerial image.

Approach — SwRI's solution to this problem for ground vehicles is to develop two related map-based localization methods that utilize cameras on a vehicle. To this end, SwRI researchers designed a pair of camera systems – a downward-facing camera with high intensity illumination and a forward-facing stereo pair – to address two related aspects of the localization problem. The downward facing camera system allows for extremely high precision localization on pre-

driven, mapped routes, while the forward facing camera system allows for localization using both maps generated on pre-driven routes, as well as maps consisting of readily available aerial imagery. By processing the real time imagery acquired with the cameras and comparing the image features/landmarks to the geo-referenced imagery that comprises the map, the location of the cameras (and thus the vehicle on which the cameras are mounted) can be determined. In addition, either camera system can be used to compute differential motion between camera frames, and thus can fill in gaps when the live imagery from the vehicle cannot be confidently matched to the map.

Accomplishments — For the ground-facing camera localization approach, a full hardware system, which includes a camera and synchronized high-intensity illumination, was designed and installed on an SwRI vehicle. An algorithmic framework based on feature matching with geometric constraints was developed as the basis of the localization approach. This approach has been shown in a subsequent analysis to have a very high success rate for positively identifying location (on a variety of road surfaces), with a very low rate of incorrect matches. Finally a simple implementation of a full localization system was implemented on the vehicle, and the ground-facing system was operated successfully in real time on the vehicle. Development of this system is ongoing. For the forward facing stereo camera localization approach, two separate algorithmic frameworks have been developed, a feature matching approach and an image correlation approach. Both methods have been demonstrated to yield successful localization on several types of data, including real projected stereo imagery. Development of this system is also still ongoing.

2012 IR&D Annual Report

Traffic Management Center Video Distribution System, 10-R8256

Principal Investigators
Robert W. Heller
Roger Strain

Inclusive Dates: 09/12/11 – 01/12/12

Background — A primary function of Transportation Management Centers (TMC) is the "detection and management" of transportation events using Advanced Traffic Management Software (ATMS). The presence of traffic measurement equipment aides in the detection, but all detected and reported events are visually confirmed with the use of roadside video cameras. Typically the roadside video is transported in digital format to the TMC and displayed on large video monitors covering the majority of a wall. Operators in small TMCs without video walls use non-integrated solutions to monitor the video. This project sought to integrate the display of video into the TMC operator's desktop.

Approach — A market survey of digital video decoding products was conducted using a list of required capabilities, which included video formats, transport mechanisms, bandwidth capabilities, installation requirements, etc. The product survey identified Video LAN Client (VLC), an open source project, as best fitting the deployment requirements. The Florida Department of Transportation SunGuide ATMS was used as a demonstration platform.

Accomplishments — The original goals of the effort were met; several small application programs were written to control the transcoding of video streams into viewer friendly formats using open source video transcoding and commonly installed viewer applications. Specifically:

- A VLC and open-source software product was used to transcode the video.
- The user could select a video to be displayed from a list of cameras.
- The IE Plug-in for Windows® Media Player was used as a video viewer.
- Video from cameras configured in a manner consistent with existing FDOT field cameras was viewable on the workstation.

2012 IR&D Annual Report

Wear Leveling in an Embedded Flash File System, 10-R8275

Principal Investigators
Sue Baldor
Robert Klar
Scott Miller

Inclusive Dates: 12/19/11 – 04/27/12

Background — This project evaluated a NAND-based flash wear-leveling algorithm in the context of typical flight software file system usage. Flash memories originally developed for the consumer market have revolutionized mass storage for space-based applications. However, flash memory cells can wear out quickly if erased frequently, degrading certain memory regions of the device enough to require replacement (not a viable option on-orbit). An algorithm was implemented that targeted the FAT filesystem – a filesystem readily available in many real-time operating systems. This algorithm was evaluated based on the number of erases per groups of clusters on the target mass memory device.

Approach — Traditionally, wear-leveling is implemented in either the hardware device or within file system software. Our approach implements wear-leveling algorithms within the device driver for the target device, the Multi-Mission Mass Memory Module (M4) mass memory board. Doing this allows us to make use of some of the features provided by the hardware design without paying the price of high overhead found in higher-level software solutions. The wear-leveling algorithm contains two main components: the logical-to-physical table (LPT) cluster mapping component and the reclamation component. The LPT maps the requested logical clusters to physical clusters on the device. Reclamation erases clusters that have been marked as free and periodically moves old clusters to new less-used locations. The number of device erases is used to determine where new data is written and where old clusters are relocated.

Evaluation of the performance of the wear-leveling solution occurs within the context of file system operation. To facilitate evaluation, we created a hierarchical driver structure utilizing the VxWorks extended block device (XBD) interface, which provides a framework for file system integration. Using the XBD interface, the device is mapped into a FAT file system. Erase statistics provide a mechanism to determine the evenness of wear as large files are written to the file system.

Accomplishments — Wear-leveling statistics collected during this work were used to evaluate the algorithm. Preliminary results show that while the algorithm shows promise for effectively managing wear on the target device, some modifications will still be necessary. Primarily, the algorithm, as implemented, displays a tendency to favor the first half of the device while neglecting clusters on the remainder of the device. Future work will be required to examine and fix this issue.

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2012 IR&D Annual Report

Investigation into Techniques for Detecting Negative Obstacles 10-R8278

Principal Investigators
Steven W. Dellenback
Jason Gassaway
Richard Garcia

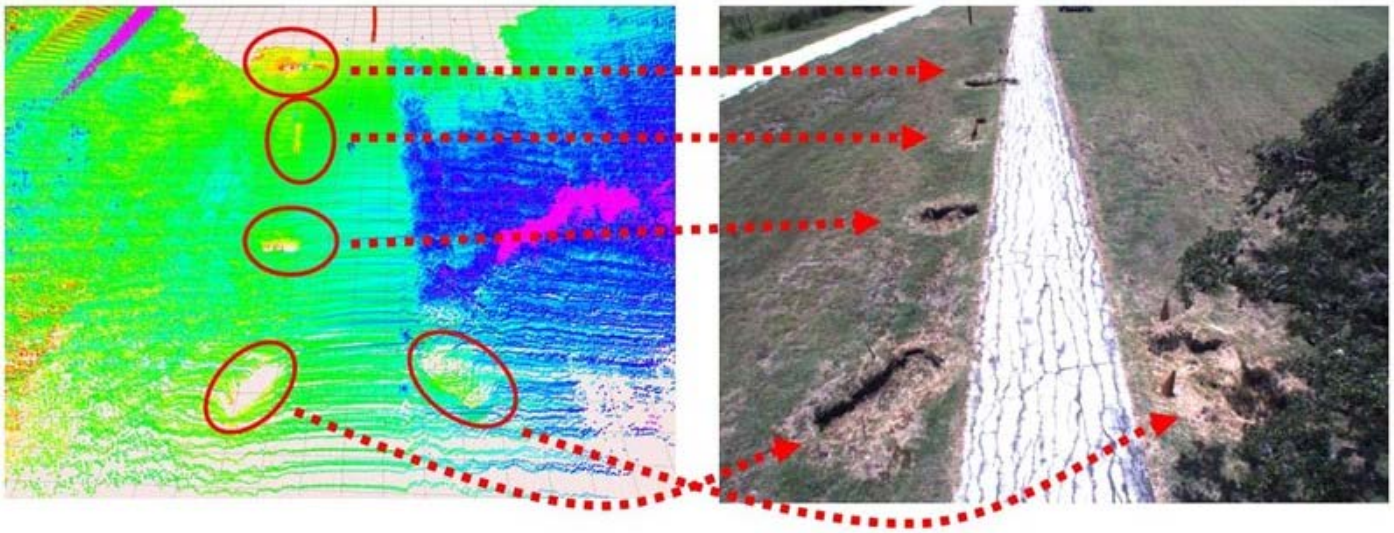
Inclusive Dates: 01/01/12 – Current

Background — The U.S. military has repeatedly stated the single most complex unresolved issue in the unmanned ground vehicle (UGV) community is the detection of negative obstacles (these are holes and troughs, anything that does not reflect or is difficult to observe). In most cases, it is simply a geometry problem because the angle in which sensors can detect a hole is not acute enough until the vehicle is too close to do anything about it.

Approach — The goal of this project is to develop techniques that facilitate the detection of "negative obstacles" for UGVs. Negative obstacles are very difficult to identify from a traditional UGV platform moving at a significant speed because the elevation of the sensors does not provide a field of view (FOV) that can identify the obstacle in enough time to perform avoidance maneuvers. Techniques currently used are to place downward-looking sensors at the front of the vehicle and have a FOV that is measured in a small number of meters with a UGV moving at a very slow rate of speed. This effort is investigating the use of sensors that will be located above the vehicle using an airborne platform.

Accomplishments — The project has completed the following phases:

- Designed and fabricated a mast structure to allow the sensors to be located 12 meters above a HMMWV.
- Designed an algorithm framework that implements a pipeline processing framework composed of the following steps: data collection, localization, filtering, analysis and detection.
- Implemented algorithms to capture data from both LIDAR and a camera attached to the mast. The sensors have captured scans of the negative obstacle test area while mounted to the mast, and early results are encouraging. The illustration depicts initial detection efforts that have been implemented.



Negative obstacles detected by sensors mounted above the vehicle.

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2012 IR&D Annual Report

Detection of Malware on Vehicular Networks, 10-R8281

Principal Investigators
Mark J. Brooks
Marisa C. Ramon
Tam T. Do
Nakul Jeirath

Inclusive Dates: 01/01/12 – Current

Background — Computers are becoming increasingly prevalent in modern automobiles. By some estimates, even low-end cars contain anywhere from 30 to 50 of these automobile computers, also known as electronic control units (ECUs). ECUs control everything from the in-car entertainment system to the braking system and the engine fuel-air mixture. Wireless connectivity in these computers is also becoming more common, with some vehicles having capabilities for cellular, Bluetooth, and even Wi-Fi connections. Given this increasing sophistication and connectivity, the modern automobile is fertile ground for the same sort of malware and malicious attacks that are usually associated with traditional computers.

Approach — The primary objective of this investigation is to demonstrate the beginning steps toward a system of vehicular malware detection. As a result of this investigation, it is expected one or more prototype algorithms will be produced that can effectively detect the presence of vehicle malware. This is expected to further SwRI's understanding of vehicle exploitation tools and techniques and position the project team to present their results at a major relevant conference.

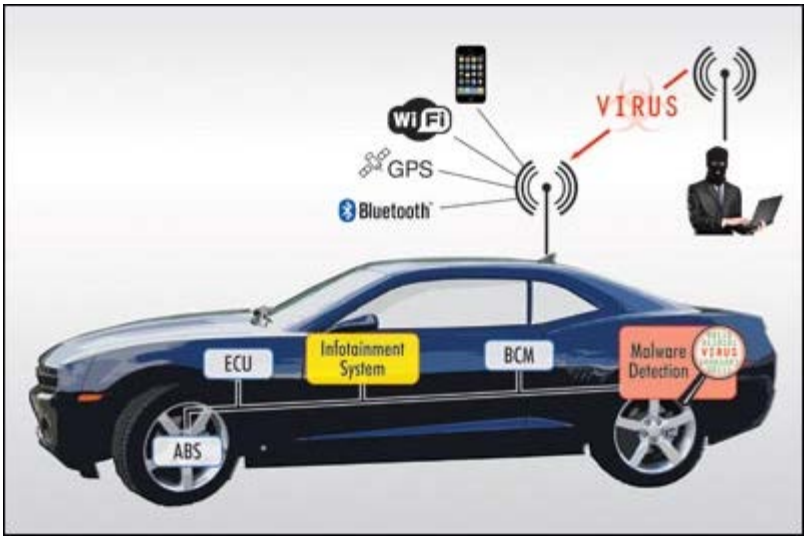

Figure 1. Potential Exploit Vectors and Busses Present on a Vehicle

Accomplishments — A vehicle security test bed has been established with several Controller Area Network (CAN) analyzer tools, several infotainment ECUs, a vehicle, and an oscilloscope with a CAN-specific analyzer. Several wireless tools were also acquired for the test bed for connecting to vehicle infotainment devices.

Using the test bed, the project team investigated vehicle vulnerabilities, patterns of malware, and detection algorithms.

- Researched vulnerabilities in the ID3 tags in the MP3 files, USB

Figure 2. SwRI's Vehicle Security Test Lab

vulnerabilities, Bluetooth vulnerabilities, and Wi-Fi vulnerabilities in the infotainment ECU.

- Investigated various malware pieces running on the infotainment ECU platform. These malware pieces attempt to reach the CAN bus once a vulnerability has been exploited.
- Recorded sample CAN traffic in a variety of scenarios and used this data to begin creating several detection algorithms based upon traffic variations. In order to test the detection algorithms, a prototype detector framework is being developed that will be used to test the detection algorithms on the CAN bus.

2012 IR&D Annual Report

Advanced Situational Awareness Experiment, 10-R8284

Principal Investigator
Michael S. Moore

Inclusive Dates: 12/27/11 – Current

Background — SwRI has supported the U.S. Army Program Executive Office for Command, Control, and Communications Tactical (PEO C3T) in development of the Vehicular Integration for C4ISR/EW Interoperability (VICTORY) architecture since 2008. This architecture provides a foundation enabling sensor and weapon system interoperability on military tactical vehicles. The VICTORY architecture will provide a core vehicle network that will enable interoperability between systems on the vehicle. Leveraging the VICTORY integration and adding an extra-vehicle mesh network to also share data between the vehicles will enable innovative new situational awareness applications.

Recognizing this potential, SwRI conducted an initial internal research project (10-R8107), resulting in new technologies. One technology receives first-hand observation inputs from multiple, disparate sensors on the vehicles and coordinates between the vehicles to develop an overall view of the local operational picture. It applies heuristic algorithms that correlate the information from the various sensors and automatically applies reasoning that is currently done manually by the soldiers. The goal is to create more actionable information for soldiers. As an example, sensors that are currently fielded have high false alarm rates and, as a result, are often disabled by frustrated soldiers. The advanced situational awareness (ASA) technology should reduce the false alarm rates by correlating information from multiple sensors and from other vehicles. The second technology integrates the operational picture with real-time battle maps and video streams, creating fused views with the goal of providing relevant, timely information to the soldier in simple views.

Approach — The technology developed in the prior project was realized and evaluated in a laboratory setting. This project is integrating experimental systems on three vehicles and executing experiments in military-relevant scenarios. The feedback obtained from the experiments is being used to adjust the approaches in the correlation and visualization tools and increase their relevance to soldiers. The objective is to quantitatively and qualitatively measure the effectiveness of the ASA technologies and mature the algorithms to meet warfighter needs. Toward this objective, SwRI is collaborating with the Army's Night Vision and Electronic Sensors Directorate (NVESD), which supports the Army Deployable Force Protection (DFP) program. They have teamed with SwRI to integrate the ASA systems with DFP systems, develop military relevant scenarios, and execute experiments.

Accomplishments — The team integrated an ASA demonstrator vehicle (a Chevrolet Suburban) to include a variety of sensors, cameras, and displays, which is being used to evaluate the technologies. The Suburban was used in conjunction with two VICTORY-enabled HMMWVs and a stationary Tactical Operations Center (TOC) to develop and test ASA technologies at SwRI. These platforms are integrated via an Extra Vehicle Mesh Network (EVMN), which enables sharing relevant situational awareness information. This shared information is presented to users on an integrated mapping application, "augmented reality" video overlays, and tabular user interfaces. SwRI then teamed with NVESD after completion of initial ASA technologies testing at SwRI in a weeklong exercise at Camp Roberts, Calif. The SwRI/NVESD team integrated a DFP-VICTORY-ASA experimental system, including three VICTORY and ASA-enabled vehicles (the Suburban and two HMMWVs), an experimental TOC, and a large-scale DFP network. Extensive experiments were conducted, and data and feedback were collected. Lessons learned from that exercise are being used to evolve and mature the ASA technologies. NVESD is funding follow-

on research, which may include a demonstration system to be fielded in Huntsville, Ala., in July 2013.

2012 IR&D Annual Report

Investigation of a General Artificial Intelligence Framework for Robotic Control, 10-R8294

Principal Investigator
Cody Porter

Inclusive Dates: 03/05/12 – 07/05/12

Background — As robotic systems become more complex, intelligent control must be applied to further advance the field of robotics. For more than two decades, SwRI has fabricated and maintained coating removal systems for large aircraft for the U.S. Air Force. These large robotic systems are currently controlled with a human operator monitoring video feedback of the coating removal process and adjusting the robot speed accordingly. A method of automating the speed control based on coating removal sensory feedback will result in greater throughput and higher reliability of these existing systems. However, traditional machine learning techniques are unlikely to be effective because of the complexity of the video data due to variance in lighting conditions, coating color and surface geometry. Therefore, this research focused on applying a general artificial intelligence (AI) framework to these robotic coating removal systems. The goal of this effort was to produce appropriate speed control decisions using AI given the input video data and to evaluate the chosen AI framework.

Approach — The AI framework was used to construct an intelligent "agent," which is the structure of how the data is passed around within the framework. The video data was first manipulated into a feature vector for the agent input. The agent was allowed to make its best guess on speed decisions based on the input feature vector. The agent was then trained by applying positive feedback for good speed decisions and negative for bad speed decisions. This feedback and performance information was stored into a knowledge base for future decisions. Finally, the agent was exposed to unseen video data to test the appropriateness of its speed control decision.

Accomplishments — The image processing algorithms produced for this agent were remarkably robust and produced a realistic feature vector for a variety of video conditions. These tools will be useful for future efforts to automate coating removal processes and for a variety of surface processing applications. These results have been shared with customers in the coating removal market and are under consideration for improving existing robotic systems. The general AI framework used for this application is a recent development that required some refinement efforts prior to testing. As a result of this effort, SwRI researchers now have an extensive understanding of the capabilities this framework and can accurately apply it to other future applications. The unique information theories and technique applied through the framework could be powerful for a variety of applications as it matures.

2012 IR&D Annual Report

High-Performance Rendering of Interactive Decision Support Visualizations in Network Restricted Environments, 10-R8296

Principal Investigator
John G. Whipple

Inclusive Dates: 04/02/12 – 08/02/12

Background — Decision support systems collect large amounts of historical data, but making decisions based on the data is difficult without summarizing visualizations. Traditional decision support visualizations allow the user to manipulate settings to view the data in a way that might make more sense; however, a round trip to a back-end server, or more recently "the cloud," is required before the visualization can be re-rendered. This is the accepted visualization paradigm; nevertheless, there are two intrinsic flaws with relying on a remote computer. First, network connectivity may not be available due to practical or procedural reasons. Second, including a network round trip limits the speed that the user can modify settings and see an updated visualization. This project investigated the high-speed rendering of interactive decision support visualizations that relied solely on the processing power of the computer hosting the visualization.

Approach — The first step to achieve the project objectives was to obtain a time-series predictive model that could be used as a basis for two custom visualizations. Data was randomly generated based on a known function that reflected a generic two-party negotiation data set. The generated data was then modeled using two different modeling techniques: neural network and Markov Chain Monte Carlo (MCMC). The focus of this research was not the quality of the model, but the quality of the visualizations and the speed at which they could be rendered. Next, the application algorithms for the modeling techniques as well as the visualizations were developed using HTML5 and JavaScript. A rendering test script was used to capture performance metrics. Test results were obtained from Internet Explorer®, Firefox® and Chrome®. An Apple® iPad was also included in the testing. An average frame rate of 15 FPS or greater was considered to be a success, as this frame rate is typical of mobile device refresh speeds and is unperceivable to the human eye.

Accomplishments — The neural network model did not pose a performance problem for any platform or browser. The frame rate consistently peaked at 60 FPS regardless of how the user interacted with the visualization. The calculations required of the MCMC were significantly more complex. The accuracy of the MCMC depended on the number of simulation iterations. It was discovered that all modern browsers running on modern hardware were able to maintain the 15FPS metric while iterating through the MCMC simulation 1,500 times. As a result of this research, it is now known that it is practical to use neural networks and, to an extent, MCMC using only Internet browser technology.

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2012 IR&D Annual Report

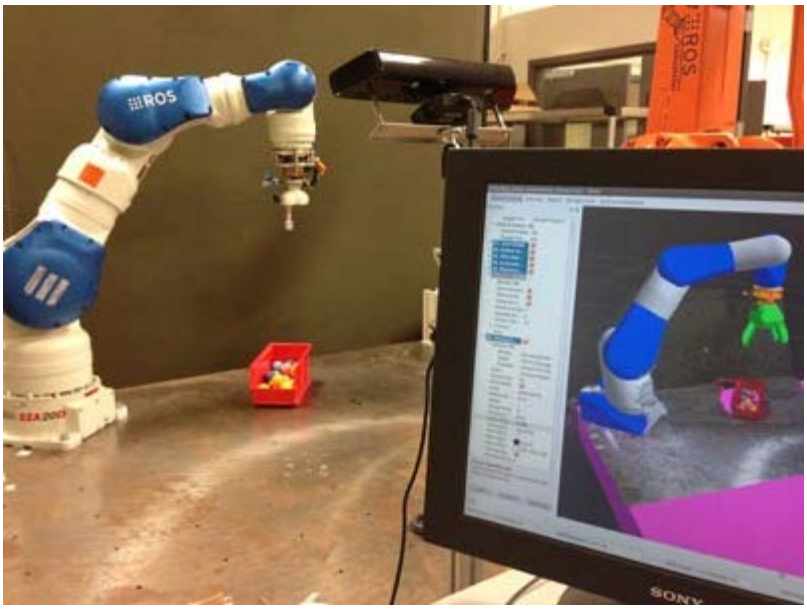
Robotic Part Handling for Unstructured Industrial Applications, 10-R8301

Principal Investigator
Clay Flannigan

Inclusive Dates: 04/01/12 – 11/01/12

Background — Recent developments in 3D sensor technologies, adaptive robotic grippers and advanced perception and planning algorithms are rapidly advancing the use of robots in complex and dynamic environments. Traditional industrial application of robots requires that parts be precisely located using dedicated fixtures so that there is little uncertainty in the location of the workpiece and condition of the workspace. More advanced industrial robotic systems use 2D or 3D vision sensing to handle minor variations in part locations. However, there are large classes of problems where high part variability or dynamic environments prohibit rigid fixturing methods and confound commercially available vision solutions. An example application is sorting residential recyclables, where there is an almost infinite variability of parts to be manipulated. Aerospace manufacturing is another market that is challenged by high-mix, low-volume processes.

Approach — SwRI has previously developed an open-source software framework for industrial robotics called ROS-Industrial that leverages the huge community of robotic researchers using the Robot Operating System (ROS). This research is extending the ROS-Industrial program through investigation of perception, motion planning, and grasp planning methods to address unstructured manipulation. Specifically, we are using the Microsoft® Kinect sensor for colorized 3D range image acquisition. Object recognition and pose estimation algorithms are being developed using the Kinect data to identify objects in cluttered environments. Both vacuum and adaptive finger grippers are being employed for grasping. Motion planning objectives include the generation of efficient and collision-free motion even in dynamic or complex scenes.



Robot cell showing Motoman Arm, Kinect Sensor, and ROS visualization.

