The Department of Mechanical Engineering at
The University of Texas at El Paso
Proudly Presents

1st Southwest Energy Science & Engineering Symposium

Saturday, April 16, 2011

The University of Texas at El Paso
500 W. University Ave.
El Paso, Texas 79968

1st Southwest Energy Science and Engineering Symposium

April 16, 2011
Hilton Garden Inn
University of Texas El Paso
El Paso, Texas 79968

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FOREWARD

Welcome to the Southwest Energy Science and Engineering Symposium sponsored by Shell. The purpose of the symposium is to encourage communication among the engineers and scientists in and around the El Paso area's universities and industries.

The following individuals and organizations are acknowledged for their assistance with the symposium.

Technical Committee:	Dr. Ahsan Choudhuri, Chair Dr. Norman Love Dr. Vinod Kumar University of Texas El Paso
Logistics Committee:	Nate Robinson, University of Texas El Paso Virginia Lee, University of Texas El Paso
Hosted By:	Center for Space Exploration and Technology Research (cSETR) University of Texas El Paso
Welcome and Introduction:	Dr. Richard Schoephoerster Dean, College of Engineering University of Texas El Paso
Session Chairs:	Dr. David Nemir, TXL Group Inc. Dr. Felicia Manciu, University of Texas El Paso Tommy Goolsby, Sandia National Laboratory John Scott, NASA Lyndon Johnson B. Space Center Dr. Evgeny Shafirovich, University of Texas El Paso Dr. Vinod Kumar, University of Texas El Paso Dr. C.V. Ramana, University of Texas El Paso Dr. Jose Espiritu, University of Texas El Paso Dr. Mir Hayder, University of Texas El Paso
Keynote Address:	Bob Malone President and CEO of the First National Bank Sonora, Texas Former Chairman and President of BP America

Southwest Energy Science and Engineering Symposium

UNIVERSITY OF TEXAS EL PASO
APRIL 16, 2011

7:00 am	**REGISTRATION**	Hilton Garden Inn	Main Lobby
8:00 am	**BREAKFAST**	Hilton Garden Inn	Del Norte Ballroom
8:30 am	**WELCOME**	Dr. Richard Schoephoerster Dean, College of Engineering University of Texas El Paso	Del Norte Ballroom
9:15 am	**PARALLEL TECHNICAL SESSIONS I**		
	Session 1-A	Materials Technology I	Room: Del Norte I
	Session 1-B	Combustion and Propulsion I	Room: A-129
	Session 1-C	Modeling and Emerging Technologies I	Room: Del Norte II
	Session 1-D	Sustainable and Renewable Energy	Room: Board Room
	Session 1-E	Materials and Design	Room: Miner Room
	Session 1-F	Advanced Aerospace Systems	Room: Del Norte III
10:30 am	**BREAK**		
10:45 am	**PARALLEL TECHNICAL SESSIONS II**		
	Session 2-A	Materials Technology II	Room: Del Norte I
	Session 2-B	Combustion and Propulsion II	Room: A-129
	Session 2-C	Modeling and Emerging Technologies II	Room: A-227
	Session 2-D	Heat Transfer, Chemistry, and Fluids	Room: Del Norte II
	Session 2-E	Materials and Geological Science	Room: Miner Room
	Session 2-F	Energy Enabling Technologies	Room: Del Norte III
	Session 2-G	Advanced Systems	Room: Board Room
11:45 am	**LUNCH**		Del Norte Ballroom
12:00 pm	**LUNCHEON ADDRESS**		Del Norte Ballroom

Bob Malone
President and CEO of the First National Bank
Sonora, Texas
Former Chairman and President of BP America

1:00 pm	**ADJOURN**

ABOUT THE SPEAKER

Bob Malone is currently the President and CEO of The First National Bank of Sonora, Texas. He was appointed by the Board of Directors in October of 2009. The First National Bank of Sonora is a $200 million community bank with branches in Sonora, San Angelo, and Boerne, Texas. Prior to his retirement from BP in March of 2009, he served as an Executive Vice President of BP p.l.c. and was the Chairman and President of BP America Inc. from July 1, 2006 until February 1, 2009. During that time he was BP's chief representative in the United States and served on BP's Executive Management team. He was based in Houston, Texas where BP business units are involved in oil and natural gas exploration and production, refining, chemicals, supply and trading, pipeline operations, shipping and alternative energy.

In the US, BP owns over $40 billion in fixed assets and employs some 37,000 people. The company is the nation's largest producer of oil and natural gas and the second largest gasoline retailer. Prior to this role, Mr. Malone was chief executive of BP Shipping Limited responsible for the operation of the energy industry's largest oil and natural gas fleet. During his tenure, BP Shipping accepted delivery of almost 50 new, double hull tankers.

During his 35 year career Mr Malone has developed a reputation for building teams, driving change, improving operating and safety performance, and changing cultures. As well as increasingly senior positions within Kennecott Copper Corporation, the Standard Oil Company of Ohio (Sohio), the Carborundum Company and BP, Mr Malone had a four-year assignment as president, chief executive officer and chief operating officer of Alyeska Pipeline Service Company, operator of the Trans Alaska Oil Pipeline.