Accomplishments — In the first six months of this 12-month project, the broad research objectives were narrowed by identifying end-user requirements and by creating a hierarchy for the problem domain. A robot cell has been integrated that includes a Motoman SIA-20 robot, Robotiq 2 and 3-finger grippers, vacuum grippers, and Kinect sensing. The robot cell has been integrated with the ROS-Industrial software and is capable of tabletop manipulation of randomly oriented objects using the vacuum gripper. A novel method has been developed for object recognition and pose-estimation based on object templates. This

perception algorithm is robust for tabletop recognition using just shape cues (visual texture is not required). Future work will include continued research on perception methods for highly cluttered scenes such as those found in bin picking. Additionally, a demonstration capability will be created that permits quantitative benchmarking of the perception and manipulation approaches.

2012 IR&D Annual Report

Mobile Persistent Stare Using Unmanned Systems, 10-R8306

Principal Investigator
Paul A. Avery

Inclusive Dates: 04/02/12 – Current

Background — Within the unmanned ground vehicle (UGV) community there has been a number of successful "short-duration" demonstrations, which perform well for 10 to 45 minutes. In order for UGVs to have long-term success in tactical situations, they will need to perform missions in duration of 4 to 12 hours. The military has indicated that system "resets" could occur during fueling operations that would need to occur at least every 12 hours. The software for these systems needs to be adaptable and flexible enough to allow a system to "correct" itself over the mission duration. Additionally, most demonstrations have used one of two sensing technologies: Light Detection and Ranging (LIDAR) or Electrical Optical (E/O); SwRI is well versed in both technologies, but fusing the two technologies (cooperatively across platforms) could dramatically improve the performance of UGVs. The scope of work in this proposal is to add several additional building blocks to the SwRI MARTI (Mobile Autonomous Research Technology Initiative) platform that are necessary for long-term viability of UGV technology. Groups of unmanned vehicles conducting long-term operations could also benefit from being linked together to form a cooperative vehicle system, which SwRI has experience in implementing for traffic scenarios.

Approach — The approach in this work is to develop hardware-agnostic software tools to automatically collect "health" status data from numerous hardware and software components of an unmanned vehicle, which can later be analyzed for long-term operational effectiveness. This tool will also be integrated into the unmanned vehicle's operating framework, which could enable a more rapid identification and notification of any system warning, error, or failure. With this tool, we will be able to conduct endurance autonomy testing with SwRI's fully autonomous HMMWV 1165. A perimeter will be identified for a surveillance mission around the SwRI facility. A cooperative perception system framework will also be developed to allow the integration of sensor and position data from a number of UGVs. We will define and develop tactical behaviors for the cooperative system and integrate these into the assessment of a cooperative vehicle mission.

Accomplishments — Hardware-agnostic software tools have been developed using the Robot Operating System (ROS) diagnostic tools for logging data related to the operation and behavior states of an autonomous vehicle platform. The specific platform that has been targeted initially is the SwRI-owned HMMWV 1165. The data logging system functions by subscribing to ROS topics that indicate the status of various subsystems, such as behavior states and health status of all included sensors. This manner of operation allows for the system to operate without any modifications to the current vehicle codebase. During operation, the data is periodically saved to a human-readable file called a YAML file, which is later moved to another computer for processing. The data can be parsed in a variety of ways, and presented visually, to further facilitate analysis of the performance of the vehicle during the test. A model of a cooperative vehicle system has been developed using agent-based methods, where a simplified UGV model (agent) is combined with other agents in a scenario of perimeter patrol. The behavioral characteristics of individual UGVs when some specified anomaly is either detected or communicated from another vehicle are being investigated regarding their effect on system-level behavior.

2012 IR&D Annual Report

Next-Generation Neutrally Buoyant Sensors, 10-R8274

Principal Investigators
Gregory C. Willden
Ben A. Abbott
Ronald T. Green

Inclusive Dates: 12/12/11 – Current

Background — SwRI had previously developed the award-winning Neutrally Buoyant Sensor (NBS) system for automatic mapping of partially water-filled caves and conduits. The technology was successfully adapted for externally funded projects with two government clients; however, newer applications require improved processing capabilities and a more flexible and capable hardware architecture.

Approach — Bringing together rapid prototyping capabilities for quickly building a waterproof housing and a small, powerful, flexible hardware system enabled the assembly of a toolkit that allows for the development and specialization of NBS systems to meet potential client needs. Competing constraints that guided the design of the toolkit elements include a low unit cost, having a modular system for rapid development and specialization, employing chirp correlation processing, and providing for flexible communication schemes.

Customer-specific system built from toolkit components

Accomplishments — The team has successfully developed an improved platform for NBS development and specialization. The new components provide higher sampling rates, onboard storage and processing capabilities, as well as rapid prototyped housing components. As part of an externally funded project, the technology toolkit was applied in the creation of a specialized NBS system for mapping and inspection of culvert conduits for a current customer. Additional toolkit components are prepared for use in services contracts that are being pursued with a variety of potential clients.

2012 IR&D Annual Report

Prevention of Ice Build-Up on Power Line Conductors and Ground Wires, 18-R8265

Principal Investigator
Sergey Vinogradov

Inclusive Dates: 10/01/11 – 10/01/12

Background — Ice build-up on electric power lines and ground wires during a winter storm is a major concern to the electric power utilities in cold climate regions. Unabated, it could cause extensive structural damage and economic loss. To protect the power lines, utilities are interested in anti-icing and de-icing methods that are efficient and economical.

Approach — Precipitation icing is the primary cause of structural damage when, during a storm, raindrops or snowflakes stick to conductors and freeze to form an ice layer. A high level of vibration acceleration is known to weaken the adhesion and friction forces between the two contacting surfaces, which separate and slide relatively freely. This effect is utilized for friction force reduction in metal working. As an anti-icing approach, longitudinal guided waves generated and propagated along the power line conductors or ground wires based on the magnetostrictive sensor (MsS) technology were proposed. A high level of vibration acceleration associated with the guided waves may weaken the adhesion and friction forces between conductors and precipitation. When raindrops or snowflakes do not adhere to conductors, they will fall off by natural forces (gravity, wind, and wind-induced vibrations) and no ice layer would be formed on the conductors as a result.

Accomplishments — The feasibility of preventing ice build-up using MsS-generated longitudinal guided waves was investigated experimentally on 0.25-inch diameter steel rods. The rod was subjected to simulated icing conditions in an environmental chamber with 20 kHz guided wave vibrations propagated continuously along its length. It was found that, with approximately 0.9 micron displacements (or 1.4×10^4 m/sec^2 vibration acceleration), which is the upper bound of the vibration displacements that could be produced continuously with the existing MsS technology, ice forming on the rod was unpreventable. Even if some much higher level of vibration accelerations could prevent the ice forming and build-up, this anti-icing approach was deemed impractical unless a simple way to produce the required level of vibration is found.

However, during the research project, it was realized that the MsS probe developed and used in this feasibility investigation produced about 30 times stronger signals than those generated directly in the steel rod using existing MsS probe technology composed of a coil and bias magnets. Recognizing that the developed MsS probe design would also eliminate the need of heavy bias magnets (which has limited a wider use of the MsS technology for cable/rope inspections and monitoring), a preliminary prototype MsS probe was developed and its applicability for cable/rope inspection was evaluated and proven on a 0.4-inch diameter ground wire. This magnet-less probe is expected to significantly expand the applications of the MsS technology for cable/rope inspection and monitoring.

2012 IR&D Annual Report

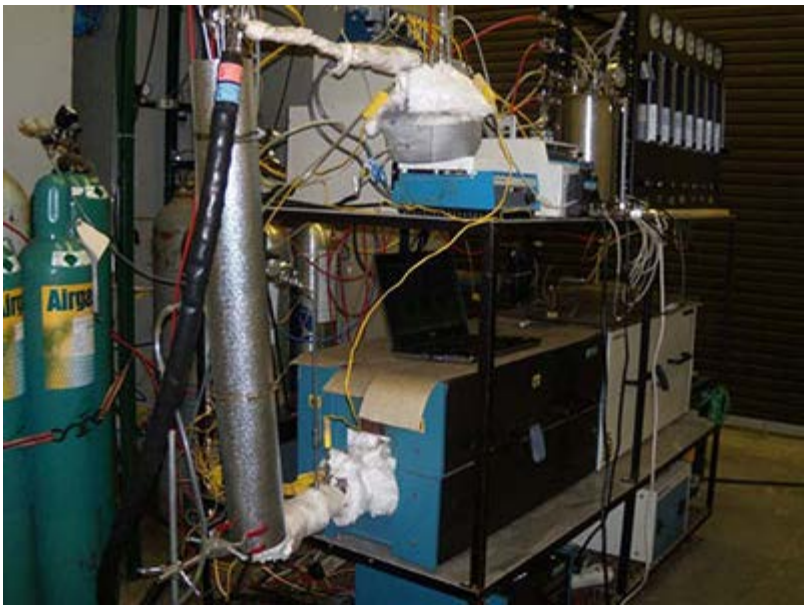
Development of a Selective Noncatalytic Reduction (SNCR) System for Stationary NO_x Emission Control, 01-R8213

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.



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.

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2012 IR&D Annual Report

Investigation of a High-Efficiency, Low-Emission Engine Concept for Heavy Duty Applications Using a Dual-Fuel Approach, 03-R8170

Principal Investigators
Michael Joo
Terry Alger
Christopher Chadwell
Raphael Gukelberger
Jacob Zuehl

Inclusive Dates: 07/01/10 – 01/01/12

Background — Diesel engine emissions regulations in the U.S. have become exponentially more challenging since the year 2002, and the most stringent ever U.S. On-Road Heavy Duty regulation went into full effect with the 2010MY. For off-road engines, the implementation of the new Tier IV Final regulations is in 2014. To meet these increasingly strict regulations, the diesel engine industry has developed and applied new technologies such as the diesel particulate filter (DPF) for PM reduction and selective catalytic reduction (SCR) devices or lean NO^x traps (LNT) for NO_x control along with exhaust gas recirculation (EGR) technology. Although the diesel industry has successfully employed these technologies to meet the U.S. 2010 on-road heavy duty regulations, the cost increase due to the very complex aftertreatment system is high and the efficiency penalty to keep the engine clean is significant. The efficiency penalty from the aftertreatment requires more expensive engine components, i.e. turbochargers, injection systems, power cylinders, etc., to maintain or improve the engine efficiency. Because of the cost increase and negative effect on the engine's fuel efficiency associated with the complex aftertreatment systems, the diesel industry, especially heavy-duty diesel engine OEMs, are enthusiastically seeking alternative technologies that provide high fuel economy and ultra-low emissions with minimal cost increases.

Approach — The objective of this project was to integrate SwRI's dual fuel HEDGE technology on a large-bore, dual-fuel engine and demonstrate diesel-like power density, high fuel efficiency and engine-out emissions compliant with U.S. 2010 heavy duty emissions standards. Specifically, the project goals were:

- Maximum power density greater than 16 bar BMEP
- Minimum fuel consumption of less than 200 g/kWhr BSFC
- NO_x emissions lower than 0.27 g/kWh $BSNO_x$
- Smoke emissions less than 0.2 FSN

Accomplishments — The minimum BSFC target of 200 g/kWh was fully satisfied. The project team was able to keep the $BSNO_x$ and FSN below the target of 0.27 g/kWh and 0.2 at almost every test point except for very high load BMEP conditions. They could also achieve 15.6 bar BMEP, which is very close to the target and surprisingly high maximum BMEP for the compression ratio of 14.5:1 with gasoline operation. With the results, the feasibility of dual fuel combustion for heavy duty application was successfully confirmed. The results are published at SAE (2012-01-1979) and presented at COMVEC 2012.

2012 IR&D Annual Report

Advancement in Fuel Injection Technology as an Enabler for Improved Engine Efficiency and Reduced CO_2, 03-R8185

Principal Investigators
Radu Florea
Sudhakar Das
Mark Walls
Nigil Jeyashekar
Stefan Simescu
Charlie Roberts

Inclusive Dates: 10/01/10 – 04/01/12

Background — Modern commercial diesel engines are expected to meet extremely strict NO_x and Particulate Matter (PM) regulations as well as upcoming fuel efficiency and CO_2 emissions standards. For the last 10 to 15 years, the diesel industry has combated smoke production through the use of ever-increasing fuel injection pressure. Current heavy-duty engines now regularly utilize injection pressure in excess of 2,500 bar. Increased injection pressure results in significant increase in engine fuel-system parasitic loss as well as engine efficiency penalty. Therefore, there is increased interest in alternative technologies that allow the effective control of PM emissions while minimizing engine efficiency losses. One such technology, called *air-assisted diesel combustion*, is proposed and investigated in the current research. It employs high-velocity air jets that aid fuel-air mixing by increasing turbulence in the diesel flame envelope and reducing PM formation.

Approach — Diffusion-controlled combustion of diesel sprays with and without air-jet assistance has been investigated for different injection pressures in an optically accessible constant volume reactor. Experiments were designed to provide a qualitative and quantitative assessment of the proposed air-assisted operation and compare it with the performance of commercially available high-pressure injection systems as well as injection systems expected to be available in the near future (up to 3,000 bar injection pressure). First, the air-assisted operation has been investigated using a computational fluid dynamics (CFD) numerical solver, the results of which guided the experimental work. Second, diesel combustion has been qualitatively investigated using high-speed Schlieren photography. This approach provided enhanced understanding of the impact of the air-assisted operation on the air-fuel mixing process as well as the temporal and spatial distribution of the fuel-rich combustion responsible for the production of in-cylinder soot. Finally, quasi-quantitative experiments using the laser-based light extinction method (LEM) measured the impact of the air-assisted combustion on the time-based evolution of soot optical thickness KL at a single location within the diesel jet.

Accomplishments — For high-pressure fuel injection, it was found that the laser extinction predicted a reduction of average KL values by a factor of two as injection pressure was increased from 500 to 2,500 bar. The air-assist jets investigated, which had momentums equivalent to a 500-bar fuel injection, produced a swirling flow field, which improved the fuel-air mixing. The air-assist technology showed promise, and while further work needs to be done before it may be ready for commercialization, this internal research project showed an alternative path towards soot reduction in high-EGR combustion systems that minimizes fuel system effort and improves the energy efficiency of the engine system. The results of this work have been detailed in an upcoming SAE publication.

2012 IR&D Annual Report

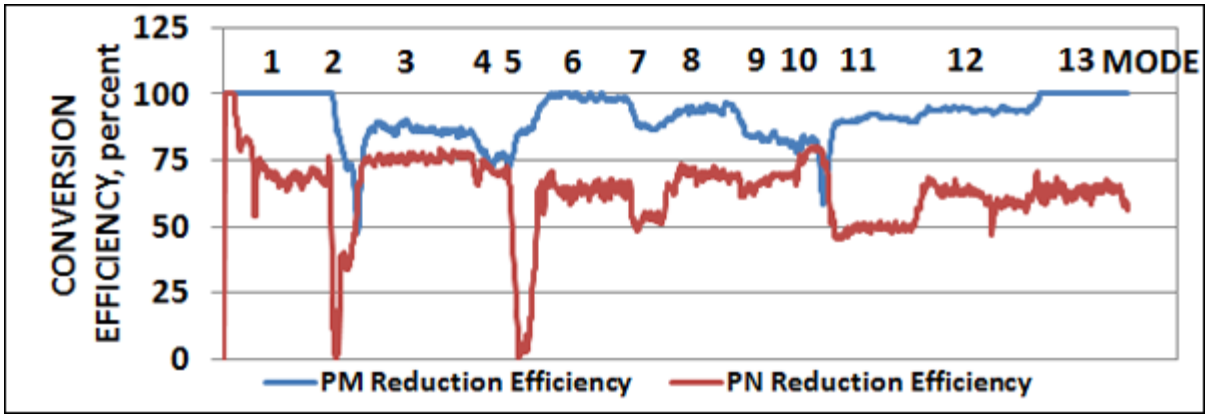
Investigation of Particle Reduction Efficiency of a Flow-Through Filter, 03-R8247

Principal Investigators
Reggie Zhan
Michael Chadwell

Inclusive Dates: 08/01/11 – 012/01/11

Background — Flow-through filters (FTF) can be a cost-effective emissions control technology to reduce particulate matter (PM) from diesel engine exhaust, though they have a lower reduction efficiency than a typical, more expensive wall-flow diesel particulate filter (DPF). A FTF system usually consists of an upstream diesel oxidation catalyst (DOC) and a downstream FTF. The DOC has two main functions: 1) oxidize nitric oxide (NO) to nitrogen dioxide (NO_2), and 2) reduce the soluble organic fraction (SOF) of the PM. In addition, the DOC can also effectively reduce carbon monoxide (CO) and hydrocarbons (HC) emitted by the diesel engine. In the downstream FTF, the solid portion of the PM, represented as elemental carbon (EC), is oxidized by NO_2. Therefore, the FTF system can reduce both SOF and EC. It was the intent of this project to benchmark the PM and particle number (PN) reduction efficiency, and the potential for soot blow-off, of a FTF system in order to determine FTF viability for various emissions regulations.

Approach — A supplier-provided FTF system was instrumented for temperature and pressure measurements. Reduction efficiencies of NO, particulate mass, and PN were then measured over the World-Harmonized Steady-State Cycle (WHSC). Using this data, soot loading and blow-off cycles were developed from the WHSC operating modes. After triplicates of each pertinent emission species were sampled, the FTF was then loaded to approximately 3.0 and 5.0 g/L, respectively. A blow-off cycle was then performed each time to measure PM and PN efficiencies in this worst-case scenario.



PM vs. PN reduction efficiency.

Accomplishments — PM and PN reduction efficiencies over the WHSC were approximately 85.0 and 62.0 percent, respectively. The tailpipe PN emission over the WHSC cycle was estimated to be 3.76×10^{13} #/kW-hr. This result does not meet the EURO 5+/6 regulations of 6×10^{11} #/kW-hr. In addition, when the FTF was loaded with soot, maximum instantaneous PN emission during a harsh acceleration event was

approximately 25 percent higher than the highest portion of the WHSC cycle on a clean FTF. The results indicate that as the FTF is loaded with soot, PN emissions increase. This behavior is the opposite of a properly functioning wall-flow DPF whose PM/PN emissions decrease with soot loading. Steps will have to be taken in-cylinder to lower engine-out PM/PN rates before a FTF can be a viable solution for sufficient PM/PN reduction to meet upcoming emission regulations.

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2012 IR&D Annual Report

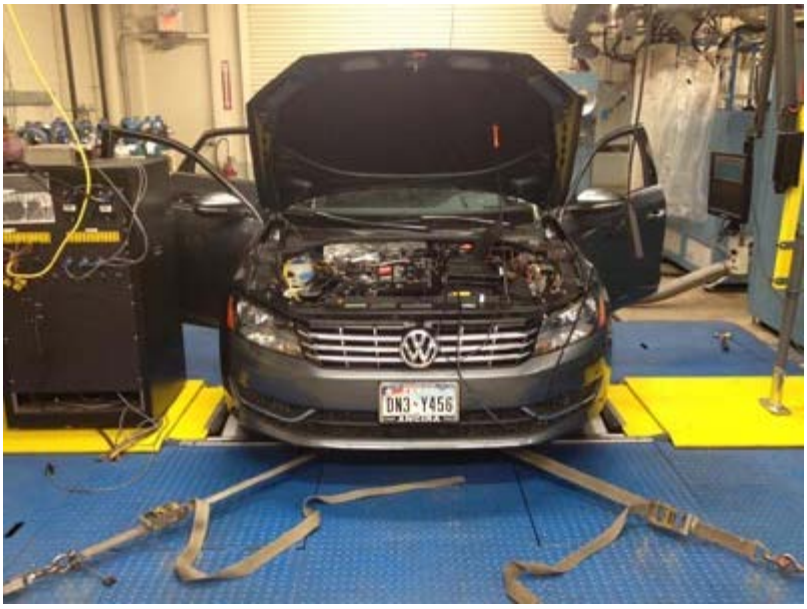
Severe Downsizing of a Three-Way Lean NO_x Trap (3wLNT) Diesel Engine, 03-R8293

Principal Investigators
Ryan Roecker
Sankar Rengarajan

Inclusive Dates: 05/01/12 – Current

Background — Increased cost is driving the diesel engine out of the compact/small car market. SwRI's concept of a three-way lean NO_x trap (3wLNT) diesel engine is a low-cost solution for light-duty diesel OEMs to meet emissions regulations without the need for exhaust gas recirculation (EGR) or an expensive SCR system. The after-treatment is essentially a three-way catalyst with a NO_x adsorbing coating. The 3wLNT is a truly cost-effective solution.

Approach — The 3wLNT engine runs lean at light-to-mid load conditions and stoichiometric at mid-to-high loads. At lean light-load operation, the after-treatment is used as a lean NO_x trap. At high loads, the after-treatment is used as a three-way catalyst by stoichiometric operation. While the concept is certainly cost-effective from a hardware point of view, there are technical challenges in the form of soot production and fuel economy. While it is accurate that stoichiometric engines without significant dilution from EGR have higher fuel consumption on a BMEP to BMEP basis, the stoichiometric diesel concept lends itself to significant downsizing potential, which may overcome this deficiency. The down-sizing potential is greater than spark-ignited engines because a stoichiometric diesel engine does not suffer from engine-damaging knock or pre-ignition. The downsizing potential is greater than standard diesel also because there is no need for EGR and excess air. Therefore the 3wLNT concept engine is expected to have lower peak cylinder pressures, allowing for higher BMEP levels to be achieved and less demanding turbo-charging requirements.



Testing FTP 75 cycle on chassis dyno with lean-stoichiometric switching.

Accomplishments — This project is on-going and currently in Phase II. The accomplishments to date are as follows:

1. Set up a valuable platform that is complete in terms of hardware and software.
2. Operated a diesel engine at stoichiometric conditions and quantified fuel penalty compared to lean burn operation at steady state.
3. Explored downsizing potential at engine loads and speeds for a typical light-duty drive cycle

(NEDC).
4. Tested the vehicle on the chassis dyno with increased inertia simulating a downsized engine.

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2012 IR&D Annual Report

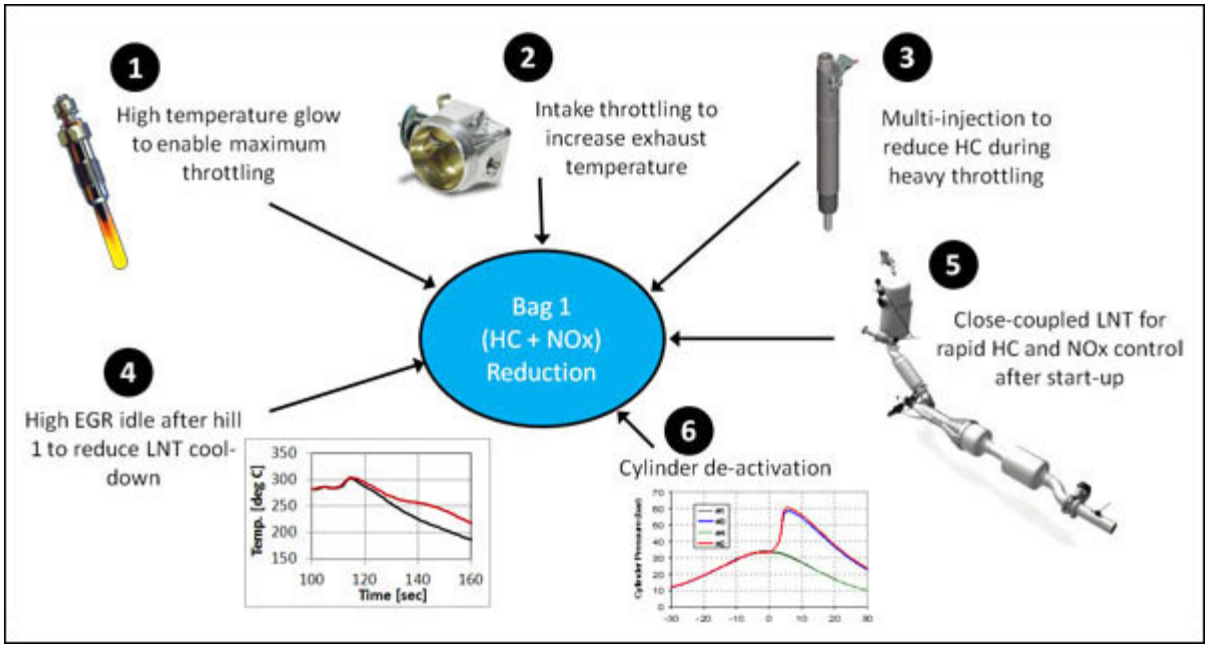
Diesel Cold Start Emission Control Research for 2015-2025 LEV III Emissions, 03-R8299

Principal Investigators
Gary D. Neely
Jayant Sarlashkar
Darius Mehta

Inclusive Dates: 04/01/12 – Current

Background — The diesel engine can be an effective solution to help vehicle manufacturers meet the impending 2017-2025 U.S. EPA and National Highway Traffic Safety Administration greenhouse gas and fuel economy standards, especially for larger segment vehicles. However, meeting the very stringent 2025 LEV III emissions standards poses a significant challenge for the diesel due to the difficulty in obtaining rapid emissions control with aftertreatment following a cold-start.

Approach — The goal of this project is to develop and evaluate a novel diesel cold-start emissions control strategy. The strategy combines several engine tuning and aftertreatment technologies to simultaneously reduce NO_x and hydrocarbons (HC) during the first hill of the FTP75. An illustration of the various technologies under investigation is shown below.



Engine tuning and aftertreatment technologies for cold-start emissions control strategy.

Accomplishments —

- Moderate intake throttling can be used to increase exhaust gas temperature without increasing HC emissions. Test data obtained at 1,200 rpm and 1.7 bar BMEP demonstrated a 50°C increase in turbine-out temperature for only a 5-percent increase in engine-out HC emissions.
- High-temperature glow plugs with improved temperature control can provide significant HC

reductions. Engine-out HC emissions were reduced by more than 50 percent from the stock glow plugs during both steady-state and transient tests with glow plug temperatures at or above 1,200°C.

- Proper tuning of the multiple injection parameters can result in an improved trade-off between exhaust gas temperature and engine-out HC emissions.
- The use of high EGR idle during the idle period between the first and second hills of the FTP75 was shown to result in a 30°C higher close-coupled catalyst temperature with a negligible HC emission increase after the DPF.
- A low HC calibration map was made that combined the above engine tuning technologies, which resulted in an additional 20 percent reduction in HC emissions and a higher closed-coupled catalyst temperature history. However, the new calibration map has higher NO_x, so future testing with a close-coupled LNT must be conducted to determine the acceptable level of engine-out NO_x.

2012 IR&D Annual Report

D-EGR™ WGS Catalyst Development and Optimization, 03-R8326

Principal Investigators
Gordon J. Bartley
Terrence Alger
Jess Gingrich
Raphael Gukelberger

Inclusive Dates: 07/01/12 – 07/01/13

Background — SwRI has been actively developing its Dedicated Exhaust Gas Recirculation™ (D-EGR™) concept and system within the HEDGE II Consortium. A key to successful application is the amount of hydrogen (H_2) that can be efficiently produced and fed back into the intake mixture. Rich operation of the D-EGR cylinder produces a significant amount of H_2, but more would be beneficial. The D-EGR cylinder exhaust also contains substantial amounts of carbon monoxide (CO) and water (H_2O). A water gas shift (WGS) catalyst can react CO with H_2O to form H_2 and carbon dioxide (CO_2), but no WGS catalyst has ever been developed for this application or environment. Catalysts that SwRI has used to evaluate the concept have been traditional three-way (TWC) exhaust formulations that have achieved about 45 percent H_2 production efficiency with minimal durability. If this efficiency can be increased to 70 percent and durability improved, an additional 2 to 3 percent brake thermal efficiency (BTE) is possible, a very significant technological advance.

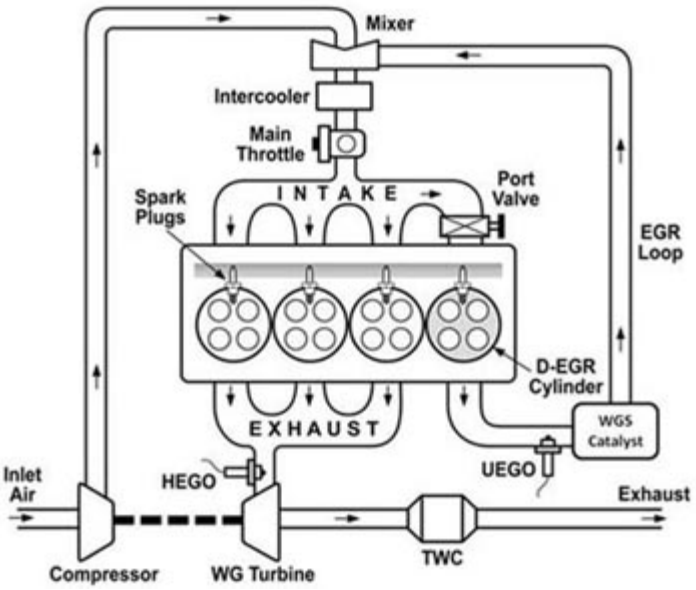


Figure 1: D-EGR Engine Overview Showing WGS Catalyst

Figure 2: SwRI's Universal Synthetic Gas Reactor®

Approach — Three different catalysts received from catalyst companies were evaluated on the D-EGR engine. The one that provided the best performance became the reference formulation for this work. The catalyst was analyzed to obtain the overall elemental composition of the catalyst washcoat. Starting with this reference formulation, a matrix of 45 varying formulations was prepared on core samples for testing. SwRI's Universal Synthetic Gas Reactor® (USGR®) is being used to perform the testing. Each catalyst's WGS activity is being evaluated over a fixed

set of test conditions. Sensitivities to individual independent and dependent variables are being used in a statistical approach to identify the direction of optimum formulation for WGS reactivity in the anticipated temperature regions. The optimum operating conditions for that formulation will also be extracted from the data.

Accomplishments — All of the matrix catalyst samples were prepared and received for testing. The initial performance testing is under way and partially complete. Already it is clear that rhodium is an important component for both activity and durability. On the other hand, palladium does not appear to benefit the WGS reaction, and actually caused coking, which fouls the catalyst and reduces the activity. The rhodium seems to reduce coking. Increased high surface area alumina appears to increase activity, and the other components appear to have minimal benefits or no effects on overall performance. It appears probable that an improved formulation will be determined that has both higher intrinsic activity and significantly improved durability.

2012 IR&D Annual Report

Design and Analysis of High-Torque, Hydraulic Wind-up Mechanism for Four-Square Gearbox Test Stand, 08-R8266

Principal Investigator
Rebecca L. Winer

Inclusive Dates: 11/02/11 – 03/02/12

Background — Testing of extremely high horsepower gearboxes rated up to 40,000 hp with output speeds as low as 118 rpm generates torques up to 4,000,000 ft-lb. Such values are representative of applications relating to submarine propellers, wind turbines and helicopter blades and have long posed significant technical, financial and infrastructure challenges to manufacturers. Four-square-type testing of high horsepower gearboxes uses two identical parallel gearboxes in a back-to-front configuration that connects the inputs and outputs of the gearboxes. In this system, the electric motor is sized to overcome the parasitic losses and desired acceleration rate in the gearboxes. Typically, these losses are only 10 percent of the total circulating power in the system, thus eliminating the need for a motor sized to provide 100 percent of the total power requirement. The function of the electric motor is predominately responsible for controlling the speed at which the system operates. To supply the torque requirement of the system, a torque-inducing mechanism is installed within the system in one of the shafts used to connect the two gearboxes. This mechanism induces the torque required for testing by twisting one part of the system's shaft relative to the other. These mechanisms are currently available for low horsepower and low speed applications, but are not available for high torque or higher speed applications. SwRI was asked to submit a proposal to fabricate a four-square test stand to test an 11,000 hp gearbox used on the U.S. Navy's next-generation hovercraft. To date, no torque-inducing mechanisms have been designed for an application at the torques and speeds required for this application. Smaller torque-inducing mechanisms have not been able to be scaled up in size because of the sealing problems associated with larger components.

Approach — In this project, a design for a 39,000 ft-lb torque-inducing mechanism that can operate at speeds up to 1,800 rpm was developed. The technical challenges associated with a hydraulic windup mechanism capable of meeting these requirements are:

- Maintaining a compact size to prevent rotational imbalances
- High-pressure hydraulic sealing on multiple rotating surfaces
- High-pressure hydraulic sealing from a stationary surface to a rotating surface on a large diameter shaft

Hydraulic rotary actuators use vanes attached to one shaft and opposing vanes attached to a second shaft. Hydraulic fluid is pumped between the two vanes, causing one shaft vane to rotate relative to the second vane, which induces

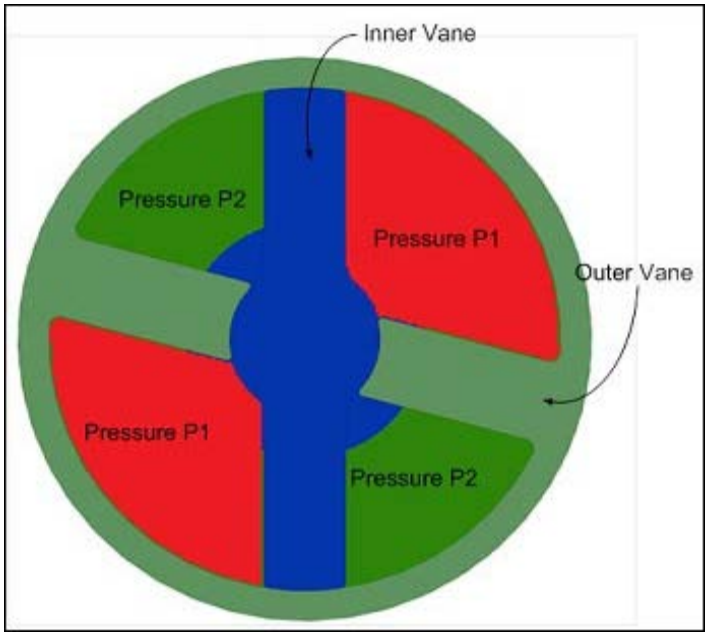


Figure 1: Cross section of the mechanism showed with

torque between the two shafts. The magnitude of the torque will vary based upon the pressure of the fluid. Both the center vane and the housing will rotate at the same speed. The shafts connected to both the inner vane and the housing vane will be supported by two double taper roller-type bearings. The inner vane and housing vane will sit inside an outer housing. The outer housing will remain stationary and provide a means for the hydraulic fluid to be routed through the device. Two specialty rotary unions are used to route pressurized hydraulic fluid to each of the four chambers via ports in the vanes. These allow for sealing of 3,600 psi fluid and can rotate up to 4,000 rpm.

relative movement between the two shafts. Here, torque is being applied in the clockwise direction because P1>P2.

Accomplishments — The results of this project allowed for the development and demonstration of the technical aspects associated with building high-horsepower wind-up mechanisms, as well as generating costs to fabricate the system. The original project this mechanism was designed for has been delayed by congressional funding mandates, but the information developed during this study has been used for other proposal efforts to clients with similar needs.

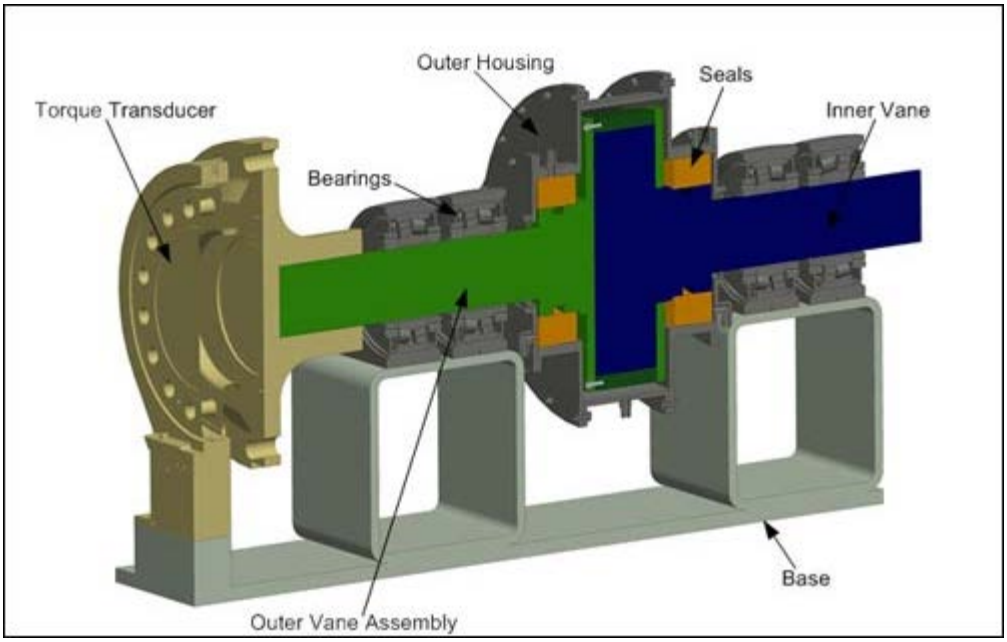


Figure 2: Overall assembly of the mechanism showing the location of seals, housings, bearings, and torque transducer all mounted on a common base structure.

2012 IR&D Annual Report

Elucidating the Effects of Lubricant Viscosity, Oxidation and Soot Loading on Total and Component Engine Friction, 08-R8300

Principal Investigator
Peter M. Lee

Inclusive Dates: 04/01/12 – Current

Background — Governmental legislation has increased pressure on vehicle manufacturers to reduce exhaust NO_x emissions. One way in which this has been achieved in diesel, and now gasoline engines, is the inclusion of exhaust gas recirculation. This technology results in increased soot levels in the lubricant, adversely affecting wear rates and frictional properties of the lubricant. Vehicle manufacturers are also increasing engine loads in an attempt to improve fuel economy resulting in higher operating temperatures, increasing thermal oxidation of the lubricants. In addition, there is a trend towards reduced lubricant viscosities, causing thinner operating films, resulting in increased component contact, which, in turn, results in higher wear rates. There becomes a point where the friction created by component contact outweighs the advantages of lower viscosity lubricants. At this time this is not fully appreciated and is little understood due to the complexities of measuring engine component friction on bench top rigs. Only measuring the friction of engine components running in an engine will allow direct comparison between results.

Approach — A single cylinder research engine will have all ancillaries removed, ensuring all friction experienced by the engine is caused by engine components only. The engine will be instrumented so total engine friction can be measured. The valvetrain will have the cam wheels instrumented to measure instantaneous friction, and the connecting rod will be instrumented to measure piston assembly friction. Bearing friction will be calculated by subtracting piston assembly and valvetrain friction from total engine friction. This will give friction for each engine component. Once operational, different soot-loaded lubricants, oxidated lubricants and viscosity lubricants will be run in the engine to measure component friction to elucidate their effects. The objectives of this project are:

- Elucidate the effect of reduced lubricant viscosity, lubricant oxidation and lubricant soot loading on engine component friction (valvetrain, bearing and piston assembly)
- Validate the results for lubricant viscosity against industry standard tests for fuel economy
- Elucidate the effect of engine load on engine component friction
- Install piston assembly friction on a Cummins ISX in the SwRI clean diesel program
- Generate unique knowledge for SwRI, giving employees more authority when talking with clients
- Create a new and unique capability at SwRI

Accomplishments — The engine, dynamometer and engine control system has been assembled in the test cell and is operational. Four different viscosity lubricants have been supplied and run in the sequence IVD fuel economy test and results reported. Special instrumentation for the engine has been designed and is currently being manufactured. The remaining months of the project will see the specific instrumentation installed on the engine, lubricants run through a special oil sooting engine for testing in the research engine and the different viscosity lubricants run through the research engine.

2012 IR&D Annual Report

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

Principal Investigators
Debashis Basu
Kaushik Das
Steve Green
Ron Janetzke
John Stamatakos

Inclusive Dates: 10/01/11 – 03/01/12

Background — Landslides and debris flows represent severe natural disasters and are a source of societal hazard 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 landslide hazards. A similar class of natural geotechnical hazards is the liquefaction of loose, saturated, cohesionless soils and other granular materials during large-magnitude earthquakes. Lateral spreading induced by seismic liquefaction causes large ground displacement and shear strains that can cause extensive damage and disruption to pile foundations of buildings and bridges, embankments, river dikes, pipelines, and waterfront structures. Most of the 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 project is to establish a generic SPH-based computational framework capable of solving problems in geomechanics that involve both small and large deformations.

Approach — This project developed a SPH-based computational framework for predicting the size, shape, and runout length of debris flows, landslide flows, and liquefaction-induced lateral ground displacement. The simulations were carried out using an adaptation of a SPH 2-Dimensional (2–D) code. The computational effort was also supported by limited experiments related to the rheology of the debris material and flow of landslide debris material along an inclined plane. The experimental test setup consists mainly of a ramp with an adjustable angle. A sample of clay slurry mud is placed in the reservoir at the top of the ramp and released. The motion of the mud down the ramp is recorded digitally through clear acrylic sidewalls. Simulated results were compared with the experimental results. A detailed analysis on the various non-Newtonian rheology models was also carried out as part of the project. These experimental investigations coupled with simulations from the SPH-based computational tool emphasized the importance of landslide and debris flow geometry, viscosity of the material and treatment of non-Newtonian viscosity. The project established a generic SPH-based computational framework capable of solving problems in geomechanics that involve both small and large deformations.

Accomplishments — One peer-reviewed conference paper and one conference presentation resulted from the project. These conference papers described the different aspects of landslides and debris flow

modeling as well as the treatment of non-Newtonian viscosity in liquefaction-induced lateral spreading analysis. An existing SPH 2–D code (SPHYSICS) was modified and further developed for implementation of non-Newtonian viscosity rheological formulae. A code for generating complex geometry for the SPH model was developed. These tools are also expected to be useful in work involving deformable geometries and coastal hydraulics analysis. Project staff used results from this completed project to prepare a National Science Foundation proposal on hybrid analysis with the SPH framework for geomaterials and SPH framework for quasi incompressible/ incompressible water flow. The SPH technique was found to be a very effective tool for modeling the spreading of liquefied soil.

2012 IR&D Annual Report

Antarctic Sea Ice Thickness from Satellite Remote Sensing and In Situ Measurements, 20-R8181

Principal Investigators
Michael Lewis
Marius Necsoiu
Jorge Parra

Inclusive Dates: 10/01/10 – 9/07/12

Background — The cryosphere is intricately linked to the global climate system and the Earth's surface energy budget. Sea ice cover is a primary component of the polar oceans and is important to the global climate system due to its prominent role in the 'ice-albedo' feedback mechanism and other factors such as heat, gas, and momentum exchange between the ocean and atmosphere and buoyancy of ocean currents. Despite increased research focus in recent years, the Antarctic sea ice zone remains one of the least-known regions of the Earth's surface due to remote location, limited extent and infrequency of direct measurements, and difficulties in validation of remote sensing products.

This project involved direct collaboration with the British Antarctic Survey (BAS) 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 improve satellite remote sensing products, allowing for improved long-term monitoring of the ice mass balance in the Antarctic sea ice zone.

Approach — The project had two tasks:

1. participation in IceBell cruise aboard the JCR to obtain detailed snow and ice measurements that are coincident with airborne and satellite remote sensing measurements, and
2. analyses of field campaign 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 Synthetic Aperture Radar (SAR) returns.

The project 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 ship schedule precluded the overlap of IceBridge flights.

Physical and geophysical measurements were obtained on sea ice floes in the Weddell and Bellingshausen seas. Installing ice mass-balance buoys (IMBs) allowed tracking of sea ice floes for months following the cruise. The acquisition of TerraSAR-X radar, Envisat radar and AMSR-E passive microwave satellite data was coincident in time and location with IMBs. A methodology was developed to analyze radar decomposition products and correlate with surface elevation, snow depth, and freeboard to allow discrimination of the (positive or negative) freeboard condition. The freeboard condition was applied to an empirical model of sea-ice thickness developed for the Bellingshausen Sea resulting in a new method that aligns closely with actual ice thickness data on the studied ice floe.

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 a Shannon Entropy product for the sea-ice floes that was subsequently 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 Shannon Entropy.
- Built successful relationships with a significant group of external collaborators who contributed to various aspects of the project. Specifically, this project has resulted in establishing/strengthening several very important international collaborations with investigators from BAS, Scottish Association of Marine Science (SAMS), German Aerospace Agency (DLR), Woods Hole Oceanographic Institute (WHOI), The University of Texas at San Antonio (UTSA), University of Manitoba (UM) and others and has resulted in several publications and proposals.
- 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.

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2012 IR&D Annual Report

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

Principal Investigators
Todd Mintz
Debashis Basu
Kaushik Das
Marla Roberts
Michael Muller
Tim Michaels

Inclusive Dates: 10/01/11 – 03/01/12

Background — The interaction of Earth's atmosphere with its geosphere through the planetary boundary layer (PBL) (i.e., land/inland water and ocean) via exchanges of energy and mass is a major driver of atmospheric phenomena and thus climate. Interaction between the ocean and the atmosphere, particularly the exchange of mass (moisture), momentum, and energy (heat) between the atmosphere and the ocean, controls atmospheric phenomena such as cyclones and hurricanes. Proper understanding of the coupling between the atmosphere and ocean is essential for accurately predicting hurricane wind intensity, trajectory, and likely landfall. As air flows over the ocean, wind stress generates surface gravity waves and drives local ocean currents and large-scale circulation. Analysis of smaller ocean mesoscale features suggests that the ocean mainly affects the atmosphere through heat exchange. Because of the importance of these two-way couplings, a fully coupled atmosphere-ocean model is necessary for accurate analysis of atmospheric phenomena.

Approach — A coupled atmosphere-ocean model has been developed using the Earth System Modeling Framework (ESMF), a general purpose software that facilitates coupling earth system modeling codes such as WRF (Weather Research and Forecasting) and HYCOM (HYbrid Coordinate Ocean Model). This coupled atmosphere-ocean model is created using the weather prediction model, Weather Research and Forecasting-CHEM (WRF-CHEM) and HYCOM. The coupled model is a flexible and efficient software framework designed to facilitate developing multicomponent Earth science modeling applications. Coupling is based on conservation of mass, momentum, and energy at the air-sea interface. The sea surface temperature (SST) is computed in the HYCOM model and passed to WRF-CHEM. SST is the primary controlling parameter that is passed from HYCOM to WRF-CHEM.