Mr. Malone was raised in the Northeast Texas town of Daingerfield. He holds a Bachelor of Science in Metallurgical Engineering from the University of Texas at El Paso, and was an Alfred P. Sloan Fellow at the Massachusetts Institute of Technology where he received a Master of Science in Management. In 2003, he was selected as a Distinguished Alumni of the Year by the UT at El Paso Mr. Malone was appointed by the Governor of California as a founding Board Member of the California Climate Action Registry, appointed by the Governor of Alaska as a founding Board Member of the Alaska Children's Trust and has served on the Board of Regent for the University of Alaska system. He has also served on the Board of Trustees of the National Urban League, the Foreign Policy Association, the Pacific Council, the National Petroleum Council, and the Museum of Science and Industry in Chicago. Until early last year he served on the Executive Committee and Board of Directors for the American Petroleum Institute (API), the Executive Committee and Board of Directors of the Greater Houston Partnership and a member of the Business Roundtable.

He currently serves as an Independent Director of the Halliburton Company, the second largest oil field service company in the world and Peabody Energy Company, the world's largest publicly owned coal company. He is also a Director of the First National Bank of Sonora. Mr. Malone and Diane Trujillo Malone have been married for over 36 years. They have two adult sons. Ryan is an engineer working in the oil industry out of Houston and son Michael is a law school student at St. Mary's University in San Antonio.

PARALLEL TECHNICAL SESSIONS I

Session 1-A: **Materials Technology I** Room: Del Norte Ballroom I
Session Chair: David Nemir, TXL Group Inc. Hilton Garden Inn

9:15 am	**Synthesis and Characterization of $NiFe_{1.925}Dy_{0.075}O_4$ for Electrochemical Energy Devices** *K. Kamala Bharathi, UTEP*
9:30 am	**Spectroscopic Analysis of WO_3 for Sensor Applications** *J.L. Enriquez, UTEP*
9:45 am	**Synthesis and Microstucture of Gd_2O_3-HfO_2 Thermal Barrier Coatings** *C.K. Roy, UTEP*
10:15 am	**Growth, Microstructure and Optical Characteristics of $W_{0.80}Ti_{0.2}0O_3$ Thin Films for h2s Sensors in Coal Gasifiers** *G. Baghmar, UTEP*

Session 1-B: **Combustion and Propulsion I** Room: A-129
Session Chair: Evgeny Shafirovich, UTEP Engineering Annex

9:15 am	**Study on the Feasibilities of Reducing the Operating Temperatures in Chemical Oxygen Generators** *A. Garcia, UTEP*
9:30 am	**Combustible Mixtures of Lunar Regolith with Metals** *C. White, UTEP*
9:45 am	**Exothermic Welding in Microgravity** *A. Delgado, UTEP*
10:15 am	**Design and Future Applications of an Optically Accessible Combustion Chamber Test Rig** *C. Navarro, UTEP*

Session 1-C: **Modeling and Emerging Technologies I** Room: Del Norte Ballroom II
Session Chair: Tommy Goolsby, Sandia National Labs Hilton Garden Inn

9:15 am	**Validation Study of a Numeric Model for Rocket Engine Cooling Channel Flow** *C. Bradford, UTEP*
9:30 am	**Applied Variational Methods for Simulations of Newtonian Flow Through Porous Spaces** *P. Delgado, UTEP*
9:45 am	**A Third Order Non-Oscillatory Transport Scheme for Atmospheric Modeling** *K. Katta, UTEP*
10:15 am	**Computational Thermal Analysis and Measurement of the Salt Gradient Stability in a Solar Pond** *E. Busquets, UTEP*

PARALLEL TECHNICAL SESSIONS I

Session 1-D: **Sustainable and Renewable Energy** Session Chair: Jose Espiritu, UTEP	Room: University Board Room Hilton Garden Inn
9:15 am	**Conceptual Development of an Expert System to Aid Designers in the Selection of Sustainability Methods** *P. Acosta, UTEP*
9:30 am	**A Multiple Objective Approach to Solve the Parallel-Series System Redundancy Allocation Problem with Environmental Constraints** *O. Moreno, UTEP*
9:45 am	**Optimization of Wind Turbine Placement Using Viral System** *C. Villareal, UTEP*
10:15 am	**A Post-Pareto Analysis to Solve the Renewable Energy System Integration Problem Considering Multiple Objectives** *N. Lopez, UTEP*
Session 1-E: **Materials and Design** Session Chair: C.V. Ramana, UTEP	Room: Miner Room Hilton Garden Inn
9:15 am	**Thermal Barrier Coatings of High Heat Flux Thrust Chambers** *C. Bradley, UTEP*
9:30 am	**Thermal Stress Analysis of Titanium Nitride Coating on Silicon Utilizing a Combined Analytical Model** *M. Hernandez, UTEP*
9:45 am	**A Finite Element Damage Model for Adhesive Failure of Mastic-Aggregate Interfaces** *M. Hossain, University of New Mexico*
10:15 am	**Effect of Dwell Time, Loading Rate and Unloading Rate on Viscoelastic Material in Nanoindentation Test** *H. Faisal, University of New Mexico*
Session 1-F: **Advanced Aerospace Systems** Session Chair: John Scott, NASA	Room: Del Norte Ballroom III Hilton Garden Inn
9:15 am	**Cryogenic Feed System Development and Condensation for LOX/Hydrocarbon Propulsion Research** *F. Pineda, UTEP*
9:30 am	**Development of a Heat Flux Test Rig to Study Cryogenic Heat Transfer Characteristics** *A. Trejo, UTEP*
9:45 am	**Modal Analysis of a Low Thrust Torsional Thrust Balance for the Performance Evaluation of 5N Class Thrusters** *J. Flores, UTEP*
10:15 am	**Development of An Optically Accessible High Pressure Turbine Combustor** *S. Sarker, UTEP*

PARALLEL TECHNICAL SESSIONS II

Session 2-A: **Materials Technology II** Session Chair: Felicia Manciu, UTEP	Room: Del Norte Ballroom I Hilton Garden Inn
10:45 am	**Thermoelectric Generation for Waste Heat Harvest** *D. Nemir, TXL Group Inc.*
11:00 am	**Explosive Consolidation of Thermoelectric Materials** *J. Beck, TXL Group Inc.*
11:15 am	**High Temperature Tolerance and Chemical Stability of YTTRIS-Stabilized Hafnia** *M. Noor-A-Alam, UTEP*
11:30 am	**Present and Future of Thermoelectrics** *H. Lopez, UTEP*
Session 2-B: **Combustion and Propulsion II** Session Chair: John Scott, NASA	Room: A-129 Engineering Annex
10:45 am	**HTP Decomposition in Millimeter Scale Channel Type Catalytic Reactors** *J. Valenzuela, UTEP*
11:00 am	**An Experimental Investigation of CH_4-O_2 Flame Stability in a Laboratory Scale Tubular Burner** *M. Islam, UTEP*
11:15 am	**Characterization of Turbulent Flow Field of Syngas Flames in a Laboratory Scale Tubular Burner** *V. Ardha, UTEP*
11:30 am	**Experimental Measurements of Radiative Heat Release Rates of CH_4-O_2 and CH_4-CO_2-O_2 Flames for Advanced Combustors** *B. Dam, UTEP*
Session 2-C: **Modeling and Emerging Technologies II** Session Chair: Vinod Kumar, UTEP	Room: A-227 Engineering Annex
10:45 am	**Short Term Electric Power Consumption Forecasting Using Linear Programming Support Vector Regression** *P. Rivas-Perea, UTEP*
11:00 am	**Scalable Three-Dimensional Geometry Preprocessor for Molecular Dynamics Analysis** *J. Motta-Mena, UTEP*
11:15 am	**Large Eddy Simulation of Flame Flashback in a Swirl-Stabilized Gas Turbine Combustor** *G. Corona, UTEP*
11:30 am	**Numerical Analysis of Drag on Non-Spherical Particles in Fluidized Beds** *M. Ruvalcaba, UTEP*

PARALLEL TECHNICAL SESSIONS II

Session 2-D: **Heat Transfer, Chemistry and Fluid Dynamics** Session Chair: Evgeny Shafirovich, UTEP	Room: Del Norte Ballroom II Hilton Garden Inn
10:45 am	**Study of the Copper-Chlorine Thermochemical Cycle for Hydrogen Production from Water** *F. Alvarez, UTEP*
11:00 am	**Study of CO_2 Reduction in the SnO_2/SnO Thermochemical Cycle** *A. Garcia, UTEP*
11:15 am	**Computational Fluid Dynamics in Veins** *C. Barraza, UTEP*
11:30 am	**Computational Fluid Dynamics for Parachute Analysis** *J. Valles, UTEP*

Session 2-E: **Materials and Geological Science** Session Chair: C.V. Ramana, UTEP	Room: Miner Room Hilton Garden Inn
10:45 am	**Effect of Growth Temperature On Optical, Structural and Electrical Characteristics of Y_2O_3 Films** *V. Mudavakkat, UTEP*
11:00 am	**A Study of WO_3 and $W_{0.95}Ti_{0.05}O_3$ Thin Films Using Comparative Spectroscopy** *Y. Yun, UTEP*
11:15 am	**Changes in the Trace Metal Chemistry of Iron-Oxides Formed in the Presense of Bacteria** *K. Schnittker, UTEP*
11:30 am	**Bioleaching of Ilmenite and Basalt in the Presence of Iron-Oxidizing and Iron-Scavenging Bacteria** *J. Navarrete, UTEP*

Session 2-F: **Energy Enabling Technologies** Session Chair: Jose Espiritu, UTEP	Room: Del Norte Ballroom III Hilton Garden Inn
10:45 am	**Hydrodynamic Analysis of a Fluidized Bed Operating with Spherical and Non-Spherical Particles** *M. Rahman, UTEP*
11:00 am	**Zero Net Carbon Study** *R. Martinez, UTEP*
11:15 am	**Point Site Selection for Sequestering CO2: Determining the Impact of an Earthquake on Seal Integrity of a Reservoir Cap-Rock** *S. Afrin, UTEP*
11:30 am	**Fundamental Study of a Beam Vibration Frequency** *R. Chacon, UTEP*

PARALLEL TECHNICAL SESSIONS II

Session 2-G: **Advanced Systems**	Room: University Board Room
Session Chair: Mir Hayder, UTEP	Hilton Garden Inn

10:45 am	**A Variational Approach to One Phase Non-Newtonian Flow in a Circular Duct** *F. Chen, UTEP*
11:00 am	**Development of a Torsional Thrust Balance for the Performance Evaluation of 5N Class Thrusters** *M. Ingle, UTEP*
11:15 am	**Spatio-Temporal Cardiac Pacing Sites Localization and Time Varying Pericadium Potential Maps Projection Using Egg Precordial Leads and a Single Moving Dipole Model** *J. De La Cruz, UTEP*

VALIDATION STUDY OF A NUMERIC MODEL FOR ROCKET ENGINE COOLING CHANNEL FLOW

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ABSTRACT

An important key to the progression of the field of engineering research and design is the ability to be confident in the work of previous researchers. This is especially important in the field of regeneratively cooled rocket engines, particularly the knowledge of the coolant behavior inside the coolant passages where high heat and stress loadings are present near combustible materials. With that prior research and the confidence in it, additional research can be conducted in the future. Additionally it is important to have confidence in the research methodology, gained by replicating the results of previous researchers. As the field of engineering increasingly relies upon complex commercially available computer software to perform simulations, confidence in the utilization of that software is also important. In the present work a previously published research reference article concerning CFD simulations of rocket engine coolants is replicated using the software FLUENT. The methodology required to do so in FLUENT is presented, and the results are compared to the results of the reference article for validation. Despite some lack of detail in the reference article and some limitations of FLUENT, both presented and discussed, the data correlation is strong.