Figure 1: Actual track for hurricane Rita

Accomplishments — A computational framework was established to carry out simulations of ocean and atmosphere dynamics. The computational framework can be used in subsequent projects to develop an atmosphere-ocean-wave model by including wave simulation software. The model also can be extended to investigate the effects of atmosphere dynamics on aerosol generation, aerosol transport, and cloud formation. Simulation of Hurricane Rita, demonstrated the importance of coupling the atmospheric and ocean model for intensity forecasts of hurricanes. The project also developed the ESMF-based computational platform necessary for simulating atmospheric dynamics and processes. The predicted intensity of Hurricane Rita was compared with the observed data. Simulations suggest that the storm intensity changes as a direct consequence of variations in the heat flux across the ocean-atmosphere interface. This showed that the coupling between WRF-CHEM and HYCOM correctly predicted the physics of the hurricane. Significant experience was gained using atmospheric modeling tools developed by the National Oceanic and Atmospheric Administration (NOAA), as well as with the ESMF computing platform and several NOAA-developed post-processing codes. This experience positions the staff to secure external projects from federal agencies, such as NOAA, National Science Foundation, and National Aeronautics and Space Administration. Two journal papers are being prepared for publication in the near future.

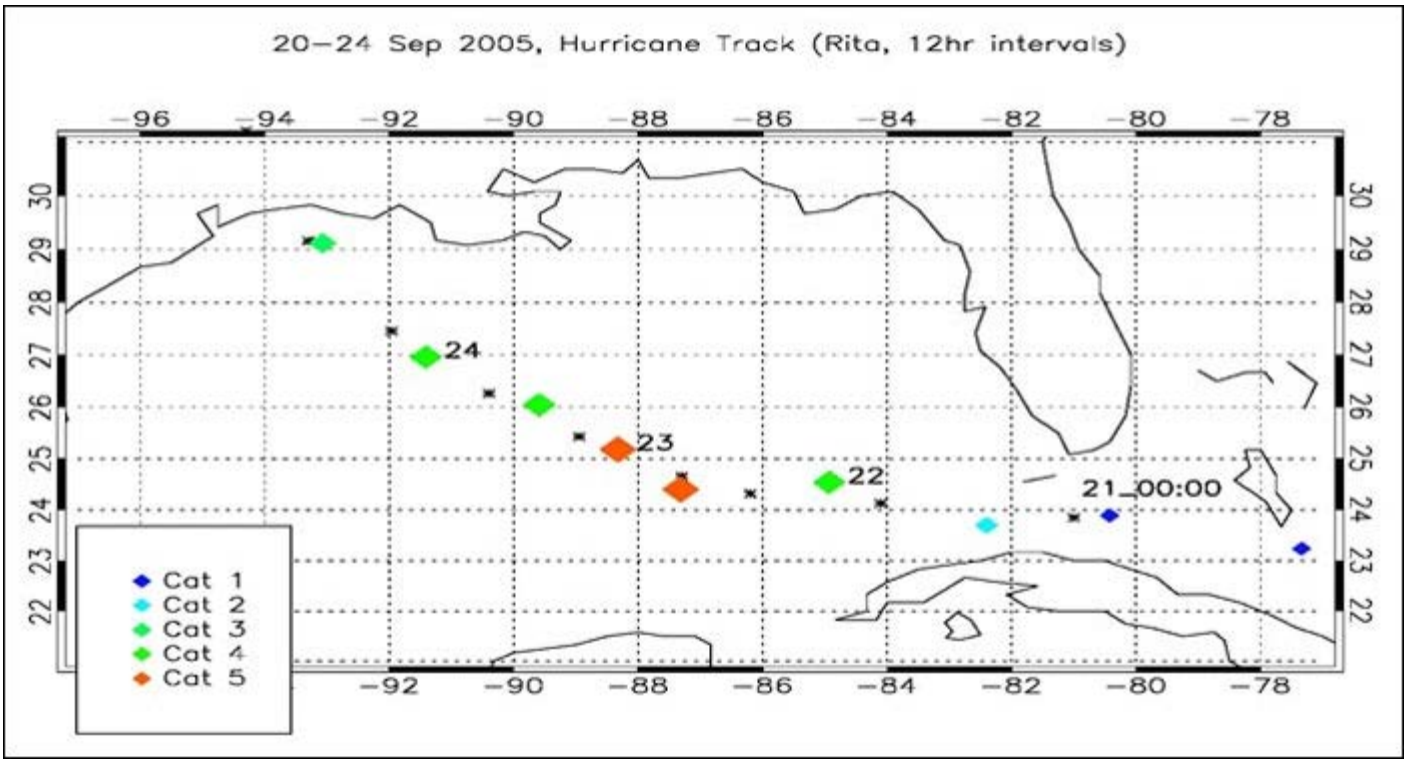

Figure 2: Predicted track for hurricane Rita

2012 IR&D Annual Report

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

Principal Investigators
Ronald Green
F. Paul Bertetti
Ronald McGinnis
Hakan Basagaoglu

Inclusive Dates: 04/01/11 – 09/01/12

Background — Increased demand for groundwater has elevated the need to better understand the hydraulics and sustainable yield of aquifers, a major source of water. 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 responses to recharge events due to 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. The objective of this project is to investigate the hydraulics of epikarst layers to understand the mechanisms of recharge and groundwater storage in regional-scale karst aquifers and to develop a 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 if not misleading. 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 (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.

Approach — The objectives of this project were to investigate the hydraulics of epikarst, to understand the mechanisms of recharge and groundwater storage in regional-scale karst aquifers, and to develop a universal model for the hydraulics of epikarst. To achieve these objectives, the following tasks were undertaken:

1. identify potential recharge zone for groundwater monitored at a representative index well and
2. quantify the delayed aquifer response and storage time of the epikarst.

Accomplishments — The project achieved its objectives of characterizing the hydraulic properties of epikarst to identify potential recharge zone for groundwater monitored at a representative index well, and to quantify the delayed aquifer response and storage time of the epikarst. A multi-variate regression model was constructed to analyze the statistical correlation between precipitation at Edwards Aquifer Authority rain gauges and changes in groundwater elevation at the Uvalde index well. The multi-variate regression model is essentially an impulse-response model, which relates changes in groundwater elevation to 15-day moving-averaged and lagged precipitation events. The statistical relationships were analyzed using daily precipitation, groundwater elevation, and river stage data.

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2012 IR&D Annual Report

Correlation between Natural Gamma Radiation and Mechanical Stratigraphy in the Cretaceous Eagle Ford/Boquillas Formation of South-Central and West Texas, 20-R8257

Principal Investigators
Alan P. Morris
Ronald N. McGinnis
Kevin J. Smart
David A. Ferrill
Mary Katherine Todt

Inclusive Dates: 10/01/11 – 01/01/12

Background — The Cretaceous Eagle Ford/Boquillas (EFB) Formation in south-central and west Texas consists of interbedded shale and limestone layers, and is one of the largest unconventional hydrocarbon plays in the United States. The success of this play is dependent on the ability to "geo-steer" sub-horizontal well legs into and through sections of the formation that are both hydrocarbon rich and intrinsically able to support hydraulic fracturing. EFB lithologies have low intrinsic permeability, and effective production requires induced fractures. Hydraulic fractures induced during well completion must be appropriately developed and must remain open after completion. Strong (more brittle) rock layers such as limestone are generally easier to hydraulically fracture, and these fractures tend to remain open; however, strong layers may have lower hydrocarbon content than weaker shale layers. Weaker (less brittle) rock layers are generally more difficult to fracture and induced fractures in such rocks often close following completion, rendering them useless in terms of production.

Geo-steering is most often accomplished by monitoring natural gamma radiation during drilling and comparing the results to a reference stratigraphic section. There is no existing direct correlation between gamma emissions and rock strength. Gamma emissions are generally high in rocks with high clay mineral content (shales) and low in rocks with little clay mineral content (limestones). Although it is generally recognized that shales are weaker than limestones, data to define a robust correlation between rock strength and gamma emissions are lacking. This data gap limits industry's ability to easily predict rock strength characteristics, needed for planning and executing hydraulic fracturing, from their navigational tool of choice (natural gamma radiation).

Approach — The objective of this project is to answer the question: What is the correlation between natural gamma radiation and rock strength in the EFB of south-central and west Texas? To answer this question, SwRI researchers established a mechanical stratigraphic section through an outcrop exposure of the EFB and matched it in detail with a natural gamma radiation profile through the same stratigraphic sequence. A hand-held radiation detector and a Schmidt Rebound Hammer were used on well-exposed sections of the EFB.

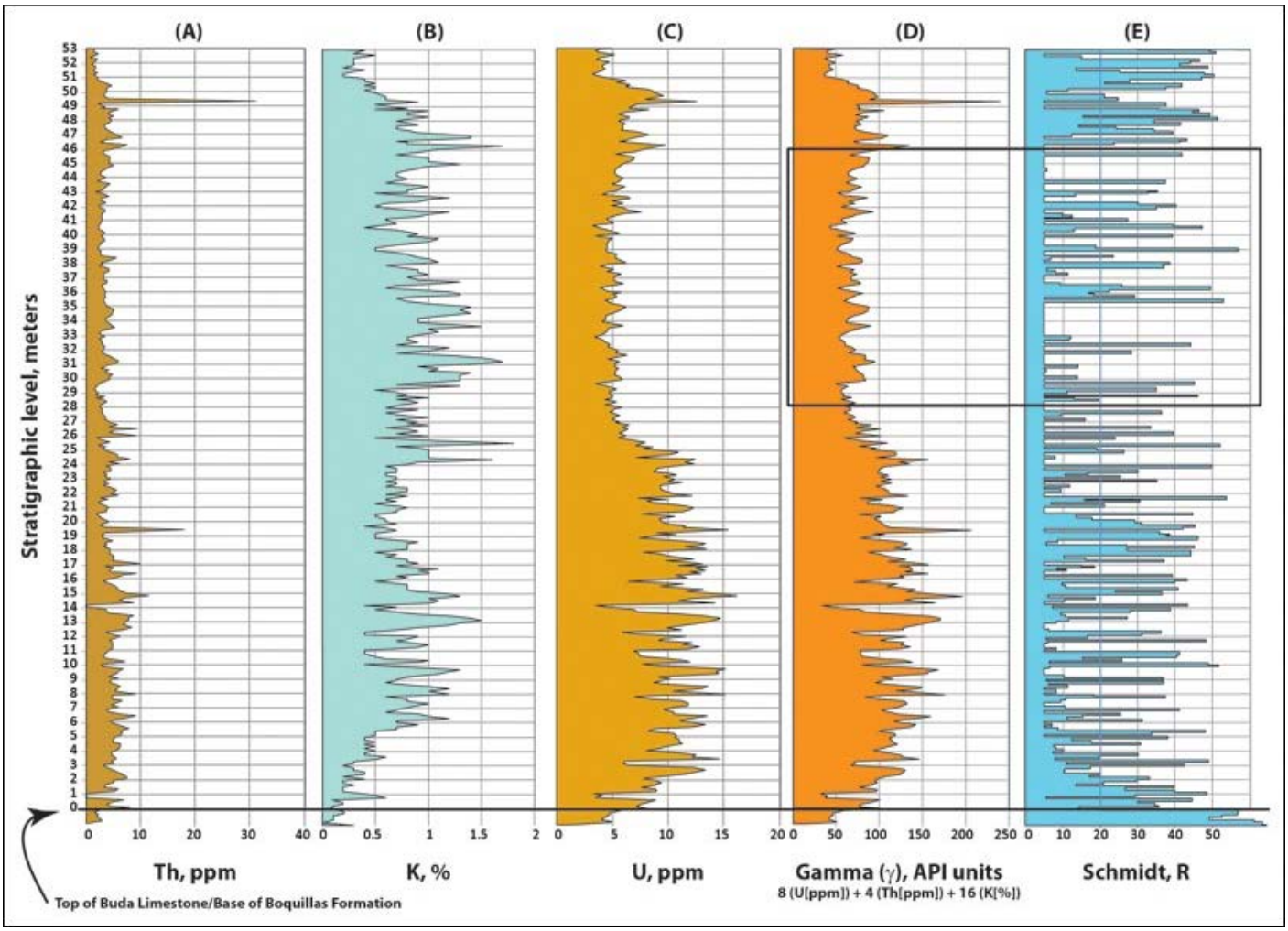

Figure 1. Spectral gamma logs for (A) thorium (Th), (B) potassium (K), and (C) uranium (U) plotted against stratigraphic position (in meters) in the Boquillas Formation with 0 m coincident with the top of the Buda Limestone. (D) Spectral gamma data has been combined to provide a log of API gamma units for direct comparison with typical hydrocarbon industry gamma logs. (E) Schmidt rebound (R) log for the same stratigraphic interval; blue line is at R = 20. Rectangle over (D) and (E) is the area illustrated in Figure 2.

Accomplishments — A correlation was established that can be used to predict rock strength from gamma log character. There is a broad, negative correlation between R and *y*. Low values of R correlate with high *y* values, and vice versa, as illustrated in the figures.

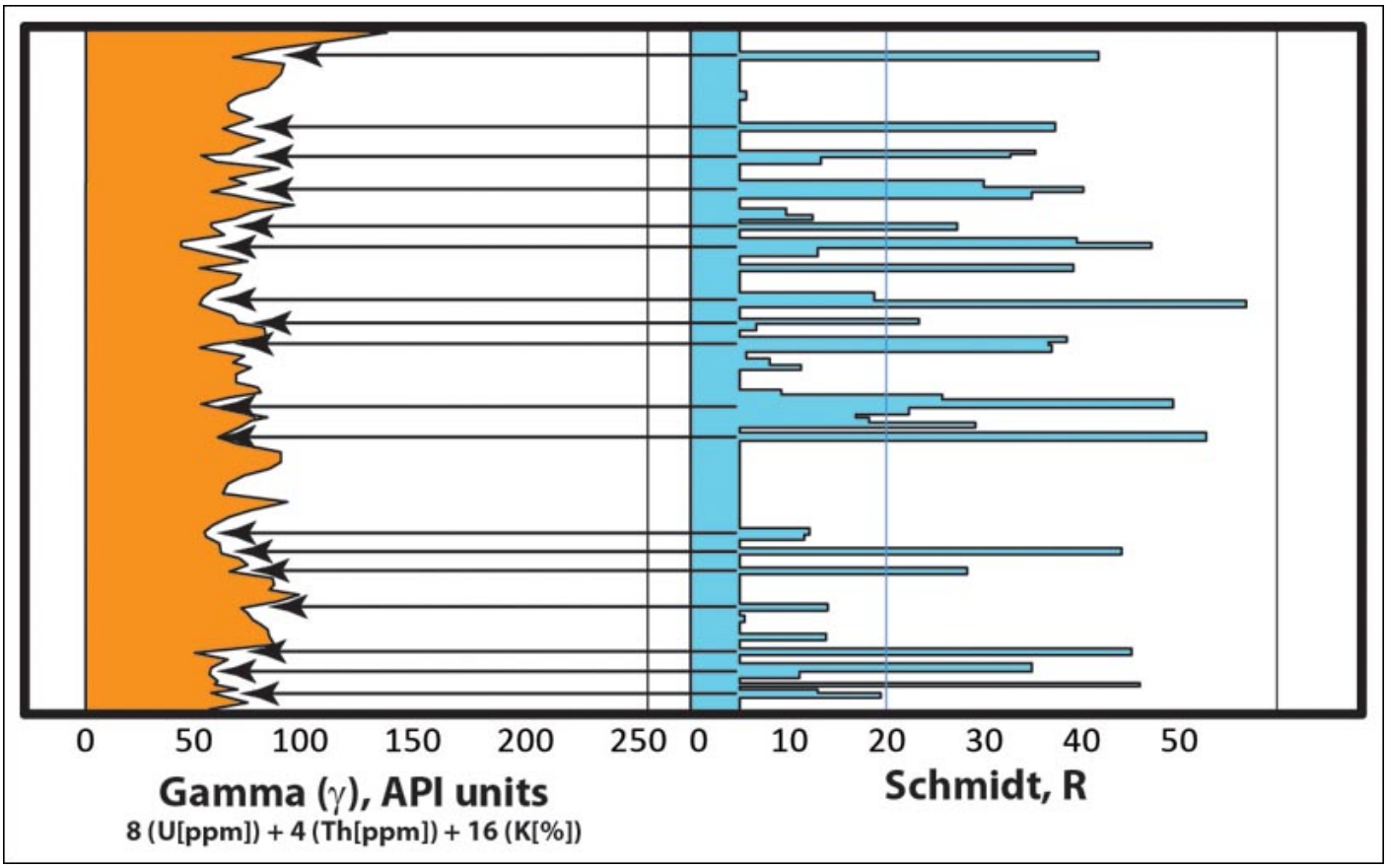

Figure 2. Detail of gamma log (API units) and Schmidt rebound log (see Figure 1 for location within the section) illustrating the near one-to-one relationship between R peaks and gamma troughs.

2012 IR&D Annual Report

Integrity Management of Nuclear Power Plant Components Subjected to Localized Corrosion Using Time-Dependent Probabilistic Model, 20-R8267

Principal Investigators
Pavan K. Shukla
Osvaldo Pensado
Jay Fisher
Gary Burkhardt

Inclusive Dates: 11/14/11 – Current

Background — The objective of this project is to develop an adaptive-predictive probabilistic model to forecast localized-corrosion-induced pit population and pit depth distributions. Nuclear power plant (NPP) operators are required to periodically inspect components by visual and volumetric examinations to maintain integrity and ensure safety. As nuclear power plants age, however, more frequent inspections are expected to ensure component integrity. A framework to define an inspection schedule based on risk considerations is needed to keep the cost of inspection constrained without compromising safety. SwRI is developing a model to forecast localized-corrosion-induced damage of NPP components based on damage measured at a given time. For example, if a component exhibits pitting corrosion in an environment, the model will be used to estimate the distribution of pit depths as a function of time and an initial state. The model is expected to account for previous inspection data, randomness of pit generation and propagation, and pit growth rate as a function of time. The model could be used to estimate probability of component failure due to pitting corrosion, and calibrate inspection schedules so that detection of corrosion-induced degradation occurs before failure.

Approach — Model development consists of the following tasks: statistical model, experiments, and data analysis and integration. Probabilities of transition between discrete states that satisfy Kolmogorov's forward equations for a pure birth process can be used to describe the evolution of depths of a population of pits. The discrete state of a pit is defined as a pit falling in a range of depths (e.g., a pit is in state 1 if its depth falls between 0 μm and 100 μm; it is in state 2 if the depth is between 100 μm and 200 μm; and so on). Thus, pit growth is conceptualized as a pit that transitions from a state to the next. Parameters to define the transition rate between states can be obtained by measuring the average pit depth as a function of time. Experiments are being conducted with coupons and tubes made of stainless steel 316. The coupons and tubes have been placed in a tub filled with synthetic sea water. Sea water is used in some NPPs as coolant in the open-cycle cooling water system. The tubes will be inspected using a eddy current technique for pit population and their depths. One-by-one, coupons will be removed from the tub at defined intervals. When a coupon is removed from the tub, it will be inspected using laser profilometry. The eddy current method will provide a coarse measurement of pit population and pit depth distribution in tubes, representative of results that would be achieved during in-service inspections of NPP components, whereas the laser profilometer will provide more accurate measurements. The data collected from coupons will be used to estimate pit depth versus time. Both coupon and tube data will be used to estimate statistical model parameters, such as transition rates, separately for coupons and tubes. The model will be used to forecast the next pit depth distribution. At the next inspection, the model will be updated with the collected data and the next forecast will be performed.

Accomplishments — A numerical solution for the system of Kolmogorov's forward equations for a pure

birth process was implemented, with non-homogeneous birth rate or transition rate to develop the model. Several dependencies for the transition rate were investigated to find a functional dependence that yields a growth rate for the average pith depth that is consistent with a time dependence empirically observed. The common growth law is of the form $d = \kappa(t + t_o)^{\nu}$, where d is a reference pith depth, t is the time, t_o is a reference time, and κ and ν are empirical constants. In the numerical solution, the empirical parameter ν is provided as an input to define state transition rates, and the parameter κ is used to map computer time to a physical time. Given an initial distribution of pit depths, the numerical solution can be used to forecast the distribution at a later time, preserving the relationship $d = \kappa(t + t_o)^{\nu}$, where d is interpreted as the average pit depth. The experimental work has been initiated, and the data from the experiments will be fed in the model to test the adaptive-predictive forecasting approach. Specifically, later stages of the project will be devoted to track pit population and their depth with time using the model, i.e., forecast the pit population and depth distribution, inspect experimental data and compare with the model forecast, and if necessary, update the model to make next forecast. This will be repeated till a satisfactory match is found between the model forecast and experimental data.

2012 IR&D Annual Report

Development of an Integrated Numerical Framework for Tsunami Hazard Assessment at Nuclear Installations, 20-R8268

Principal Investigators
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Kaushik Das
Ron Janetzke
John Stamatakos
Todd Mintz
Rob Sewell, Consultant

Inclusive Dates: 11/14/11 – 09/01/12

Background — Tsunamis are a series of long ocean waves generated by large-scale earthquakes or landslides that occur along active faults near continental margins or subduction zones. The primary aim of the ongoing work is to develop an integrated tsunami analysis method for risk assessment at nuclear installations. The analysis is primarily focused on earthquake-generated tsunamis. The developed method calculates parameters such as maximum wave runup height, impact velocity, and inundation area from an earthquake generated tsunami. The generation stage of tsunami evolution includes the formation of the initial disturbance of the ocean surface caused by earthquake-triggered deformation of the sea floor. Subsequently, this initial disturbance of the water surface evolves into a long gravity wave radiating from the earthquake source. Developing an integrated tsunami analysis method will include predicting the initial wave height that is linked to the earthquake source mechanisms.

Approach — This ongoing research has resulted in the development of an integrated computational methodology to simulate the generation, propagation, and impact of an earthquake-generated tsunami. Developing this integrated approach involved developing a tsunami source model that takes into account local geological and tectonic processes as well as observed seismic and geodetic (sea floor and land deformation) data. In addition, accurate and finely resolved bathymetric and topographic data were used to generate the far and near-field computational grids. After generating the grid, numerical simulations were carried out to model tsunami generation, propagation, and runup. Simulated results were compared to available field data and observations.

The tsunami waves were simulated using the fully nonlinear and dispersive Boussinesq wave model FUNWAVE-TVD. Appropriate methodology is being adopted based on existing literature to select the earthquake source to be used in the tsunami model. For the present work, three tsunamis will be studied and modeled. The first is the 2011 Tohoku-Oki tsunami that took place on March 11, 2011, from a magnitude 9.1 earthquake. Geophysical records of the earthquake and the resulting tsunami from seismometers, Global Positioning System receivers, tide gauges, ocean bottom pressure sensors and other instruments, as well as various other observations provide significant documentation of this tsunami.