As part of the 1st Southwest Energy Science and Engineering Symposium, held at the University of Texas El Paso, continuing research information not found in the above article will be discussed.

* The material is based upon work supported by NASA under award No(s) NNX09AV09A

APPLIED VARIATIONAL METHODS FOR SIMULATION OF NEWTONIAN FLOW THROUGH POROUS SPACES

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ABSTRACT

Variational method is a promising way to study the kinetic behavior and storage potential of carbon dioxide (CO2) at the porous scale in the presence of other phases. The current study validates variational solutions for single and two-phase Newtonian flow through angular pores for special geometries whose analytical and/or empirical solutions are known. The hydraulic conductance for single phase flow through a triangular duct was also validated against empirical results. These results were validated against empirical results derived from lubricant theory. The variational method predicted flux and hydraulic conductance through the chosen geometries within 2-5% error with one parameter, and <2% for two parameter in circular geometry ratio of inner to outer radius <0.2). The results of this study indicate that this technique can potentially be applied to non-Newtonian and multiphase flow, and flow domains with irregular geometries. This provides a powerful technique for pore-scale network modeling of carbon sequestration reservoir flow.

STUDY OF THE COPPER-CHLORINE THERMOCHEMICAL CYCLE FOR HYDROGEN PRODUCTION FROM WATER

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ABSTRACT

Thermochemical cycles possess a potential capability in the field of hydrogen production from water, with no greenhouse gas generation. One promising candidate is the copper-chlorine cycle, which requires relatively low temperatures. This attribute makes the cycle suitable for using with supercritical water-cooled and fast sodium-cooled nuclear reactors as well as with solar power towers. However, one step in this cycle, viz. the hydrolysis reaction of cupric chloride, presents challenges such as a parallel thermolysis reaction, which decreases the yield of the desired product (copper oxychloride), and the need for excess steam. The objective of the present work was to enhance the hydrolysis of copper chloride in the laboratory reactor developed in Argonne National Laboratory. Specifically, this research effort was intended to experimentally verify the predicted positive effect of low pressure on the hydrolysis of copper chloride. The reactor was modified to allow operation at reduced pressure. The conducted experiments, followed by chemical and X-ray diffraction analyses, have confirmed that the hydrolysis reaction is enhanced as the reactor pressure is reduced. Since the conversion rate is improved at lower pressures, the amount of required water can be reduced, decreasing the capital cost of the process in industrial application.

*This work has been supported by DOE and NSF (Faculty and Student Teams Program). The authors thank Magali Ferrandon and Michele Lewis of ANL for their collaboration.

STUDY OF CO_2 REDUCTION IN THE SnO_2/SnO THERMOCHEMICAL CYCLE

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ABSTRACT

The increasing concentration of CO_2 in Earth's atmosphere is a matter of great concern when discussing energy and sustainability topics. Also, the United States' dependence on imported oil is an immediate, more urgent matter to address. One approach for confronting both problems is splitting of the CO_2 molecule into C, CO, and O_2. The obtained C and CO can then be converted (with addition of H_2) into synthetic liquid fuels, using available technologies. Currently, CO_2 splitting can be achieved by high temperature (> 3000 K) decomposition, which is not practical. The proposed project focuses on an alternative pathway to split CO_2 that occurs at lower temperatures. This pathway involves solar thermochemical cycles including: oxidation of some materials by CO_2 and regeneration of these materials using concentrated solar energy. In the present work, thermodynamic analysis for the material oxidation (i.e., CO_2 reduction) step in the SnO_2/SnO thermochemical cycle is conducted. The results predict a rather wide temperature range where full conversion of CO_2 to C occurs. The results of an attempt to verify the predictions experimentally are reported.

*The University Research Institute program has supported this work

STUDY ON THE FEASIBILITIES OF REDUCING THE OPERATING TEMPERATURES IN CHEMICAL OXYGEN GENERATORS

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ABSTRACT

Although chemical oxygen generators are widely used in aircraft, submarines, spacecraft, and other applications, problems such as combustion instabilities and a risk of fire still remain. For example, due to malfunction of an oxygen generator, fire occurred onboard the Mir Space Station in 1997. It is thus important to improve the process stability and fire safety of chemical oxygen generators. Chemical compositions for oxygen generators include an oxygen source such as sodium chlorate (NaClO3), a transition metal oxide as a catalyst, and a metal fuel to provide energy for self-sustaining combustion. Eliminating or decreasing the metal fuel would decrease the operating temperatures and improve the fire safety of the generators. To make a well-founded conclusion on the feasibility of this approach, information on the decomposition and adiabatic combustion temperatures of $NaClO_3$-based compositions with different concentrations of catalyst and metal fuel is required. In the present paper, thermogravimetric analysis of $NaClO_3$ mixtures with different concentrations of Co_3O_4 catalyst and metal fuel (iron and tin) is conducted. For the same mixtures, thermodynamic calculations are carried out. A strong effect of nanoscale Co_3O_4 powder on the decomposition temperature of $NaClO_3$ is reported. For each mixture, comparison of the measured decomposition temperatures and calculated adiabatic combustion temperatures provides the values of temperature margin available for heat loss in the oxygen generator. In addition, a feasibility of decreasing the decomposition temperature of $NaClO_3$ by high-energy mechanical milling of its mixtures with Co_3O_4 is studied. A planetary ball mill (Frietsch Pulveristte 7 premium line) is used for these experiments.