Two tsunami cases are being studied for the United States, one for the east coast and another for the west coast. Bathymetric data were used to generate a topographic grid to simulate the wave propagation in the far field and near field. Both the tsunami far- and near-field coastal impacts will be analyzed. For the analysis of the near-field coastal impacts, the effect of the tsunami waves on the structures will be calculated, which will provide a more realistic estimate of damage from the wave and the impact of debris on the power plants and facilities. Finally, the proposed work will try to estimate structural damage (loss in dollars) caused by tsunami forces using the simulation results of tsunami inundation and geographic

information system analysis of post-tsunami survey data. This will lead to a new quantitative understanding of the relationship between local damage and tsunami hazards. Presently, tsunami hazards are assessed either by analyzing historic data or by using shallow water wave solvers. The overall analysis also will include comparisons of the predictions with the observations.

Accomplishments — Project staff members have so far obtained bathymetric data for the different sites, and have completed FUNWAVE-TVD simulations for the Diablo Canyon site. The problem domain was limited by the available bathymetry data (238.51 to 239.17 E longitude, 35.07 to 35.34 N latitude). The horizontal bathymetry resolution for this simulation was 100 meters. The simulations revealed that FUNWAVE-TVD is able to provide a realistic prediction of the wave propagation and the variation of the wave height for the Diablo Canyon site. Project staff members have also started simulations of the Diablo Canyon site using FLOW–3D. FLOW–3D is a Navier Stokes solver and is primarily being used for the near-shore region. One of the aims of this project is to compare FUNWAVE-TVD and FLOW–3D for simulations of near-shore hydrodynamics. Project staff members also evaluated different slip distribution inversions that provide the information to calculate the complex sea floor patterns associated with major earthquakes, which will be used as the initial condition for the tsunami models. Two abstracts were submitted to the 23rd International Ocean and Polar Engineering Conference (ISOPE–2013). Once the two abstracts are accepted, full-length papers will be prepared.

2012 IR&D Annual Report

Soil-Structure Interaction Assessment of New Modular Reactors, 20-R8270

Principal Investigators
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Kaushik Das
Larry Miller
Sui-Min Hsiung
Todd Mintz

Inclusive Dates: 11/14/11 – Current

Background — To meet the growing demand for inexpensive power, the nuclear industry is developing several new, advanced nuclear reactor designs with scalable modules. Each module will produce relatively small amounts of electricity compared to current nuclear power plants. To meet the power demand and infrastructure constraints, several modules of these reactors can be installed at a given site, as needed. Because the construction is relatively simple and small in size, the lead time to start power generation is shorter. Each of these new reactors consists of an integrated reactor module and a reactor containment vessel. These containment vessels are located below the ground surface and are either fully or partially submerged in water. In addition, these containment vessels are attached to the support structures via seismic damping systems. These new reactor designs pose a complex soil structure-fluid interaction problem from earthquake-induced ground motion. Understanding this soil structure-fluid interaction phenomenon is essential to designers and regulators to ensure adequacy of the seismic damping/isolation system for safe operation of the modular reactors during seismic events.

Approach — This project uses a simplified, sequentially coupled analysis methodology for assessing the response of a containment structure housing a small modular reactor during a seismic event using the geomechanical code FLAC and the computational fluid dynamics (CFD) package ANSYS-FLUENT. The FLAC code analyzes the amplification of the earthquake motion as it propagates upward through the geological medium and to the containment structure. The time-dependent forces or velocities at the containment structure wall boundary from the FLAC analysis are used as the perturbation to initiate fluid sloshing simulated in the ANSYS-FLUENT package. The force generated by the sloshing process from the ANSYS FLUENT will be recorded and can be used, in turn, as an internal boundary condition in the FLAC analysis at a later time step.

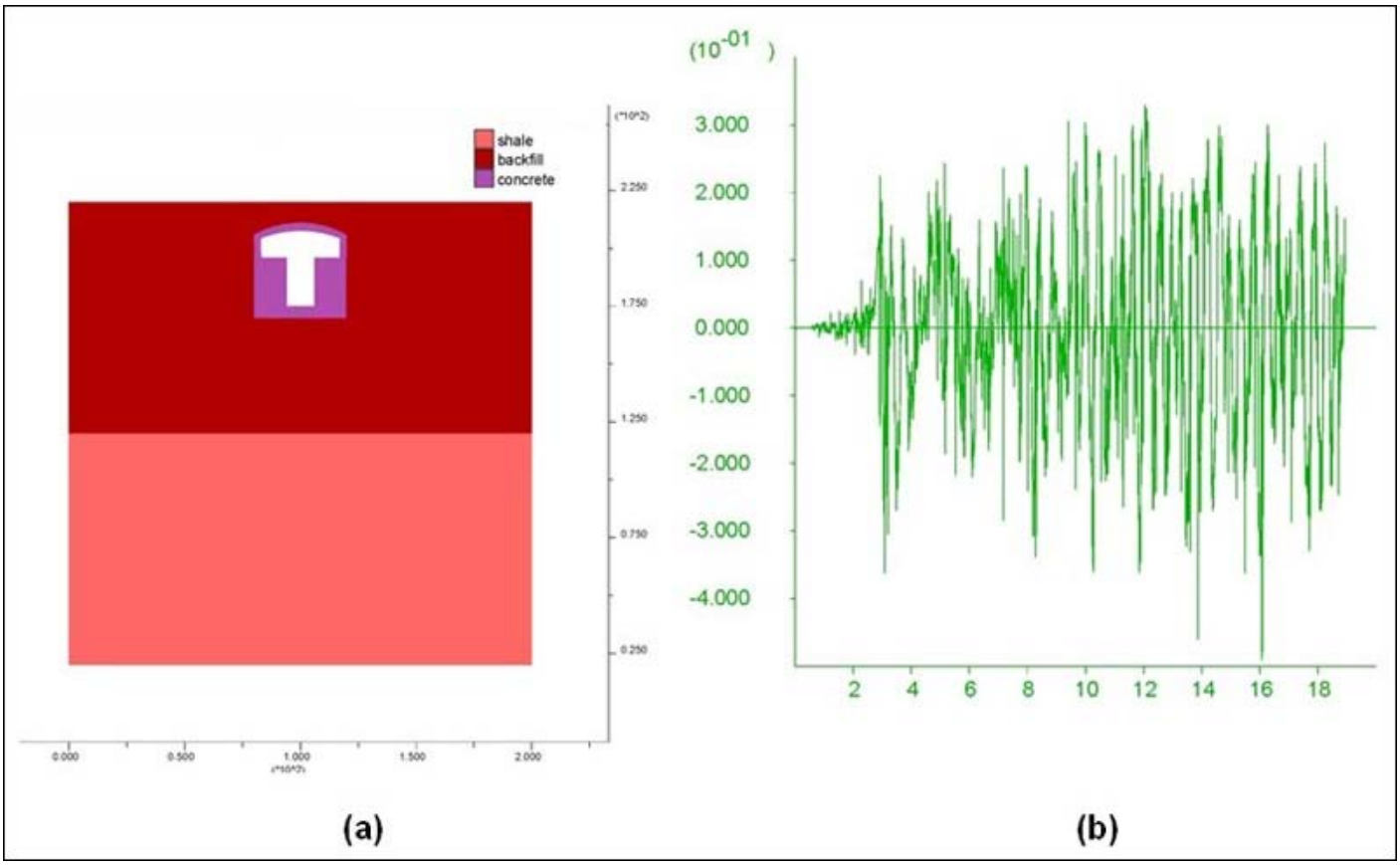

Figure 1. Soil-structure (modular reactor) interaction analysis under seismic load. Figure 1(a) shows the model dimension in meter. Ground acceleration (m/s^2) calculated at the base of the reactor is shown in Figure 1(b) as function of time (second).

Accomplishments — A site response analysis was conducted considering a hypothetical site to study the amplification of seismic waves while propagating from the bedrock to the ground surface and resulting soil-containment structure-fluid interaction with a modular reactor. Figure 1(a) shows the model used for soil-structure interaction analysis under seismic excitation. Ground acceleration at the base of the reactor from a strong-motion earthquake in California is shown in Figure 2(a). A simplified CFD model in two-dimensional space was developed to understand fluid sloshing in response to ground motion. As the wall viscous effect is expected to be negligible compared to the fluid sloshing impact, grid clustering was not done in the near-wall region. The water contained within the structure was set to have a sloshing motion in response to the applied acceleration signal. The sloshing motion continued after the input acceleration signal stopped. The vertical force on the reactor due to sloshing is shown in Figure 2(a) (negative sign because the forces are acting downwards). A representative water surface profile to highlight the sloshing motion in the reactor is shown in Figure 2(b). It shows the free water surface at an angle with the horizontal plane, indicating fluid motion and deformation due to external disturbance.

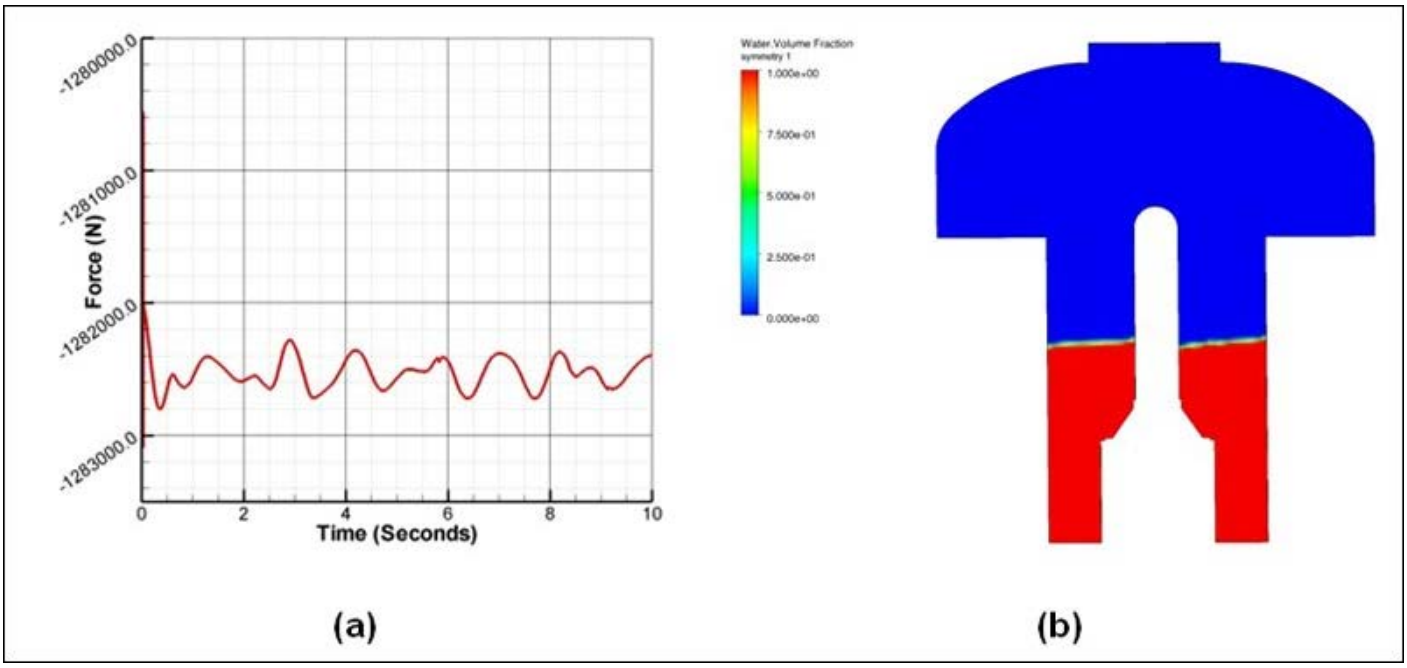

Figure 2. Computational fluid dynamics analysis for sloshing motion in a small modular reactor.

2012 IR&D Annual Report

Assessment of the Viability of Electronic Components in a High-Radiation Environment, 20-R8291

Principal Investigators
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Ben Abbott
Roland Benke
David White
Ryan Wilson
Jay Fisher
John Hageman
Keith Pickens
Glenn Light

Inclusive Dates: 02/01/12 – 05/01/12

Background — SwRI has developed a class of wireless sensor networks to sense, detect, and measure a wide range of environmental state variables and properties. Sensor networks have remotely measured and characterized underwater caves, conduits, and pipes. SwRI was asked to evaluate the potential of this sensor technology to assist in characterizing damage to the interior of the Fukushima Daiichi reactors. This sensor technology is of interest because of its ability to remotely map and characterize chambers and conduits not easily accessible using conventional technologies.

The reactor core and pressure vessels at Fukushima Daiichi incurred damage during the earthquake/tsunami disaster in March 2011. The full extent of that damage has not yet been adequately characterized. Characterization is difficult because of high radiation levels present at, and proximal to, the Fukushima reactors. The usefulness of sensors to characterize the interior of the Fukushima reactors is contingent on the sensors ability to remotely operate in a high-radiation environment. There is interest in modifying existing SwRI sensor technology to be applicable to this characterization activity.

Approach — Analysis and testing of the electronic components of the wireless sensors were undertaken to ascertain whether sensor technology used at SwRI can successfully operate in the high-radiation environment at the Fukushima reactors. Analyses were conducted to approximate the radiation dose anticipated for the interior of the reactor containment vessel and to estimate the expected performance of common electronic components to that level of radiation. Specific electronic components used in wireless networks developed at SwRI were then exposed to radiation consistent with levels estimated for the reactor containment vessels after nuclear criticality has ceased.

Accomplishments — Results from these tests indicate that existing electronic components used in wireless sensor networks will be viable for reasonable durations (i.e., about one hour or more) when deployed in high-radiation fields up to 25 krads/hr. With the exception of the camera, additional radiation hardening does not appear necessary for the candidate electronic components to remain operational and produce useable data in the high-radiation environments expected at the Fukushima Daiichi reactors.

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2012 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 wall of the pipe. Several experimental programs 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 (<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 testing 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

Figure 1. Iso-kinetic Sampling System for Measuring Liquid Entrainment at High Pressure.

Figure 2. High-Pressure Multiphase Flow Visualization Device.

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. The testing will be conducted at the MFF under various superficial gas velocities, liquid volume fractions, and various pressures. Methane gas and a hydrocarbon liquid will be used as the test fluids to simulate field-like conditions. The modeling on the 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 — The accomplishments to date are:

- 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.
- An iso-kinetic sampling system was designed and built for measuring the fraction of liquid entrained in the form of droplets in a high-pressure gas stream. The sampling system can be used at pressures up to 3,600 psig and in pipe sizes up to 6 inches in diameter. Figure 1 shows a picture of the liquid entrainment measurement device developed on this project.
- A high-pressure flow visualization device was designed and fabricated. This device allows visualizing the flow through a 3-inch pipe without introducing any perturbation on the flow and without affecting the flow pattern. A photograph of the flow visualization device is shown in Figure 2.
- A customized test section was designed and installed at the MFF for conducting high-pressure entrainment testing. The test section included the injection of the liquid phase into a gas phase stream, a 60-ft long flow development section to allow a fully-developed flow pattern, the liquid entrainment measurement section using the iso-kinetic sampling system (Figure 1), and the high-pressure flow visualization device (Figure 2).
- Testing at high pressure was conducted using hydrocarbon fluids at various gas and liquid rates and various pressures. The data collected during the experimental program are being compared against predictions obtained from existing models and correlations and will be used to validate an improved model for estimating the liquid entrainment in high-pressure systems.
- Modeling efforts have concentrated evaluating existing models and correlations found in the literature and incorporating the high-pressure effect on the entrainment prediction models.

2012 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 the increasing application of these bearings 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 utilize a gas, for example, 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.

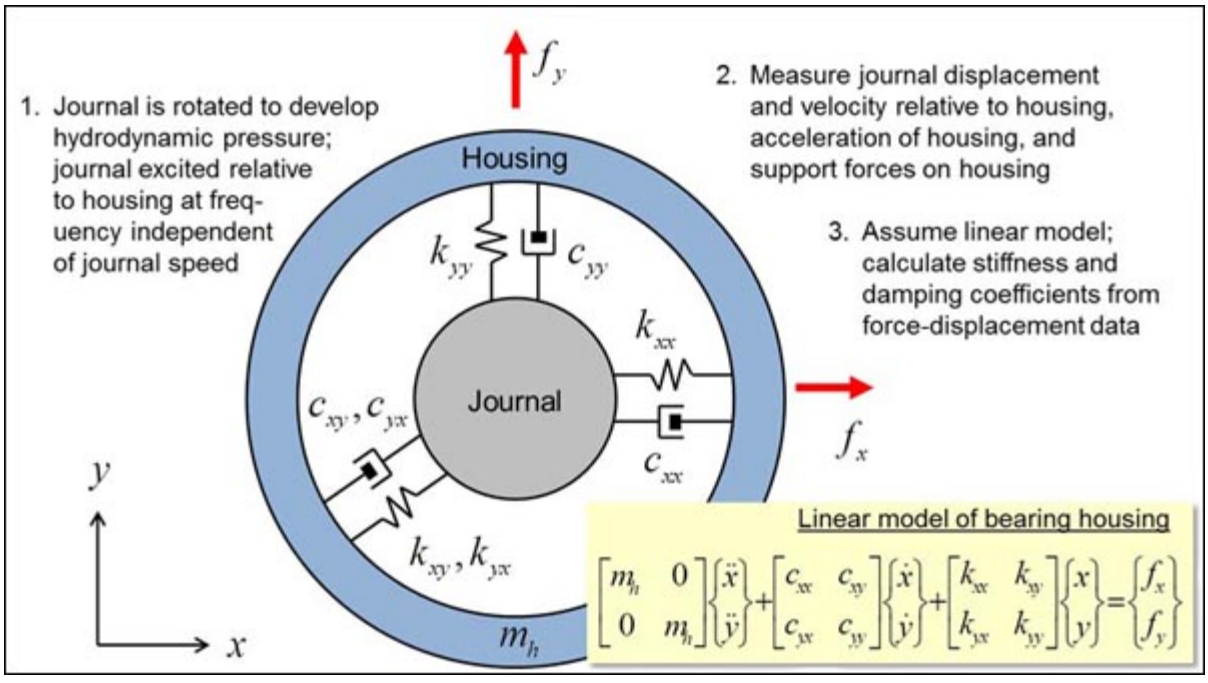

Figure 1. Model of a bearing using linearized stiffness and damping coefficients. Spring and damper elements represent dynamic behavior of lubricating film in series with mechanical structure of top foils

and undersprings.

Approach — The approach used for this project is both experimental and analytical. An experimental test rig is capable of measuring frequency-dependent stiffness and damping coefficients of foil gas bearings for journal speeds up to 60 krpm. A key component of the test rig is the ability to excite the journal in forward or backward whirl with the use of a bi-directional rotating inner shaft mechanism. A pressure chamber may permit testing of various gaseous working fluids from sub-atmospheric pressures up to 635 psig. The analytical method applies 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 can allow modeling of the complex structures of foil gas bearings, and it may be general enough to be applied to a wide range of foil gas bearing geometries and extensible to other turbomachinery components such as seals.

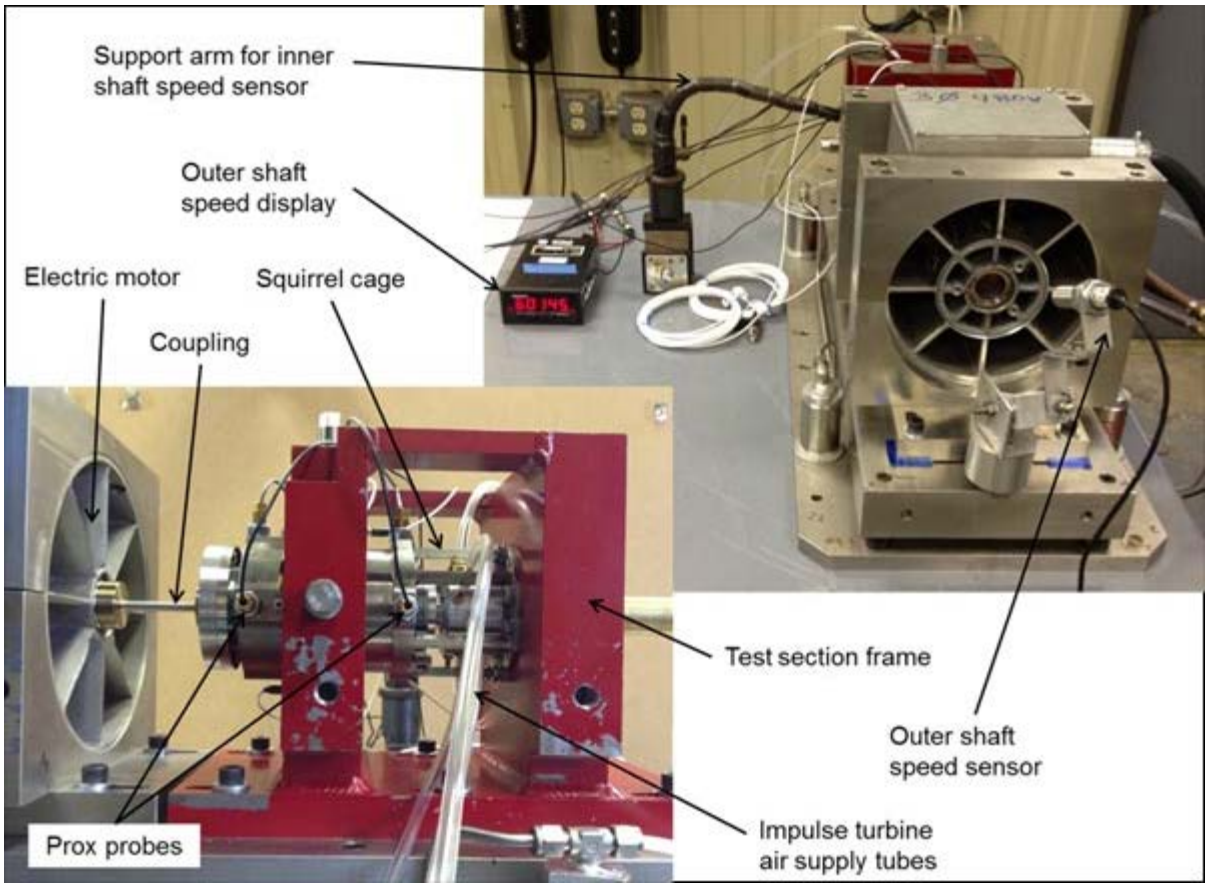

Figure 2. Photographs of test rig demonstration setup. Outer shaft capable of being driven up to 60 krpm while inner shaft capable of being driven at ±60 krpm.

Accomplishments — The design of the test rig was completed, and all features of the rig were fully demonstrated. The algorithms necessary to extract frequency-dependent stiffness and damping coefficients from the measured data have been tested extensively and have been validated with various test cases. The transient analytical 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. Comparisons of the new and established methods showed excellent agreement for the simple geometry, and parameter studies of transient time-step resolution and mesh density provided insight to optimal simulation settings. A novel "growing rotor" technique for starting a simulation with preloaded foil bearings was developed, and the ability to model compliant, spring-supported bearing foils in a steady-state simulation was demonstrated.