*This work was partly supported by NASA through a subcontract from Jacobs Technology. The authors thank Dion Mast and Steve Hornung of NASA WSTF for their collaboration.

LARGE EDDY SIMULATION OF FLAME FLASHBACK IN A SWIRL STABILIZED GAS TURBINE COMBUSTOR

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ABSTRACT

Future generation turbine system for power production by using coal as a primary fuel source is expected to increase for ensuring domestic and global energy issues. General Electric and Siemens Power Group incorporated with National Energy Technology Laboratory are developing a fuel flexible (syngas or hydrogen) gas turbine for integrated gasification combined cycle (IGCC) applications that are capable of 45-50% HHV plant efficiency, near-zero emissions. The flame dynamics of hydrogen content fuel, especially syngas (primary constituents are H_2 and CO) deviates from established models built on hydrocarbon fuels and has limited data available for modeling. However, swirl stabilized lean premixed combustor has brought a concern, flame flashback, where the flame, instead of stabilizing completely within the combustion chamber, propagates upstream into the premixing zone against the gas stream. Accurate modeling of flashback phenomena is very important for the development of future generation gas turbine combustors. Recent advances in Large Eddy Simulation (LES) allows us to model time dependent problems unlike conventional Reynolds Average models in which the velocity is a function of space only. In LES the large scales or the energy containing scales are resolved and the smaller scales are modeled. The advantages of LES over RANS have received attention due to high computational cost. The current work aims to develop a combustion model using LES to simulate the flashback phenomena for methane and syngas fuels using both commercial codes and open source codes. An LES model is developed for both isothermal and reacting flow in a laboratory scale gas turbine combustor using Fluent and OpenFoam. The isothermal model is then validated against experimental data obtained from the high speed Particle Image Velocimetry (PIV). The ultimate objective of the project is to match the combustion model with the experimental results obtained from the high speed PIV, and then modify the geometry and operating conditions of the model to explore ways to mitigate Combustion Induced Vortex Breakdown (CIVB) flashback.

* This work has been supported by U.S. Department of Energy, under awards DE-FG26-08NT0001719.

COMBUSTIBLE MIXTURES OF LUNAR REGOLITH WITH METALS

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ABSTRACT

Future exploration missions to the Moon and Mars will involve construction of habitats, radiation shields, landing/launching pads, roads, and other structures on the lunar surface. The construction materials could be produced *in situ* from regolith by sintering at high temperatures. Heating the regolith, however, would require significant energy input. An alternative approach, advanced in the present work, involves combustible mixtures of regolith with metals such as aluminum and magnesium. An important advantage of this method is that a relatively small amount of energy is required for ignition, while the high temperatures during the combustion process are generated by the reaction heat release. In the present paper, the adiabatic flame temperature and combustion products were calculated for the mixtures of JSC-1A lunar regolith simulant with aluminum and magnesium, as well as with titanium/boron pair. It was shown that at the additive concentrations of 20-30 wt%, magnesium exhibits the highest temperatures. Combustion of magnesium/JSC-1A mixture pellets was studied experimentally in argon environment. To facilitate ignition and achieve stable combustion, the original JSC-1A powder was ground in a ball mill. It was shown that with increasing the milling time of JSC-1A, the combustion front velocity of Mg/JSC-1A mixture increases. A decrease in argon pressure from 90 kpa to 10 kPa does not influence the front velocity.

* The material is based upon work supported by NASA under award No(s) NNX09AV09A

A THIRD-ORDER NON-OSCILLATORY TRANSPORT SCHEME FOR ATMOSPHERIC MODELING

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ABSTRACT

Atmospheric numerical modeling has been going through drastic changes over the past decade, mainly to utilize the massive computing potential of petascale systems. This obliges modelers to develop grid systems and numerical algorithms that facilitate exceptional level of scalability on these systems. The numerical algorithms that can address these challenges should have the local properties such as the high on-processor operation count and minimum parallel communication i.e. high parallel efficiency, it should also satisfy the following properties such as inherent local and global conservation, high-order accuracy, geometric flexibility, non-oscillatory advection, positivity preservation. In the present work, a third-order semi-discrete genuinely multidimensional central scheme for systems of conservation laws and related convection-diffusion equations, is considered to address the challenges mentioned above, this scheme is constructed by Kurganov et al. The construction is based on a multidimensional extension of using more precise information of the local speeds of propagation, and integration over non-uniform control volumes, this scheme is a simple genuinely multidimensional semi-discrete scheme. A two-dimensional piecewise quadratic non-oscillatory reconstruction is employed which ensures the high resolution of the scheme. The scheme is demonstrated for different problems in 1-D, solid-body rotation and deformational flow tests are considered to test the scheme mentioned above in 2-D, some accuracy tests were also performed to test the scheme. The main aim of the project would be to extend the considered scheme to solve compressible Euler equations. Further, to extend the same for Shallow Water model on a cubed sphere.