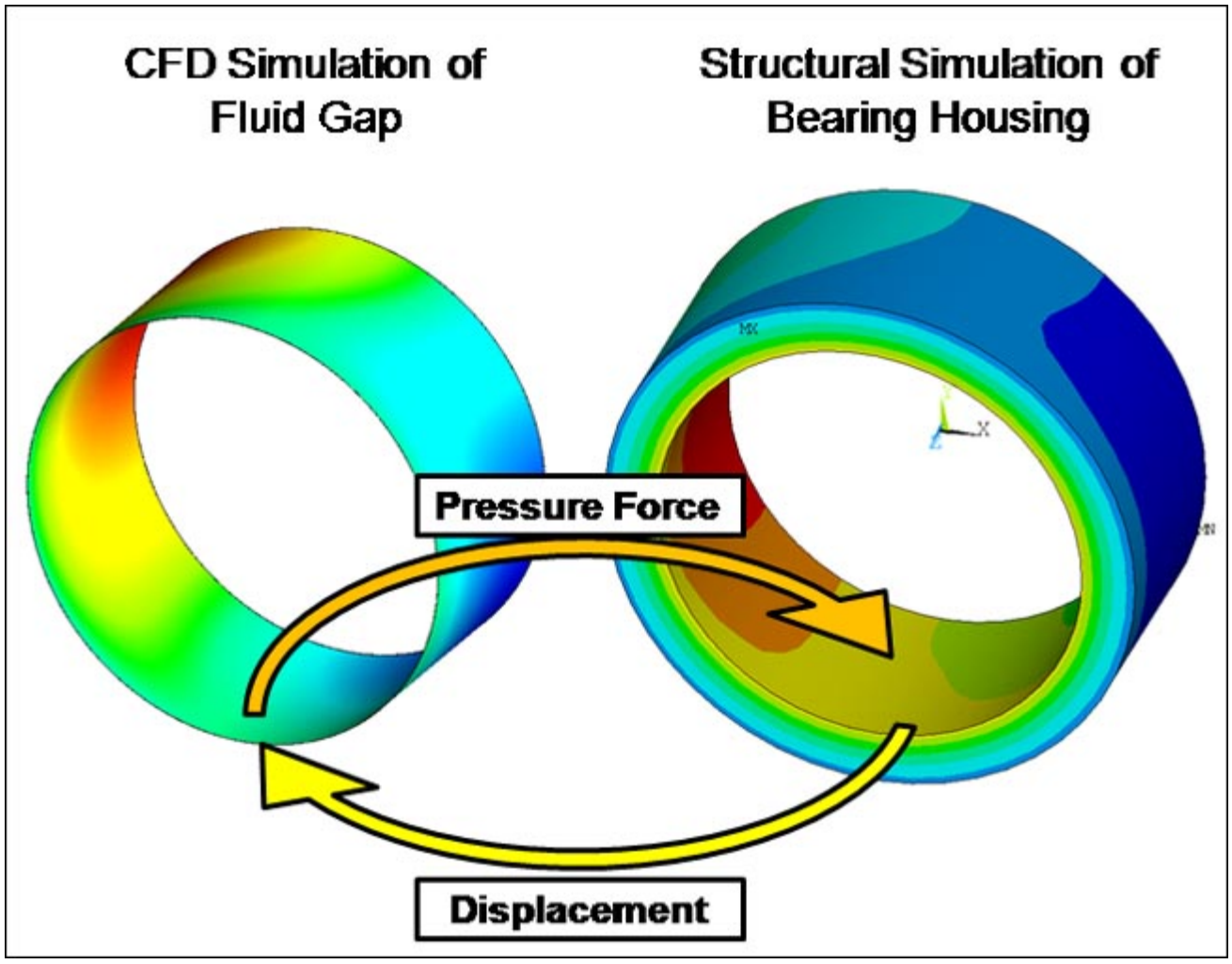

Figure 3. Fluid-structure interaction (FSI) couples the fluid and mechanical simulation results.

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2012 IR&D Annual Report

Optimized Robust Compressor Station Design Methodology, 18-R8218

Principal Investigators
Benjamin A. White
Barron J. Bichon
David L. Ransom
Eugene L. Broerman

Inclusive Dates: 04/01/11 – 09/28/12

Background — Machinery reliability assessment has long been a significant portion of the work performed at SwRI. Since 1952, SwRI has provided gas compressor installation design analysis service to the natural gas industry. In the process of designing a gas compression facility, typically for pipeline applications, it is important to ensure the mechanical reliability of the system through proper analysis of the fluid and structural systems. Pulsation and structural models of reciprocating compressor systems are developed to study the dynamic pressure, flow characteristics and structural responses for the planned operating conditions. The predictions are then used to identify potential problems, and design modifications are studied to eliminate the problems. Machinery reliability is also addressed, and SwRI has worked with NASA and other organizations over the past two decades to develop a world-class approach to probabilistic design analysis. This work is performed using SwRI-developed commercial analysis tools known as NESSUS® and CENTAUR™. This project was focused on the developing methodologies for designing an "Optimized Robust Compressor Station." The goal was to develop a design practice that better incorporates the characteristics of the fluid and structural systems and efficiently determines the preferred robust, least-sensitive compressor pulsation filter bottle and piping system design.

Approach — The primary objectives of this project were:

- Develop an optimization methodology for the design of gas compression stations to maximize station reliability and efficiency.
- Develop a robust design methodology to minimize design sensitivity to typical operational variability and degradation of mechanical systems, such as piping restraints, over time.

Accomplishments — This project has been completed. The following key accomplishments were made during this project.

- Developed a new pulsation code post-processor for increased automation and cross platform compatibility necessary to perform the optimization and robustness tasks and added significant new capabilities to the structural model to allow for automation and importation of excitation loads from the fluid domain.
- Developed a simple one-cylinder compressor and piping model for testing and optimization of both fluid domain and structural characteristics.
- Developed computer coding that will automatically identify the worst load cases from the fluid system, optimize the full system to reduce vibration and bottle weight and recheck key parameters such as pressure drop and dynamic stress after the optimal solution is found. The robustness of the design can be checked after an optimal design is found or the robustness can be included as part of the design optimization.
- Demonstrated the feasibility of the optimization and robustness processes as applied to compressor design. The optimization process was able to provide improvements to the traditional design methods in several simultaneous areas (such as reducing bottle weight and vibration).

Additionally, the reliability-based design optimization is able to successfully produce a design that is both optimized and robust to typical installation tolerances or identify a design that is not robust.

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2012 IR&D Annual Report

Implementation of a LED-Photodiode and CMOS Camera System for Water Detection and pH Measurement in a Multiphase System, 18-R8245

Principal Investigator
Leonardo J. Caseres

Inclusive Dates: 07/25/11 – 11/25/11

Background — Determination of free-water content in a multiphase fluid is of great practical interest to the oil and gas industry from the point of view of corrosion monitoring and mitigation. The presence of free water in crude oil during transportation in offshore and onshore pipelines has been associated with accelerated corrosion rates in oil and gas production operations. Today, portable devices for rapid analysis of free-water content in crude oil in deep-sea environments are lacking. As a result, there is a need for a tool to measure the presence of free water in a multiphase system for both offshore and onshore applications. In addition to the detection of free water in crude oil, it is of critical importance to determine the properties of the free water in a multiphase system, such as its pH. Accurate pH measurement allows for more accurate selection of appropriate completion materials and effective planning for scale formation treatment and inhibition. Numerous corrosion predictive models are being developed to accurately predict corrosivity as a function of pH and other parameters in multiphase and define accurate limits of use of carbon steel pipes. However, many of these models are overly conservative or focus only on a narrow range of parametric effects, thereby limiting their scope of applicability. Thus, there is a need to measure and validate the pH in the field by using a tool capable of measuring *in-situ* pH in multiphase pipelines.

Approach — The objective of this project was to test and validate a proof of concept consisting of a combination of an LED/photodiode and a CMOS color camera/pH-sensitive coating for measuring the amount of free water and pH in a multiphase system. The sensor prototype (Figure 1) consisted of two sealed prisms, 4-inches long, 2-inches high, and 3-inches wide made of transparent acrylic. One prism contained three off-the-shelf LEDs (RGB type LED, white, and an infrared LED) and the other prism contained a CMOS color camera as well as two photodiodes. For simplicity, the CMOS color camera, LEDs, and photodiodes were hardwired to a data acquisition unit. Then, the surfaces containing the electronic components in both prisms were coated with a commercially available oleophobic coating. A mixture of the oleophobic coating with a bromocresol green pH indicator was applied in front of CMOS camera. The sensor prototype was exposed to varying mixtures of crude oil and 3.5%wt NaCl solution to attain water fractions from 0 to 100 percent at flow rates of 70 and 100 mL/min. The distances between the sensing elements were set to 1.6, 3.175, and 5 mm. Sensor results were correlated with the mixture flow rates, water fraction, and distance between the LEDs and photodiodes. In addition, an ac impedance technique was used to compare the results obtained by the proposed optical measurement.

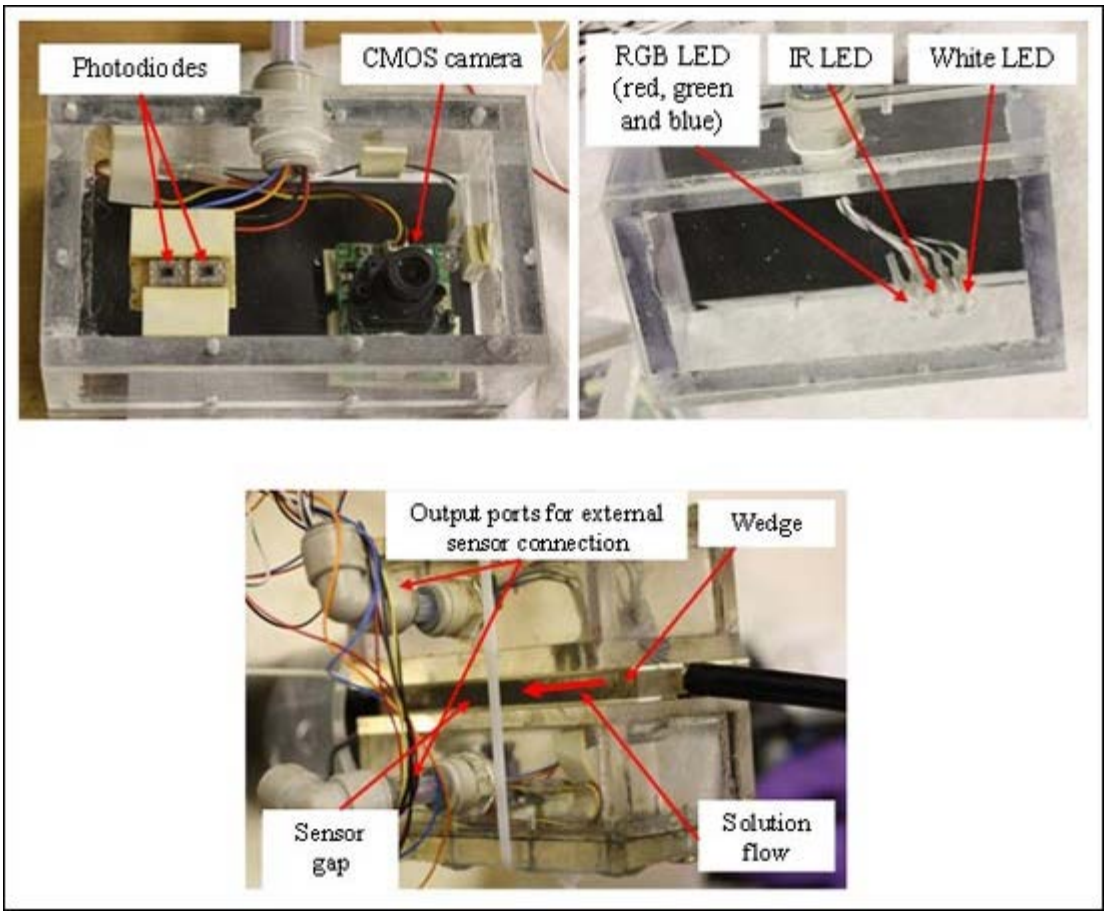

Figure 1: Pictures of the multiphase sensor prototype.

Accomplishments — SwRI has successfully tested and validated a cost-effective optical measuring device for water fraction determination and pH in multiphase systems. The results of the pH measurements showed that the CMOS camera in conjunction with the pH-sensitive coating was effective in the determination of solution pH. The sensor response to water fraction determination demonstrated that the IR LED/photodiode proved to be the best combination for measuring water fraction in crude oil in the range from 1 to 100 percent (Figure 2). An increase in water detection sensitivity, especially for small water fractions, can be increased by reducing the separation between the LED source and photodiode. The results also showed that flow rates lower than 100 mL/min did not have an influence on the water detection. However, it is expected that for higher flow rates water detection might be affected. If this is the case, increasing the sampling time could resolve this potential issue. In addition, the optical measurement technique proposed here was far more sensitive to water detection in crude oil than the ac impedance technique, especially at water fractions lower than 20 percent.

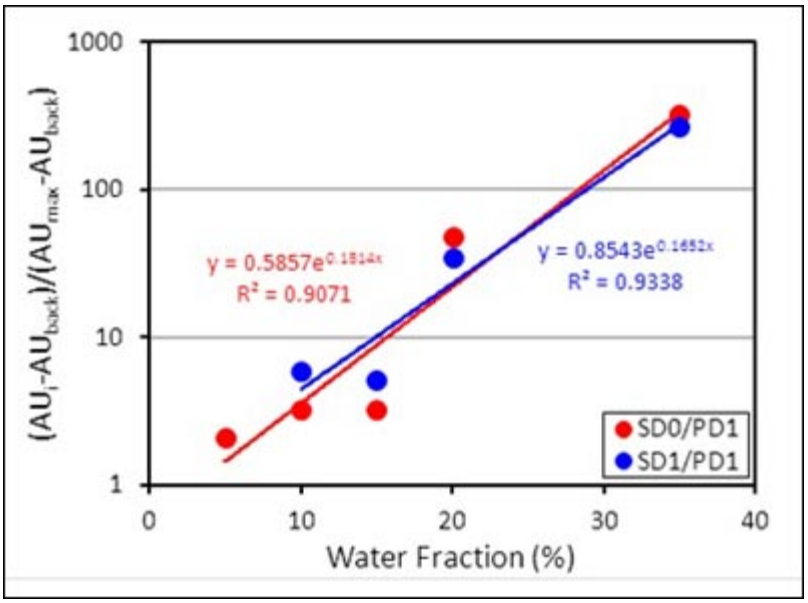

Figure 2: Sensor response to various mixtures of oil/3.5% NaCl solution

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2012 IR&D Annual Report

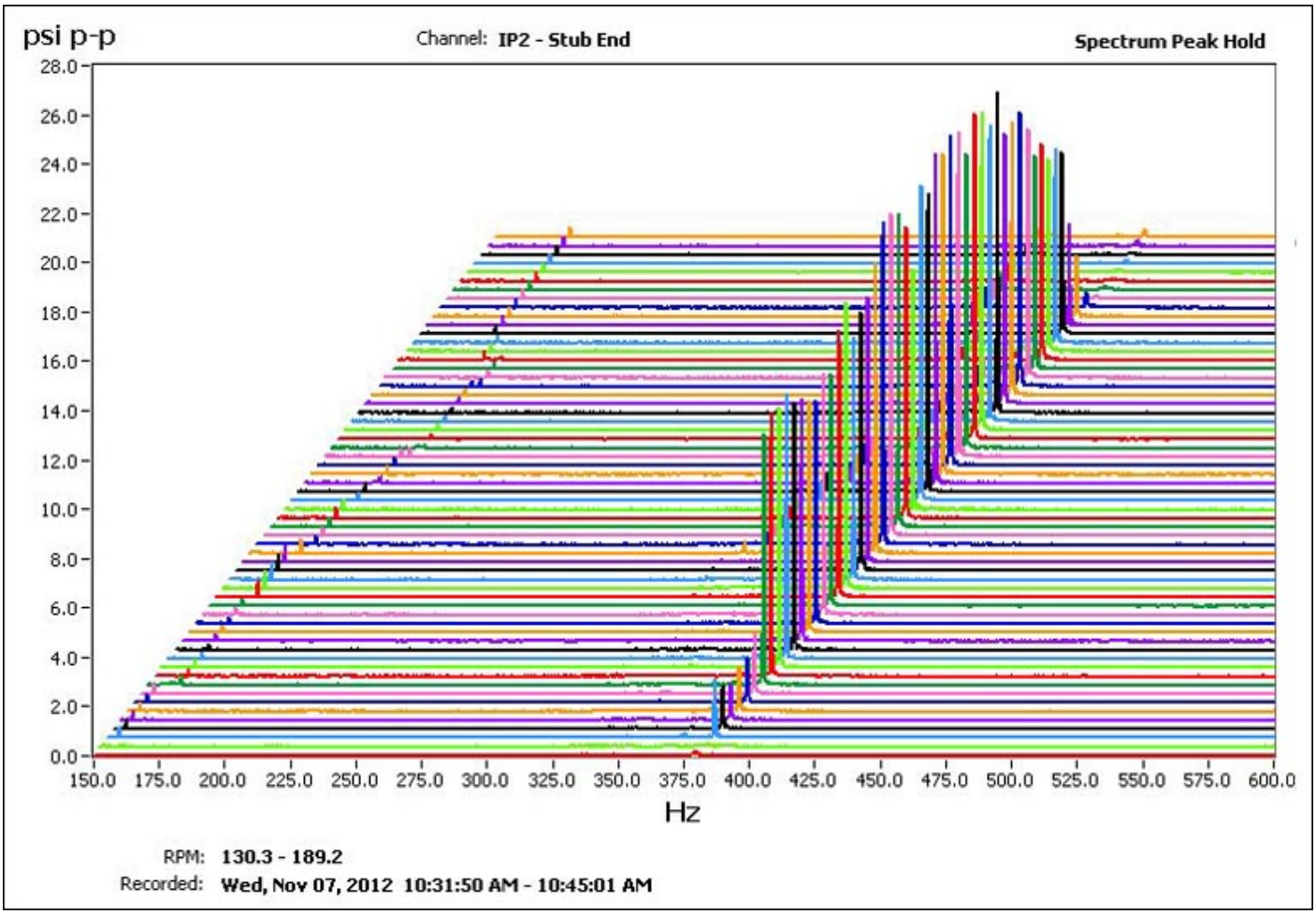
A Comprehensive Approach to Predicting Vortex-Shedding-Induced Pulsation Amplitudes in Piping Systems, 18-R8325

Principal Investigators
Eugene L. Broerman
Sarah Simons
Rebecca Owston
Aaron McClung
Nathan Poerner

Inclusive Dates: 07/01/12 – Current

Background — One of the major design criteria for centrifugal compressor piping systems is preventing piping system vibration and valve failures resulting from vortex-shedding-induced (VSI) pulsations. In recent years, computational fluid dynamics (CFD) has been used to theoretically predict the dynamic shaking forces that cause vibration when the subject phenomenon occurs in piping systems. However, a practical validated approach to applying these theoretical methods has yet to be developed. SwRI's current approach to address this concern is a screening type vortex-shedding analysis ("Strouhal analysis") for determining whether there is a coincidence associated with the frequency of the vortex-shedding of the gas flow and the acoustic natural frequency of piping stubs. If a coincidence is predicted based on the screening analysis, piping changes are recommended to avoid the coincidence. These piping changes are typically expensive, time consuming, and possibly unnecessary in some circumstances. There is currently no way to determine the severity of the resulting pulsation amplitudes and, therefore, the severity of possible piping vibration. The lack of an accurate prediction method requires added conservatism that has forced many operators to reduce operating flexibility or make costly piping changes that could otherwise be avoided. VSI pulsation amplitude predictions would allow SwRI to offer a significant cost-saving service to its clients.

Approach — This project is a combined experimental and analytical effort. An experimental Strouhal test program is being conducted in conjunction with a supporting effort that utilizes a commercial CFD package to provide supplemental pulsation amplitude predictions in order to populate pulsation amplitude response surfaces. The response surfaces will be used as the basis for developing a new boundary condition to be implemented in SwRI's proprietary Transient Analysis Pulsation Solver (TAPS). The new boundary condition will incorporate a source term representing the acoustic excitation due to Strouhal-related shedding at a piping stub. This new simulation capability will augment the current SwRI Strouhal screening methods by providing a means of predicting pulsation amplitudes when acoustic resonance cannot be avoided. The primary objectives of this project are to (1) develop validated simulation capabilities (i.e., using TAPS and CFD) to accurately predict the amplitudes of vortex-shedding-induced piping pulsation and (2) gain knowledge during the execution of this investigation that will enable the definition of design guidelines for using clamps to restrain shaking forces resulting from acoustic coincidences in small-bore piping.



Dynamic pressure (pulsation) data measured in a test stub.

Accomplishments — An experimental test matrix has been developed that includes mainline piping diameters ranging from 3 inches to 6 inches, flow conditions associated with Reynolds numbers that range from $2(10)^5$ to $4(10)^6$, and branch piping diameters that range from 1.5 inches to 3 inches. Test sections have been fabricated such that appropriate measurements (dynamic pressure, temperature, static pressure, flow, etc.) can be obtained during each data sampling. Laboratory testing is currently under way, and preliminary results show good agreement between the calculated/predicted acoustic natural frequencies and the measured natural frequencies. Vortex-shedding frequencies have also been observed to be at approximately the predicted frequencies. Some of the measured pulsation amplitudes have been lower than anticipated; therefore, additional testing is planned to provide more insight into this unexpected result. In particular, future testing will be performed in a system in which much higher Reynolds numbers can be achieved (approximately $1.7(10)^7$). Appropriate CFD software packages and turbulence models have been assessed and model verification has begun. Investigations are under way to determine an acceptable numerical approach that will minimize required computational resources.

2012 IR&D Annual Report

Improvement of Wet Gas Compressor Performance using Gas Ejection, 18-R8327

Principal Investigator
Grant Musgrove

Inclusive Dates: 07/02/12 – Current

Background — During upstream production of natural gas, the gas brought to the surface is compressed so that it can be injected into a pipeline and transported elsewhere. Sometimes the gas brought to the surface is a mixture including a small amount of liquid hydrocarbons, up to 5% volume fraction. Because a compressor is designed for dry gas only, the mixture of gas and liquid degrade the performance of the compressor to require much more power. By requiring more power, large drivers are needed that increase the cost and size of the compressor system. However, the required size of the driver is not known because a proven method does not exist to accurately predict compressor performance under wet gas conditions. The current solution is to avoid the problem of wet compression altogether by separating the gas and liquid at the well-head. Again, the cost and footprint of the system is increased because of the separation equipment. Therefore, the one attractive option to solve the wet gas problem is to modify the compressor such that wet gas has little effect on performance. Fundamental aerodynamic testing of airfoils in air-water flows have indicated that aerodynamic losses are likely responsible for the increase in power required of wet gas compression. Observations are reported that the liquid in contact with the airfoil surface in the form of droplets and film is to blame for the airfoil performance loss; however, the results lack detailed measurements and flow observations that can be applied to compressor operating conditions. Detailed information about the aerodynamic effects of wet gas flows and a solution to recover lost performance is needed to improve compressor designs to handle wet gas flows.

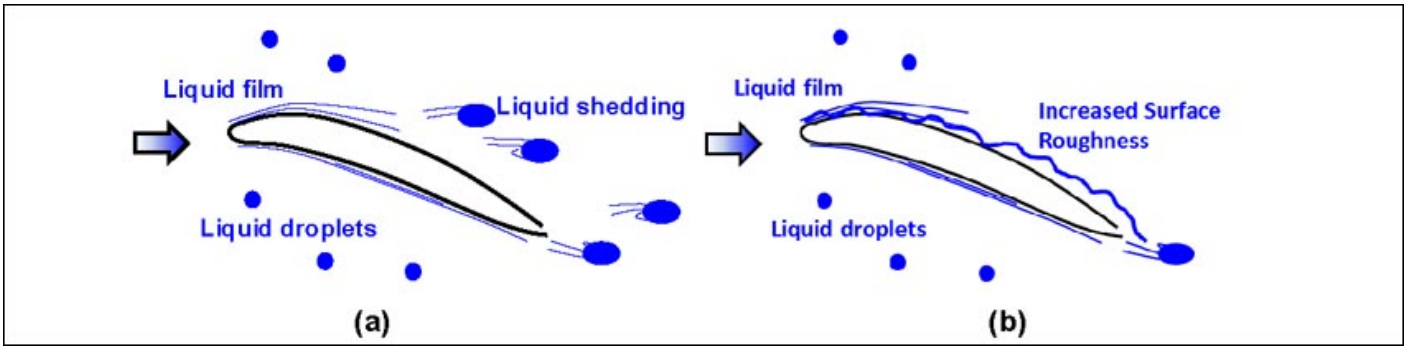


Figure 1. Potential influence of wet gas a) liquid droplets leading to premature flow separation or b) liquid film significantly increasing surface roughness.

Approach — In this IR&D project, a NACA 0012 airfoil is studied in a large-scale wind tunnel using air and water to simulate wet gas conditions. The objective is to both study the effects of wet gas on aerodynamic performance as well as develop a concept to use air ejected from the airfoil surface to create a film barrier to keep the liquid from coming in contact with the airfoil surface. Aerodynamic performance is evaluated from measured lift, drag, and surface pressures along an airfoil in wet-gas flow, including highly resolved particle image velocimetry (PIV) methods. This project is conducted in two phases using computational predictions and experimental measurements. In the first phase, the effects of airfoil

performance with wet gas over a range of operating conditions are studied with experimental measurements and computational predictions using a lattice-Boltzmann fluid solver; whereby the computational predictions can be directly compared to measurements. During the second phase, gas ejection concepts are studied using computational simulations before measuring the performance of the best gas ejection concept.

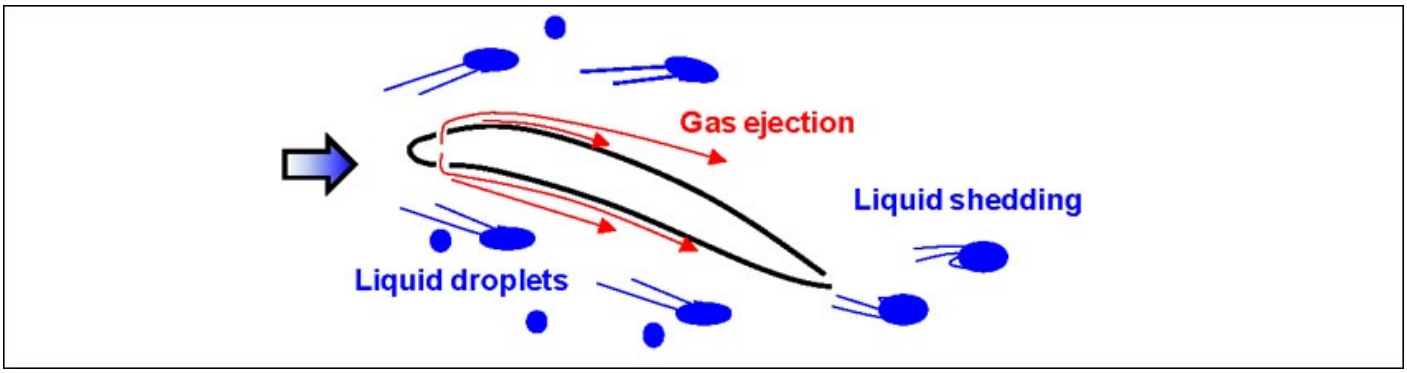


Figure 2. Gas ejection along blade surface can control boundary layer, thus negating some of the detrimental effects of liquid droplets in the flow stream.

Accomplishments — Accomplishments include the wind tunnel and airfoil test article design and construction. The airfoil is constructed using Fused Deposition Modeling (FDM), a rapid prototyping technique, to reduce hardware cost and allow complex internal geometries planned in phase 2 of the project. In parallel, a lattice-Boltzmann solver is being developed to simulate the airfoil performance in air-water flow at the planned test conditions.

2012 IR&D Annual Report

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 during obscured environmental conditions caused by phenomena such as clouds, fog and 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, the objective of this internal research project was to reliably and consistently detect the RF signals caused by the firing of automatic weapons at a distance of over one-quarter mile (400 meters) and to understand the phenomenology associated with the cause of the RF signal.

Accomplishments — The team developed a test plan and assembled the appropriate antennas and test equipment to collect RF and video data at the SwRI ballistics outdoor range and in an SwRI indoor shielded enclosure during the firing of a small arms automatic weapon. Although the team did capture valid RF signals again during the testing performed, the signals did not occur every time, and the signals did not provide an adequate signature to differentiate them from other external transmitters.

Consequently, for the particular automatic weapon and the particular test equipment used, this internal research did not reveal the presence of the necessary RF signatures for detection of the firing of weapons at a useable distance. Although this latest research did not reveal sufficient RF signal detection, further research using a different approach or using different test setups could still potentially reveal a solution for achieving positive identification of the firing of automatic weapons at practical distances. This conclusion is based on the following facts:

- Testing has shown that during the firing of an automatic weapon, the barrel and the bullet develop significant voltages that can serve as a power source for subsequent high-speed discharges.
- Testing has shown that the firing of a weapon does produce RF signals of sufficient strength for detection at adequate standoff distances.
- Testing has not shown that the detected RF signals have a unique signature.
- Testing has not determined the precise phenomenology associated with the RF signal generation.

2012 IR&D Annual Report

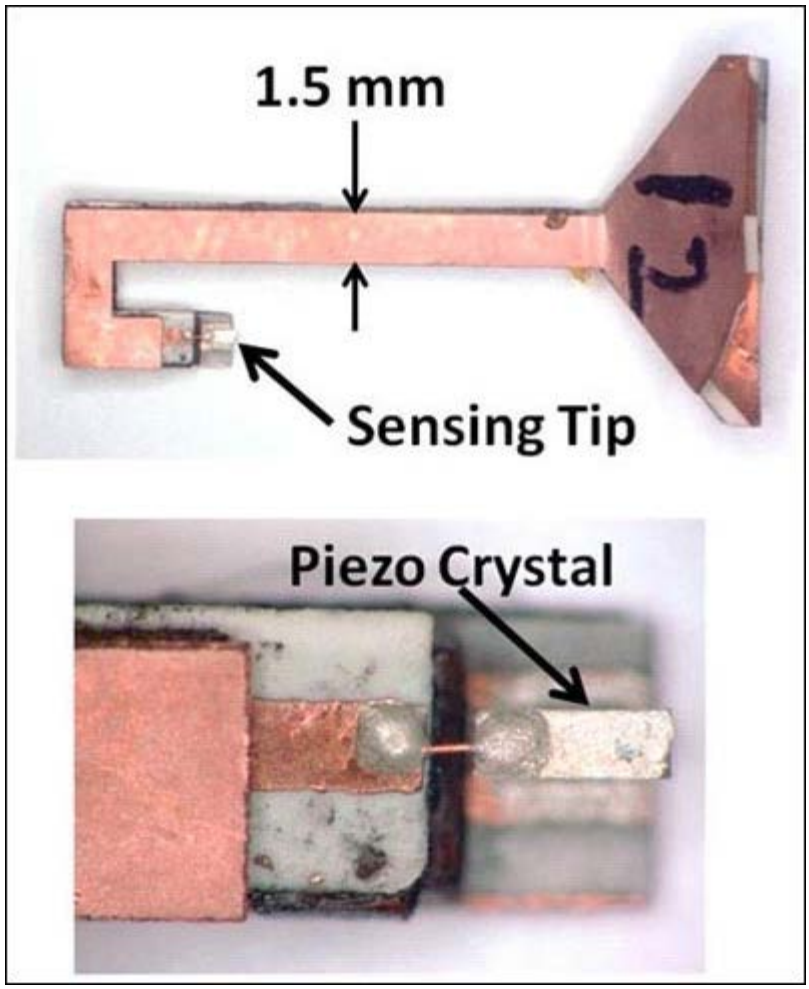
High Resolution Laser Photolithography for Fabrication of Specialized, Miniature Devices, 14-R8302

Principal Investigators
W. Royall Cox
Jerome A. Helffrich
John D. Harrison

Inclusive Dates: 04/01/12 – Current

Background — Developing custom devices of ever-decreasing size has been an ongoing activity for many years. The overall objective of this project is to expand significantly the process capabilities of SwRI's Advanced Electronics Laboratories to enable the creation of specialized circuits and sensors with smaller feature sizes and enhanced capabilities.

Approach — The primary processes to be optimized are laser micromachining, photolithography, and various combinations of these technologies. SwRI will upgrade the optics of the micromachining tool to reduce the minimum focal spot size of the UV (ultraviolet) laser, thereby enabling the fabrication of circuits having smaller circuit features. In conventional photolithography an optically sensitive coating (resist) is applied to the surface of the substrate then exposed to UV light through a mask to define an electrical circuit pattern (after subsequent development, etching and removal of the remaining resist). Each iteration of the pattern design requires a new, relatively costly, mask. SwRI will develop a laser writing process to create circuit patterns by exposure or removal of the resist, thereby eliminating the need for a mask. After optimizing the various device fabrication processes, SwRI plans to demonstrate its new capabilities by making three different types of miniature devices of potential interest to clients. The first will be a miniature ultrasonic transducer for broadband sound detection, which consists of a piezoelectric element attached to a multilayer copper/polymer circuit (as



Prototype miniature ultrasonic transducer for broadband sound detection.

shown in the figure). The second will be a miniature electronic filter with dimensions as small as 160 microns. The last device will be a miniature quartz tuning fork scanning probe for detection of metal surfaces.

Accomplishments — The reduction in laser spot size was achieved, enabling the micromachining of features as small as 50 microns. Laser writing processes were developed for exposing or removing resist coatings ranging in thickness from 2 to 250 microns. A miniature transducer was developed, and work was begun on the miniature electronic filter.

2012 IR&D Annual Report

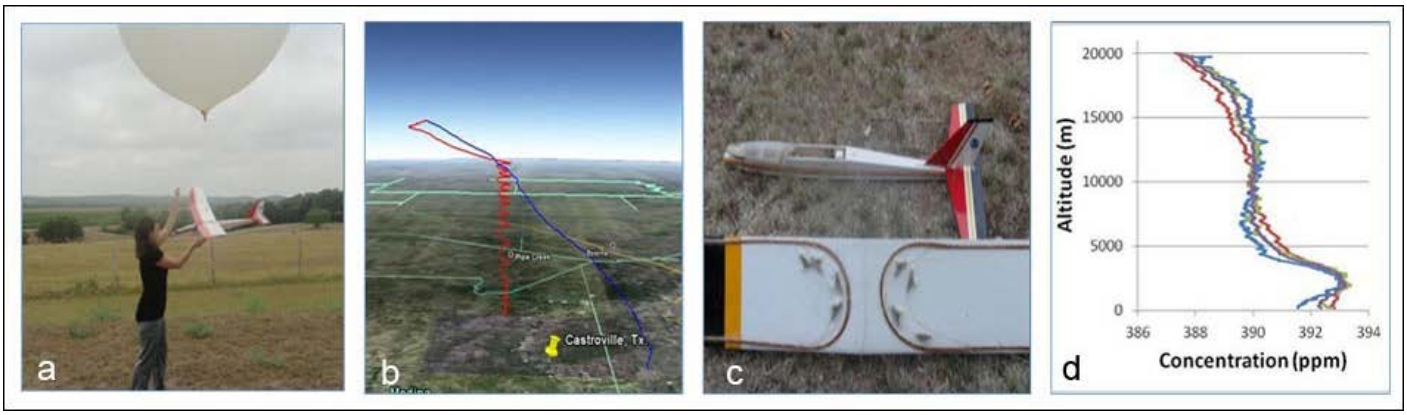
Aircore® System Miniaturization, Validation and Verification, 16-R8166

Principal Investigators
Thomas H. Jaeckle
Kristin A. Favela

Inclusive Dates: 07/01/10 – 12/31/11

Background — Researchers at the National Oceanic and Atmospheric Administration (NOAA) have recently developed and reported a novel air collection device for measuring vertical profiles of trace gases in the atmosphere, which has been applied to carbon dioxide and methane so far. The device consists of a long stainless steel tube that is prefilled with calibrated gas and allowed to ascend on a weather balloon. During ascent, the device is evacuated as it equilibrates with the decreasing atmospheric pressure. During descent, the tube is filled with atmospheric gas in an ordered manner. The diffusion rate inside the tube is slow enough that the collected gas remains ordered. Miniaturization was desirable given logistical issues with launch and recovery.

Approach — In this new manifestation of the device, the stainless steel tube is replaced with Hydroguard® fused silica tubing (0.53 mm × 30 m) and two lightweight valves having a total mass of less than 28 g. This micro-AirCore device was deployed on the SwRI-developed unmanned SkyWisp glider. Profiling of carbon dioxide in the atmosphere proceeded via mass spectrometric detection. A laboratory-based validation system was used for evaluating the micro-AirCore function, including accuracy and precision, for carbon dioxide. The diffusion profiles of carbon dioxide, argon, oxygen, and methane were also investigated.



The system was deployed on a glider (a) at a site in south-central Texas (b). Fused silica tubing was affixed to the bottom of the glider wing (c). The graph (d) shows the concentration of gases measured by the micro-AirCore devices.

Accomplishments — Overall, the micro-AirCore demonstrated an accuracy error of 2 percent ($^{12}CO_2$) and minimal diffusion over a period of 16 h (peak width increased by a factor of 1.6). Even after 63 h, mixing of the gases inside the tube was not complete. A triplet of micro-AirCores was deployed on the SkyWisp glider yielding a relative standard deviation of 0.08 percent, or 0.3 ppm, for CO_2. The profile collected resulted in observation of the boundary layer with elevated CO_2 levels, a region in the free troposphere with relatively constant CO_2 mole fraction, and a gradual decrease in CO_2 above 10,000 m.

This microdevice has broad applications extending beyond vertical profiling. Fitting the device with a metering device could enable horizontal collection of gases.

Preliminary results were presented in August 2011 at the meeting of the American Meteorological Society. Final results were published in the peer-reviewed journal *Analytical Chemistry*, "Microcollection of Gases in a Capillary Tube: Preservation of Spatial and Temporal Resolution," K.H. Favela, P. Tans, T.H. Jaeckle and W.S. Williamson (Vol. 84, pages 8310-8316, 2012).

2012 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

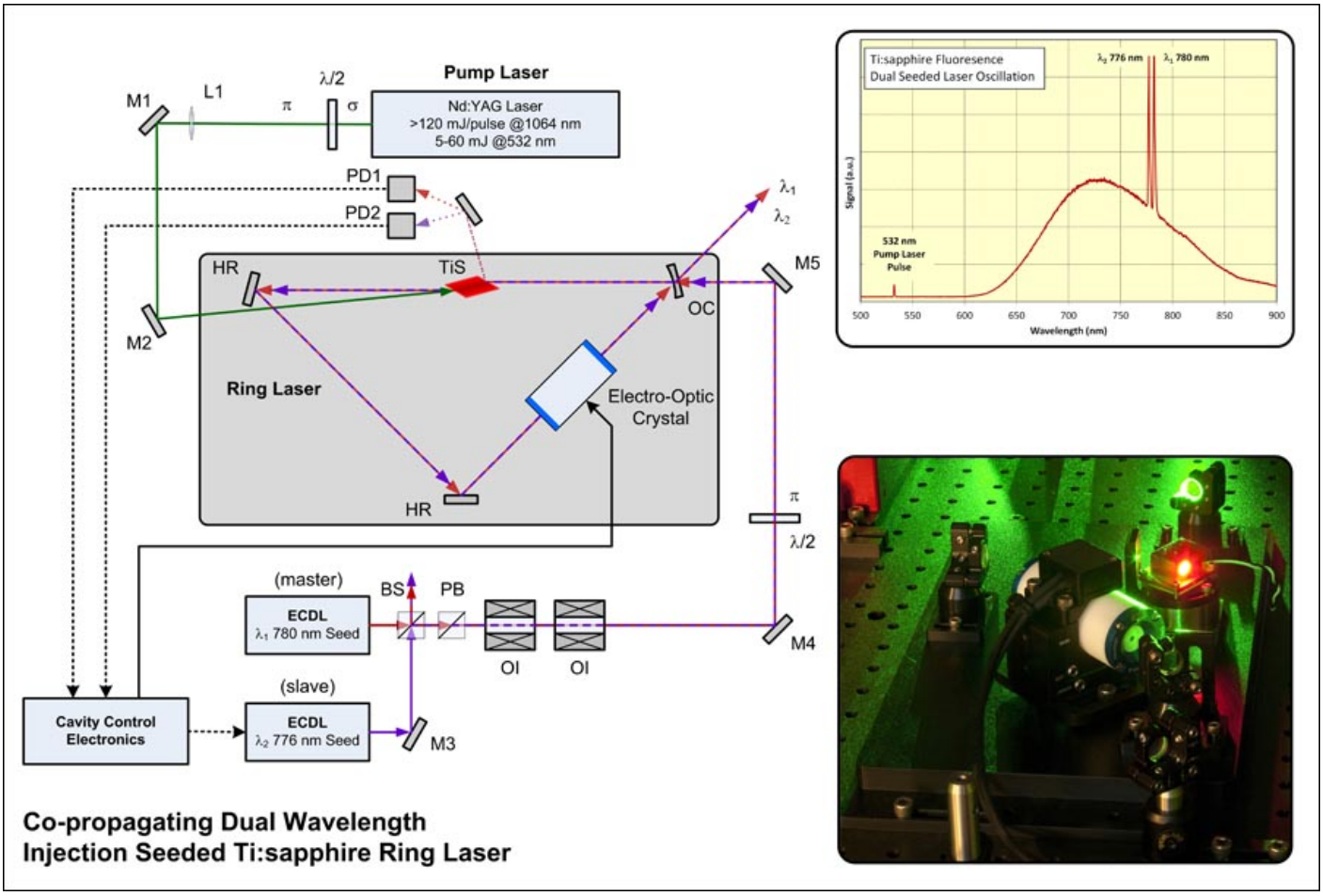
Inclusive Dates: 07/01/10 – 12/01/11

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 laser resonance ionization. Work on developing a portable Laser Desorption Resonance Ionization Mass Spectrometer (LDRIMS) instrument by SwRI space researchers led to a need for several specialized laser systems. The LDRIMS instrument performs 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 the atom or molecule. The LDRIMS system, as it exists today, utilizes seven lasers 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. All these increase the possibility of using this technique in a space mission.

Approach — SwRI developed a unique approach for generating two wavelengths simultaneously. In addition, the laser output operates near the Fourier transform limit and provides stable output with immunity from mechanical vibration throughout the acoustic range. The system has the potential to reduce the number of lasers needed by the LDRIMS system by 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 center wavelengths of the laser system is provided by two independent seed lasers, which are injected into the cavity via the output coupling mirror and propagate within the ring laser cavity. Alternatively, intra-cavity frequency selection optics such as angle-tuned interference filters, birefringence filters, prisms, or etalons may be used in lieu of the seed lasers when laser line width is not a critical factor. Enhanced noise immunity and the ability to achieve Fourier transform limited output are accomplished with the use of a nonlinear electro-optic crystal and a Ramp-Hold-Fire (RHF) cavity control technique. The RHF technique utilizes a KD*P crystal to modify the phase of the seed light propagating within the ring cavity until the light is resonant within the cavity. Once the resonance condition is detected, the resonance is held for a short period of time until the laser is fired, resulting in seeded Fourier transform limited laser output. If the time between the cavity resonance detection and laser fire is less than 30 μs, the laser output will be immune to acoustic noise. The laser system and techniques developed at SwRI represent a substantial step forward in multiple wavelength pulsed laser design.

Accomplishments — SwRI has successfully developed a Ti:sapphire ring laser with the capability to produce injection seeded laser output at two discrete wavelengths. Furthermore, SwRI has shown that this method can be extended to produce laser output at multiple discrete wavelengths with four or more

seed lasers. Feedback control of the slave ring laser cavity using a KD*P crystal to phase modulate the seed light propagating within the slave oscillator has also been demonstrated. SwRI used a RHF technique for seeding the dual-wavelength laser system to generate 20 ns output pulses. Immunity to noise throughout the acoustic range can be achieved with the RHF technique provided the laser is fired within 30 µs of the resonance detection. The RHF technique may also be adapted to many other types of injection-seeded solid state laser systems to produce Fourier transform limited output. Laser performance measurements indicate that the slave oscillator is properly seeded and producing Fourier-transform limited pulsed laser output. SwRI has also demonstrated the capability of the seed lasers to drive the D2 transition of Rubidium 87 and the ability to continuously tune the laser wavelength from 776 nm to 790 nm.



Ring laser overview

2012 IR&D Annual Report

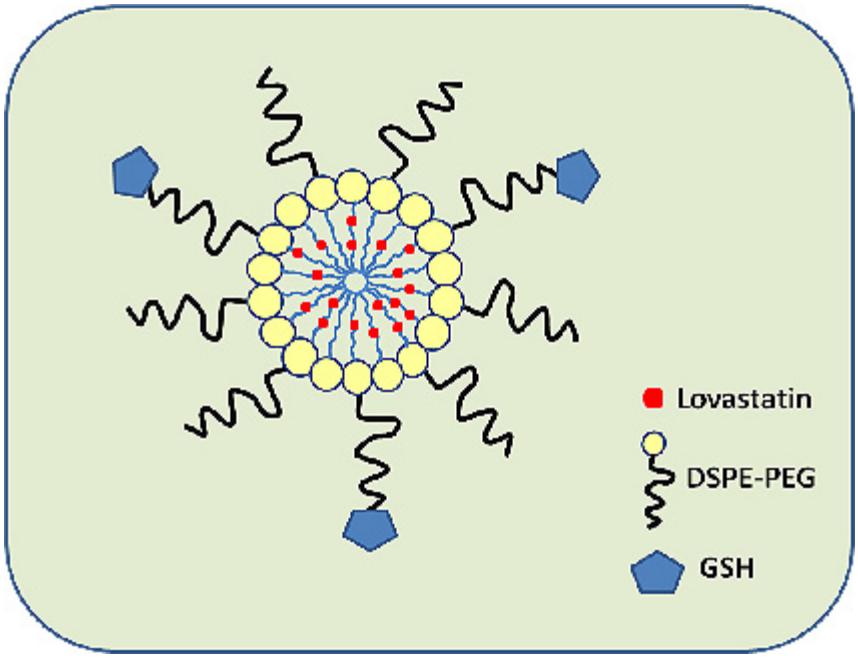
Targeted Formulation to Treat Spinal Cord Injury and other Neurological Disorders, 01-R8183

Principal Investigators
Gloria Gutierrez
Gianny Rossini

Inclusive Dates: 10/01/10 – Current

Background — There is a great need for effective therapies for spinal cord injury (SCI). Current global estimates indicate that the incidence of SCI ranges from 14.5 to 57.8 cases per million. To date, attempts to overcome some of the destructive neurological effects have resulted in some degree of functional improvement. However, the complexity of SCI obviously demands a multifactorial repair approach. Apart from this, the challenge in treating most brain disorders is surmounting the difficulty of delivering therapeutic agents to the brain by crossing the blood-brain-barrier. Statins, or 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMGR) inhibitors, are front-line therapeutic agents for the prevention of cardiovascular disease and atherosclerotic disorders related to hypercholesterolemia. In addition to their potent anti-atherosclerotic and cardioprotective effects, compelling clinical and preclinical studies delineate the neuroprotective efficacy of statins in various neurological disorders including spinal cord injury, where they have been shown to prevent endothelial dysfunction, facilitate neuroprotection, and promote locomotor recovery following spinal cord injury. The challenge in treating most brain disorders is overcoming the difficulty of delivering therapeutic to the brain by crossing the blood-brain-barrier.