THERMOELECTRIC GENERATION FOR WASTE HEAT HARVEST

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ABSTRACT

Materials that directly convert heat to electricity are said to have a thermoelectric property. Thermoelectric generators that are built from these materials have no moving parts, are scalable and can capture value from relatively low absolute temperatures and temperature differences. This presentation will review the underlying physics for thermoelectric phenomena and the way in which devices are presently built, highlighting the challenges that traditional materials and manufacturing techniques most overcome for the cost effective capture of electrical energy from waste heat streams. Current work by TXL Group addresses the need for cost reduction by using spraycasting for device preparation. Spraycasting lends itself to high volume production and by building thermoelectric elements into the walls of heat exchangers, electric generation can be implemented as a byproduct of heat exchange. Since every power generation plant and refinery has numerous heat exchangers in boilers, recuperators, condensers and chillers, this presents an opportunity to enhance operating efficiencies throughout the systems by capturing value from otherwise wasted heat energy.

CHANGES IN THE TRACE METAL CHEMISTRY OF IRON-OXIDES FORMED IN THE PRESENCE OF BACTERIA

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ABSTRACT

Bacterial surfaces can act as templates for mineral formation and influence grain sizes, lattice spacing, surface defects, and the amount of trace metals present in the resulting precipitates. These changes can impact the surface reactivity of iron-oxide minerals in natural systems on Earth, but might also be used to identify biologic activity in Martian rocks rich in iron-oxide minerals. For this study we will explore the differences in trace metal incorporation in iron-oxide precipitation experiments with and without the presence of *Pseudomonas Mendocina* (*P. Mendocina*). Precipitation of 2-Line Ferrihydrite (amorphous $5Fe_2O_3 \bullet 9H_2O$) was induced by rapidly raising the pH of an acidic $Fe(III)_{aq}$-bearing electrolyte solution. 2-Line Ferrihydrite is a hydrous ferric oxyhydroxide mineral with an amorphous structure. It is composed of grains smaller than one tenth of a micrometer (i.e., nano-sized particles) and produces only two diffuse peaks when analyzed using powder X-ray Diffraction. Trace metals like Cd, Mn, Co, etc., can substitute into the lattice structure of the amorphous mineral. Over time the ferihydrite transforms into a more crystalline structure (such as Hematite α-Fe_2O_3 or Goethite α-FeOOH), but the trace metals remain trapped within the mineral.

With the use of an Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES) we will measure the amounts of trace metals incorporated in ferrihydrite formed during biotic versus abiotic precipitation pathways. In addition to the possible identification of biosignatures, these results have implications for natural systems because ferrihydrite can control the distributions of trace metals in surface waters and influence their transport from the continent to the oceans. Future work will consist of using different bacteria types and precipitation pathways. Furthermore, we will explore the possibility of altering the mineral properties with bacteria to achieve enhanced performance of iron-oxides used for industrial purposes like photovoltaic coatings.

DESIGN AND FUTURE APPLICATIONS OF AN OPTICALLY ACCESSIBLE COMBUSTION CHAMBER TEST RIG

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ABSTRACT

This paper is intended to describe in detail the design process and considerations made for the development of a Multi-Purpose Optically Accessible Combustor (MOAC). The MOAC is intended to be used for experimentation and research of combustion of liquid and gaseous non-toxic propellants, for the development of single rocket combustion elements, and for fluid mechanics analysis by means of optical diagnostics. Discussion on optical accessibility and geometry required for testing and experimental analysis is explained as well as performance targets that drive the design of the combustor. The material selection for best compatibility with propellants, temperature, and pressure considerations are also discussed. Furthermore, structural analysis by finite element method is used to identify optimum dimensions of the chamber as well as evaluate the chamber's stress and strain structural behavior under predicted pressure and temperature conditions found while operating. Also, there is a discussion about the design process followed to make the chamber modular and accessible for maintenance of optical windows made out of Quartz glass. Sealing and assembly of the entire chamber integration is described along with gasket materials and bolting structure. Considerations for instrumentation, ignition ports and the influence the combustor geometry has on these elements are discussed. Finally, intended uses for the MOAC as well as required injector and ignition parameters are summarized.

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COMPUTATIONAL THERMAL ANALYSIS AND MEASUREMENT OF THE SALT GRADIENT STABILITY IN A SOLAR POND

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ABSTRACT

Thermal Energy Storage (TES) systems are a group of technologies employed for the storage and reuse of energy in the form of heat. A promising technology which has proven to be efficient is the solar pond. Solar ponds combine solar energy collection with long-term storage and can provide reliable thermal energy at temperature ranges from 50 to 90°C. An extensive analysis of the stability of a small scale solar pond prototype is performed. The apparatus, which is composed of an acrylic tube with a hot plate emulating the solar thermal energy input, serves as a model to study various saltwater gradients. The Solar Pond consists of three distinct zones. The first zone, which is located at the top of the pond and contains the less dense saltwater mixture, is the absorption and transmission region, also known as the upper convective zone (UCZ). The second zone, which contains a variation of saltwater densities increasing with depth, is the gradient zone or non-convective zone (NCZ). The main purpose of this zone is to act as an insulator to prevent heat from escaping to the less dense zone, maintaining higher temperatures at deeper zones. The last zone is the storage zone or lower convective zone (LCZ). In this region, the density is uniform and near saturation. Furthermore, two-dimensional computational studies of the heat transfer phenomena using Fluent are performed utilizing user-defined parameters. The results from both the experimental setup and the computational analysis are compared and a Stability Margin criterion is established.