Approach — The goal of this proposal has been to develop a nanoparticle drug delivery system to target the central nervous system using a linear or optimized branched polyethylene glycol (PEG) coating on the liposome surface with glutathione as the targeting ligand to reach the central nervous system. Glutathione is specifically and actively taken up by specialized transporters at the blood-brain barrier and the PEG coating provides prolonged systemic circulation to deliver statin nanocarriers to the spinal cord injury site, exerting controlled release of lovastatin to counteract the reactive oxygen species and suppressing inflammatory response generated by the injury. Thus it is desired that the formulation demonstrates controlled release of lovastatin and accumulation in the site of injury to enable rapid and uniform treatment and avoid unnecessary systemic exposure. SwRI researchers



Schematic representation of micellar drug delivery system. Glutathione (GSH) has been conjugated to the tips of a PEGylated phospholipid (DSPE-PEG) for enhanced lovastatin delivery to the brain.

developed and are characterizing *in vitro* cell binding and permeability across the BBB of ligand-targeted PEG-liposomes and micelles. Researchers have conjugated these linear and branched PEG moieties to glutathione molecules using maleimide chemistry followed by liposome or micelle formulations. They have tested the linear PEGylated formulations in the transcytosis assay with and without targeting and with and without the active drug. They have also established the neurite outgrowth assay *in vitro* and have been able to quantify neurite formation in response to these formulations. The rate of lovastatin release *in vitro* was also characterized over time.

Accomplishments — The project team was able to confirm glutathione conjugation to the maleimide moiety in micelles by means of nuclear magnetic resonance spectroscopy. Researchers have completed the major goal of developing and testing targeted and non-targeted liposomes and micelles, using a phospholipid linear PEG2000. The delivery system is able to provide controlled-release of lovastatin (approximately 70% release in 72 hours) improving bioavailability of the drug. They demonstrated cellular uptake and transcytosis of rhodamine-labeled micelles and liposomes in a human brain vascular endothelial cell line, hCMEC/D3 (obtained under license from INSERM, France) (approximately 30% transport across the blood-brain-barrier for targeted micelles and liposomes compared to undetectable levels for non-targeted formulation. They have also been able to prove efficacy of the formulations in the neurite outgrowth assay.

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2012 IR&D Annual Report

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

Principal Investigators
David E. Camann
Alice Y. Yau

Inclusive Dates: 06/27/11 – 12/28/11

Background — The developing fetus is particularly vulnerable to adverse effects from pharmaceutical and exogenous chemical exposure. No biomarkers exist to retrospectively assess prenatal and early post-natal exposure to many chemicals, including analgesics, organophosphate (OP) insecticides, and diester phthalates because the parent compound is rapidly metabolized and the metabolites are quickly excreted. An urgent need exists to identify perinatal exposure biomarkers of such chemicals for use in assessing their contribution to risk for epidemic pediatric neurodevelopmental disorders such as autism. The enamel and primary dentin of the crown of each deciduous tooth form during a specific period from initial dentin calcification within the second trimester *in utero* through crown completion within the first year after birth. Tooth concentrations of sequestered substances may provide useful biomarkers of exposure during its formation. It was hypothesized that organic chemicals or their metabolites circulating in the bloodstream during deciduous tooth formation may sorb along with calcium and other nutrients and remain sequestered when the tooth is shed.

Approach — The objectives were to devise analytical and preparation methods for potentially toxic or beneficial organic chemicals or metabolites in deciduous teeth, to discover if some were stored in teeth, and to estimate their detection frequency in deciduous molars. Tooth preparation, extraction, and analytical methods were developed for analgesics and specific and non-specific metabolites of OP insecticides and phthalates by tandem liquid chromatography/mass spectrometry, and for polyunsaturated fatty acids and insecticides by gas chromatography/mass spectrometry.

Accomplishments — The analgesic acetaminophen was stored at greater concentration in a child's second molar than a first molar, consistent with intake, suggesting that acetaminophen concentration in molars may be a biomarker of acetaminophen exposure during molar formation. Chemicals detected by liquid chromatography/tandem mass spectrometry in molars of 21 typically developing children include the endocannabinoid anandamide (86 percent of children), the analgesic acetaminophen (43 percent), and the specific metabolites mono-2-ethylhexyl phthalate (MEHP, of plasticizer di-2-ethylhexyl phthalate, 29 percent), 3,5,6-trichloro-2-pyridinol (TCPy, of OP insecticide chlorpyrifos, 10 percent), and 2-isopropyl-6-methyl-4-pyrimidinol (IMPy, of OP insecticide diazinon, 10 percent). None of these chemicals has previously been detected in human teeth. Molars from the two oldest subjects contained the largest concentrations of MEHP, TCPy, and IMPy. Potentially protective fatty acids detected by gas chromatography/mass spectrometry after derivatization include docosahexaenoic (19 percent), arachidonic (100 percent), and linoleic (100 percent). Validation studies are necessary to verify that each detected chemical in molars provides a biomarker of perinatal exposure.

2012 IR&D Annual Report

Combined Laser and Medicated Scar Improvement Therapies, 01-R8276

Principal Investigators
Gianny J. Rossini
Gloria E. Gutierrez
Lucy M. Kimmel
Alda E. Flores

Inclusive Dates: 01/01/12 – 01/01/13

Background — Ablative CO_2 laser resurfacing of the entire skin surface has been the FDA-approved standard of care for cosmetic enhancement and scar improvement, albeit with considerable risk of infection and loss of efficacy for deep burn scars and for wounds of large area extent. This procedure creates a tissue column or skin poration of about 2-mm deep and 300-µm wide named microablative zone (MAZ) using the focal thermal power of a CO_2 laser. After a short period of time, the MAZ is replaced by cell migration from the adjacent healthy tissue. However, this method appears to be useful only for relatively shallow scars not penetrating into the dermis. Therefore, to improve the laser procedure, drug enhancers, such as corticosteroids and similar derivatives, are commonly used as injections or creams; however, corticosteroids are quite hydrophobic and form a suspension containing crystals of wide size distribution (greater than 10 µm). It is unclear how effectively they can penetrate the skin through the MAZ. Clearly, specially designed formulations with improved permeability and controlled-release characteristics and delayed controlled-release of commonly used corticosteroids such as triamcinolone acetonide are needed. These formulations may not present known side effects such as skin atrophy and associated infections and might be able to enhance the anti-scarring effects providing physicians with additional options when treating large scars, in particular the ones seen after burns.

Approach — The project team developed advanced dermal drug delivery formulations known as flexible liposomes, cubosomes, ethosomes, and transferosomes; each of these technologies offers nonoverlapping benefits. For example, cubosomes use waxy lipids and starch and are good for loading hard to dissolve drugs. Ethosomes are made with flexible lipids and a high content (20 to 30 percent) of ethanol to make them highly efficient in penetrating the stratum corneum of the skin. Transferosomes are made with flexible lipids and surfactants to increase surface fluidity and to permeate the stratum corneum of the skin. For these basic formulations, the use of additives such as natural-derived detergents and others were investigated in order to improve dermal permeation, while at the same time avoiding the use of cholesterol or other rigid chemical structural components. Carbopol was also included as a thickening agent to allow for easier application to the skin. As a standard procedure, nanoparticle size was measured using photon correlation spectroscopy (PCS) particle analyzer and surface charge using a ZetaPal analyzer. Formulation flexibility index is measured by extrusion across a nanoporous membrane under constant pressure; permeability testing is assessed with a Franz cell device using skin from cadavers obtained under Institutional Review Board (IRB) regulations or using synthetic membranes that mimic skin permeability. Efficacy of dermal formulations is determined *in vivo* in a rabbit ear scar model, a well-established model for testing scar medication. In addition, this standard model will be investigated to also test laser therapies, a valuable tool for research of new dermal formulations for scar improvement.

Accomplishments — Flexible dermal formulations known as cubosomes, ethosomes, and transferosomes loaded with corticosteroids were fabricated and characterized for drug loading, drug

release, particle size, and drug permeability using human cadaver skin and artificial skin substitutes. A pilot study with a small number of rabbits is in progress; this study will establish the model and allow for future testing of lead formulations *in vivo* with and without ablative laser procedures.

2012 IR&D Annual Report

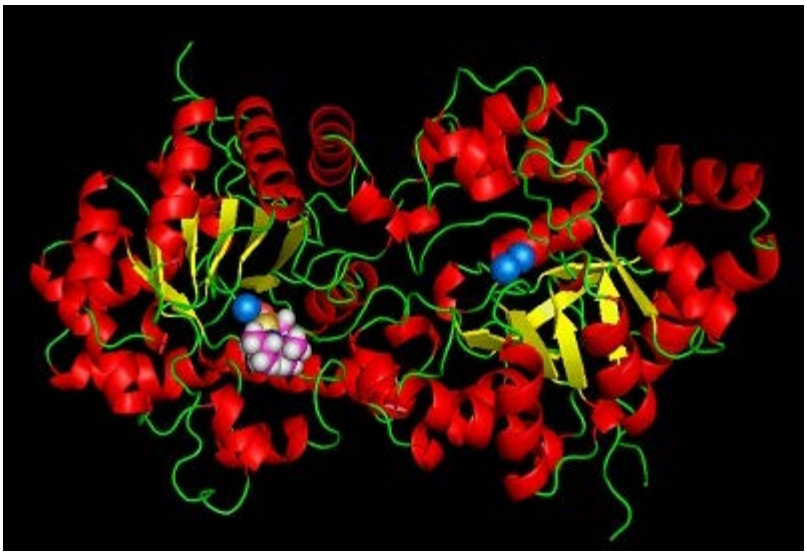
Humanized Organophosphorus Hydrolase Expressed in Human Embryonic Kidney Cells: Pharmacokinetics in the Guinea Pig Model, 01-R8280

Principal Investigator
Tony E. Reeves

Inclusive Dates: 01/02/12 – Current

Background — Current proteins under consideration for use as prophylactic drugs in the treatment of organophosphorus nerve agent intoxication lack sufficient circulatory half life to afford reasonable *in vivo* protective efficacy for extended periods of time. Most are cleared from circulation rapidly and possess half lives on the order of hours. The vast majority of proteins found in the blood/plasma are glycosylated, meaning they have carbohydrates (sugar molecules) covalently linked to their surface. Using exogenous or "non-self" proteins with different properties, or entirely lacking this glycan surface modification, makes them susceptible to clearance from the blood stream by multiple mechanisms and it is generally accepted that this rapid clearance results from the carbohydrate decoration on the surfaces of these proteins and not the protein sequence itself. Of those proteins under investigation, the most promising are of nonhuman origin (bacterial) or utilize nonhuman expression systems for their production (bacterial, plant, transgenic animals). To extend the circulatory half lives of these molecules to days, rather than hours, it is necessary to modify their surface decorations. Using an expression system that can accomplish this during expression is a significant cost-saving measure over post-purification modification by chemical means.

Approach — To address the issue of "non-self" carbohydrates, this project is using human embryonic kidney cells (HEK 293) to express a protein encoded by a gene of bacterial origin. This protein has been successfully expressed and glycosylated in transgenic corn.



Three-dimensional structure of OPH with a molecule of the nerve agent VX bound in one of the two active sites.

Accomplishments — The genetic information encoded by the bacterial organophosphorus hydrolase (OPH) gene has been optimized for expression in human cells. To achieve this, the codons for each amino acid of OPH were modified to maximize translation efficiency for high levels of protein expression. The humanized OPH gene was used to generate transient and stably transfected HEK cell lines, and these transgenic cell lines express functional humanized OPH at a constant level over time. Preliminary data indicates the protein hydrolyses the pesticides paraoxon and demeton-S, as well as the nerve agent VX, but is not glycosylated as expected. It has not been determined if the protein is never glycosylated or if it is but then is processed in the cell removing the carbohydrates. Detailed mass analysis is planned for peptide fragments to determine

if there is carbohydrate remains on the amino acid attachment sites to answer this. New gene constructs are being developed to have the expressed protein secreted from the cell into the media as it is being expressed to alleviate intracellular processing.

2012 IR&D Annual Report

Applied Dermal Delivery Nanoformulations, 01-R8321

Principal Investigators
Gianny J. Rossini
Lucy M. Kimmel
Alda E. Flores

Inclusive Dates: 07/11/12 – 11/11/12

Background — Transdermal drug delivery represents a promising alternative to oral, intravascular, subcutaneous and transmucosal routes of delivery. Gels, patches, and creams are the most frequent and effective alternatives to oral delivery, and after an oral route, are the most common way to administer drugs. In addition, transdermal delivery provides convenient and pain-free self-administration for individuals who need daily medications. It eliminates frequent dosing administration and plasma level peaks and valleys associated with oral dosing and injections; dermal delivery can maintain a constant drug concentration even if the drug has a short half-life in blood. Additionally, the transdermal drug delivery market was worth $12.7 billion dollars in 2005 and is expected to reach $32 billion by 2015. Advanced dermal delivery using nanoformulations is the topic of Project 01-8276, "Combined Laser and Medicated Scar Improvement Therapies." The objective of that project is to develop advanced flexible liposomes known as ethosomes, transferosomes and cubosomes, which have been validated for penetration of skin barriers. Flexible liposomes loaded with corticosteroids will be used as an anti-scarring agent to be used in combination with a carbon dioxide fractional ablative laser. The concept is that the ablative laser will produce a micro array of small pores on the skin, providing an ideal dermal drug delivery opportunity for flexible liposomes. During the execution of 01-8276, the project team developed a network of collaborators that have interest in dermal formulations for their drug candidates. The goal of this project is to formulate those drugs and supply the investigators with samples to conduct animal testing and collect preliminary data.

Approach — Flexible liposomes are made by self-assembled nanoprecipitation of lecithin, or similar phospholipids, from an ethanol solution into a nonsolvent designed for the specific drug-lipid combination. Hydrophilic drugs are loaded in the aqueous core compartment and hydrophobic drugs are normally loaded in the lipid compartment. Basic formulation detergents, such as oleic acid, sodium cholate, turocholate and other additives, are added to modify flexibility and stability. Cubosomes, another kind of flexible liposome, are made with waxy lipids and sticky solids such as monoolein plus a starch coating. It was found that a water-soluble, noncohesive starch coating on the waxy lipid prevents agglomeration and allows control of particle size and control-release rates; in addition, the continuous nature of the particles allows dissolution of otherwise hard to dissolve compounds. The third kind of liposome, transferosomes, are made by the classic thin film method where a lipid/chloroform solution is dried in a round bottle to form a thin film, followed by hydration in buffer and reduction of particle size by extrusion in a stack of nanoporous membranes. Flexibility is generated with the use of detergents such as oleic acid and others increasing membrane fluidity and creating disruptions in the liposome membrane. Avoiding the use of cholesterol or other rigid structural components is also important to maximize flexibility of liposomes. Nanoparticles are measured using a photon correlation spectroscopy (PCS) particle analyzer. Flexibility index is measured by extrusion across a nanoporous size membrane under constant nitrogen pressure. Skin permeability is tested using a Franz cell device setup with skin from cadavers obtained under Institutional Review Board (IRB) regulations or most commonly using synthetic membranes that mimic skin permeability. The procedure is started by applying a full load of samples under occlusive conditions and collecting fractions over time and analyzing to measure drug content, usually 7 hours for human skin

and 24 hours for synthetic skin. To measure efficacy of formulated drugs on a skin sample, we use a real-time reverse transcription polymerase chain reaction (RT-PCR) technique that allows us to monitor gene expression at the messenger ribonucleic acid (mRNA) level.

Accomplishments — Flexible dermal formulations such as cubosomes, ethosomes, and transferosomes have been prepared and characterized for drug loading, drug release, particle size, drug permeability, and drug efficacy by RT-PCR. Collaborators at national research laboratories will test SwRI's samples using animal models of Leishmaniasis, a dermal parasitic disease. Leishmaniasis is commonly found in many tropical and subtropical countries and is also found in parts of about 88 countries around the world.

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2012 IR&D Annual Report

In-situ Mass Spectrometry of Cave Atmospheres, 15-R8254

Principal Investigators
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Kathleen Mandt
Joseph Mitchell
Evelynn Mitchell
Kerri Younkin

Inclusive Dates: 09/08/11 – 01/03/12

Background — The motivation for this project was the desire to use field-deployable mass spectrometry as an analytical chemistry tool in the harsh environment of caves. Such an application has potential benefits for cave biologists studying the disease white nose syndrome (WNS), which has killed millions of bats in the Northeastern United States. Field deployment of mass spectrometry in the harsh and poorly understood environments of caves is also an analog for a number of comparable engineering constraints imposed upon analytical instruments designed for planetary surface environments. In repeated searches of the scientific literature, no record could be found for the field deployment of a mass spectrometer in a cave environment, though many caves samples had been returned to the laboratory for subsequent analysis. Numerous groups currently developing mass spectrometers for analytical purposes have the capability to field-deploy instrumentation in caves. Furthermore, the recent discovery of caves on the surface of the Moon and Mars made successful deployment of mass spectrometry into caves relevant to future goals of NASA and the space science community. For these reasons, rapid deployment of a prototype instrument was essential for establishing SwRI as a leader in deploying mass spectrometry in harsh environments.

Approach — A prototype mass spectrometer was constructed from a commercial off-the-shelf (COTS) residual gas analyzer (RGA). The RGA was serviced by a miniature turbomolecular pump and four-stage diaphragm pump. The completed prototype system was tested in the laboratory prior to field deployment. A number of cave locations were investigated and the four selected for analysis were Bracken Bat Cave, Natural Bridge Caverns, Robber Baron Cave and Wurzbach Bat Cave. Tyvek® suits, respirators and decontamination protocol were used in Bracken Bat Cave due to the hazardous environment posed by airborne microbes, flesh-eating insects and toxic levels of ammonia and urea from millions of Mexican

Robber Baron Cave was one of four investigated by the project team.

Freetail Bats. Air samples at Bracken Bat Cave were also obtained using stainless steel canisters for subsequent laboratory analysis by gas chromatograph mass spectrometry. In addition to these four cave sites, air from two aquifer wellheads was monitored by the cave mass spectrometer (CMS) employing a second diaphragm pump for drawing well air to the CMS from 60 meters below the surface. Atmospheric data from outside each cave and wellhead were also obtained for comparison with the cave and well data.

Accomplishments — Approval for the CMS project was granted September 9, 2011, and at 2:41 p.m., on Friday, September 16, 2011, a prototype CMS was carried into Bracken Bat Cave. It is believed that this is the first deployment of a mass spectrometer in a cave. The humidity was at 99 percent and the temperature was 110 degrees F. Data from each cave showed expected increases in CO_2 concentration. Peculiar to the toxic environment of Bracken Bat Cave were data suggesting elevated levels of oxygen. The second wellhead exhibited no detectable air flow, but air at the first wellhead was moving at a significant velocity. This first wellhead also showed detectable levels of volatile, low-mass hydrocarbons. Subsequent examination of the Bracken Bat Cave air samples showed numerous organic compounds, including aldehydes, ketones and nitriles, and also suggested further investigation of this environment should be a priority for the cave, bat and environmental science communities. The prototype CMS concept was proven to be a valid analytical approach for future cave investigations.

2012 IR&D Annual Report

Combined Numerical and Experimental Studies for Release Kinetics of Embedded Drugs from Deformable Engineered Vectors in Response to External Stimuli, 20-R8305

Principal Investigators
Hakan Başağaoğlu
Gianny Rossini
John T. Carrola Jr.

Inclusive Dates: 01/04/12 – Current

Background — The main objective of this study is to develop a novel two- and three-dimensional numerical model to simulate (i) the fate and transport of nano- to micron size deformable capsules with embedded nanodrugs; (ii) releases of embedded nanodrugs in response to cumulative mass erosion on the particle surface induced by dynamic flow shear rates; and (iii) local concentrations of the released nanodrugs along the flow pathways of deformable particles. To our knowledge, there has been no numerical model developed with these capabilities. The project also includes experimental tasks focusing on (i) fabrication of deformable capsules, (ii) flexibility measurements of the capsules, and (iii) release kinetics of embedded drugs under controlled shear rates. To date, only limited and incomplete experimental data on release kinetics of embedded drugs from deformable particles have been presented in the literature. In this project, experimental data will be used to validate and enhance the numerical model.

Approach — A new numerical model, based on the lattice-Boltzmann method, will be developed to simulate trajectories of deformable particles in a transient flow field. As part of this model, a new algorithm, based on the Catmull-Rom Splines method and topological relations, will be developed to keep track of all interior and exterior boundary nodes in the vicinity of an arbitrarily deformed surface of a mobile particle, which will be central to deformable particle-fluid hydrodynamics calculations. Moreover, a new equation based on existing literature data will be formulated to calculate shear-induced cumulative mass erosion rates on deformable particle surfaces as a function of local shear stress and flow velocity at particle boundary nodes. To simulate local concentrations of the released nanodrugs from deformable particles, a stochastic-differential equation will be formulated. The new algorithm and the new equations will be integrated into the master code, which we developed previously. For the experimental tasks, new capsules (liposomes) will be developed with tunable flexibilities using different surfactants. The flexibility (deformability) test will be performed using a Lipex extruder to quantify flexibility indices. Release kinetics of embedded drugs will be quantified after flow pressure generated by circulating the sample using a peristaltic pump through narrow capillary tubing mimicking the conditions of in vivo capillary blood circulation. Experimental data on the release kinetics of Fluorescein from deformable capsules will be used for model validation.

Accomplishments — SwRI researchers successfully developed a new algorithm, a Triangular Caging algorithm, as a stand-alone module to locate all interior and exterior boundary nodes of an arbitrarily deformable surface of a mobile particle. A new equation was formulated and coded as a standalone module to simulate shear-induced release kinetics of nanodrugs from mobile deformable particles. For the experimental tasks, surfactants were used to successfully fabricate three different types of flexible capsules, each with different degrees of flexibility, and measured their flexibility indices in repeatable experiments. Findings were presented November 2 at the American Society of Mechanical Engineering

Conference in Houston. After completing scoping analysis, proposals will be prepared for the Defense Advanced Research Projects Agency and the National Institutes of Health.