SCALABLE THREE-DIMENSIONAL GEOMETRY PREPROCESSOR FOR MOLECULAR DYNAMICS ANALYSIS

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ABSTRACT

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is a classical molecular dynamics code developed by Sandia National Laboratories, which can be used to model atoms or, more generally, as a parallel particle simulator at the nano, meso, or continuum scale. Molecular dynamics simulations involve the interactions of atomic force fields and atomic potentials between different molecules and the particles that compose them. This technique has been extensively used for the stydy of proteins, biomolecules, as well as inorganic compounds. Interpretation of the molecular structure by LAMMPS specifications is a time consuming task for which an automated method has not been developed. A parametric script is in development, which will enable the user to rapidly organize and compile the necessary parameters for a molecular dynamics simulation using the aforementioned open-source code. The script will gather the necessary information from a series of databases developed in conjunction with the code, will organize the data in a format specified by LAMMPS, and will output a data file and an input file, in agreement with the specific problem at hand, to run the simulation. Furthermore, the script structure allows for the interpretation of a wide variety of compounds and molecular arrangements. The databases and preprocessor will be made an open-source code for anybody wishing to perform molecular dynamics simulations using LAMMPS.

SYNTHESIS AND CHARACTERIZATION OF $NiFe_{1.925}Dy_{0.075}O_4$ FOR ELECTROCHEMICAL ENERGY DEVICES

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ABSTRACT

Being multi-component Fe oxides, ferrites exhibit properties such as various redox states, electrochemical stability, pseudocapacitive behavior by virtue of which they find applications in sensors and supercapacitors. Recently, ferrite compounds have drawn considerable attention for their potential application as electrode materials in Li-ion batteries and solid oxide fuel cells. The structure and electrical properties of Ni ferrites play a key role in the designing of magnetic, electronic and electrochemical devices. For instance, capacitors, batteries, rf circuits, high-quality filters, antennas, transformer cores, read/write heads for high speed digital tapes and operating devices require controlled electrical properties of Ni ferrites. Improved electrical properties of Ni ferrites would be advantageous in such applications. In the present case, an analysis of the growth, structural properties, electrical properties and a correlation derived between microstructure and electrical properties in Dy doped Ni-ferrite nanocrystalline films is presented. Disprosium doped nanocrystalline nickel-ferrite ($NiFe_{1.925}Dy_{0.075}O_4$) films were fabricated using sputter-deposition. Structural, electrical and optical properties of $NiFe_{1.925}Dy_{0.075}O_4$ were investigated. The grain-size (L) and lattice-expansion effects are significant on the electrical and optical properties of $NiFe_{1.925}Dy_{0.075}O_4$ films. Annealing (T_a) in at 450-1000 ^oC results in the formation of nanocrystalline $NiFe_{1.925}Dy_{0.075}O_4$ films, which crystallize in the inverse spinel structure, with L=5-40 nm. Lattice constant of $NiFe_{1.925}Dy_{0.075}O_4$ increases compared $NiFe_2O_4$ due to Dy-doping. DC conductivity was found to decrease exponentially with decreasing the temperature from 300 K to 120 K which indicates the semiconducting nature of the $NiFe_{1.925}Dy_{0.075}O_4$ films. Room temperature conductivity of $NiFe_{1.925}Dy_{0.075}O_4$ is seen to decrease from 1.07 Ω^{-1} m^{-1} to 3.9 x10^{-3} Ω^{-1} $m^{-1}$with increase T_a from 450 to 1000 C. Band gap increases from 3.17 to 4.08 eV for $NiFe_{1.925}Dy_{0.075}O_4$ films with increasing T_a from 450 to 1000 ^oC. A correlation between grain-size, electrical properties and optical properties in nanocrystalline $NiFe_{1.925}Dy_{0.075}O_4$ films is established.

SPATIO-TEMPORAL CARDIAC PACING SITES LOCALIZATION AND TIME VARYING PERICARDIUM POTENTIAL MAPS PROJECTION USING ECG PRECORDIAL LEADS AND A SINGLE MOVING DIPOLE MODEL

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ABSTRACT

A new method is proposed for the spatiotemporal localization of the sites of strongest cardiac activity, and for the creation of time varying Pericardium Potential Maps (PPM), with the use of patients' ECG precordial leads. The spatial properties added to the ECG analysis allow for the localization of specific regions inside the human heart where potential cardiac malignancies are suspected to occur. The proposed MATLAB-based software uses the single-moving dipole model, optimized in location and magnitude with respect to the measured leads, and of a realistic FEM torso model. The PPMs are displayed simultaneously with precordial leads to allow a visual synchronization between the time varying color coded potential map and the ECG waveforms. This provides a 3D color view of the physical location of observed ECG waveform peculiarities, thus indicating potential cardiac malignancies. The proposed software was implemented for the analysis of 15 normal patients and 15 patients with cardiac abnormalities. For each case, 20 different sites inside the heart were considered as possible origins of cardiac activity at each instant of time during a complete cardiac cycle. Results show that for normal patients, sources of strongest cardiac activity were located in the atrial region for Q-wave, and the in the ventricle region for both QRS complex and T-wave, whereas for abnormal patients there was no consistency in such locations. Software identified potential cardiac malignancies and its location in 93.33% of the abnormal patients.

PRESENT AND FUTURE OFTHERMOELECTRICS

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ABSTRACT

Thermoelectrical devices are currently confined to either super high-tech applications or seen as a interesting gadgets by engineers, scientists and experimentalists. This *mis-a-côté* of such promising technology has been the result of various factors, scientific and economical, but new developments in thermoelectrical devices and thermoelectrical generators (TEGs) will widen the application spectrum through higher performance at a lower cost.

Through research and innovation, the implementation of thermoelectrical devices in a near future is foreseeable for energy harvesting purposes and for high-efficiency dual purpose HVAC devices (heating and cooling in one unit) either for the transportation industry or for commercial and residential buildings. The energy harvesting would recuperate wasted heat or take advantage of existent thermal gradients in order to cogenerate electrical current in a dynamical system along with wind mills and PV-arrays.

Finally, we expect that TEGs will help ease the national dependency on foreign fuels-evidently an issue of national security- through highly efficient industrial processes and thermoelectrically-assisted geothermal powerplants operating in a totally environmentally-friendly manner.

HTP DECOMPOSITION IN MILLIMETER SCALE CHANNEL TYPE CATALYTIC REACTORS

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ABSTRACT

There is a strong need to develop miniature chemical propulsion systems for Class II (1-5 kg) and Class III (< 1 kg) spacecrafts, currently chemical propulsion hardware do not exists for the attitude control system of these classes of spacecraft. Various physical and manufacturing constraints limit the miniaturization of conventional chemical thruster design to mN ranges. Thus new concepts and technologies for micro combustors and microreactors have to be developed. Motivated by these issues the present investigation is aimed at studying microchannels and monoliths based catalytic microreactors. Conventional catalyst chamber used pallet type reactor bed to decompose the propellant. However, miniaturization of monopropellant thrusters to mN-μN thrust range requires chamber dimension in the order of 0.1-0.01 mm with pallet sizes ranging from 1 to 10μm. Clearly pallet type catalyst bed with this length scale will have serious performance penalty due to high degree of boundary effects. Thus technology for new microcatlayst reactors have to be developed to meet the miniaturized monopropellant systems. Microchannel or ceramic monolith catalytic bed technologies are new concepts which offer significant advantages for miniaturized chemical thrusters while providing minimum boundary and surface effects. Using recently developed micro and mesoscale manufacturing technologies these catalytic reactors can be fabricated in submillimeter dimension to provide superior diffusion transport characteristic and better thermal management. Due to low radial diffusion times these catalytic reactors can achieve very low residence time distribution (RTD) highly suitable for miniature monopropellant thrusters. However, hydrodynamic and kinetic behaviors of this new generation of microreactors have to be systematically investigated for propellants such as H_2O_2. The primary emphasis of the present work is to identify, configure and optimize catalyst microreactors to decompose HTP for mass-flow rate suitable for mN- μN range thrusters. Mesofabricated silver channel reactors are used to study the decomposition behavior of 90% H_2O_2 (by weight) in millimeter scale geometries. Due to short radial diffusion time microchannel/monolith reactors can provide rapid heat and mass-transfer rates, narrow residence time distributions and short response time. Effects of channel length and aspect ratio on the decomposition efficiency are evaluated. Experiments are performed at different reactant flow rates and initial reactor bed temperatures. Temperature variations within the catalyst bed different reactor operating conditions are also reported.

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EXOTHERMIC WELDING IN MICROGRAVITY

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ABSTRACT

Success of long-duration spaceflight and future space exploration missions will be highly dependent on maintenance and repair challenges. Because of mass and volume constraints to carry spare parts onboard spacecraft, an evaluation of new approaches for maintenance and repair is necessary. Exothermic welding is well known as a reliable, low-energy consuming method for connecting copper wires or cables. However, this method typically relies on Earth's gravity for moving the molten metal from the combustion zone to the welding zone as well as for separation of slag. The proposed experiment for NASA Microgravity University – Systems Engineering Educational Discovery Program will test the special approaches and design we have developed for conducting the exothermic welding process in a reduced gravity environment. The testing apparatus involves a set of industrial devices used for exothermal welding, modified for operating in a microgravity environment. The devices are placed in a sealed chamber, which, along with other safety measures, ensures safe testing onboard the reduced-gravity aircraft. After the flight, using characterization techniques available at UTEP, the quality and properties of the welds obtained in reduced gravity will be compared with those of the welds obtained in a standard 1-g environment.

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NUMERICAL ANALYSIS OF DRAG ON NON-SPHERICAL PARTICLES IN FLUIDIZED BEDS

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ABSTRACT

Gasification is a process that converts carbonaceous materials, such as coal into CO and H_2 (syngas) by reacting the raw material at high temperatures with a controlled amount of oxygen and/or steam. For this purpose, a fluidized bed is used. Nonetheless, the most common particles in this type of chemical process are non-spherical. The modeling of these particles can be determined only through the understanding of flow characteristics such as drag coefficient and terminal velocity. Correlations for defining drag coefficient and terminal velocity are presented in the literature. Most of the work found in literature was carried out in an experimental environment, where empirical equations for the drag coefficient and terminal velocity of non-spherical particles are derived.

In this paper, the calculation of drag coefficient of a solid non-spherical particle moving at the terminal velocity is studied. The numerical approximations are done using the CFD solver FLUENT on a moving grid. The non-spherical particle shape simulated in this study was elliptical with a major diameter of 9.76 mm and its minor diameter of 2.65 mm. Numerical drag results are compared to experimental data for validation. To carry out the drag analysis, a 2D-mesh with triangular elements was created. Moreover, three flow cases were analyzed in order to compare drag force obtained from the simulation and validated with the experimental method. The first case is steady flow passing by the stationary non-spherical particle. In case 2, the non-spherical particle was set to move downwards at free-fall conditions with only vertical motion (without rotation). A moving mesh condition is assigned to the domain. For case 3 the particle is set to move downwards with free-rotation allowed. Flow was simulated for 10 ms with a time step of 0.1 ms.

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SYNTHESIS AND MICROSTRUCTURE OF Gd_2O_3-HfO_2 THERMAL BARRIER COATINGS

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ABSTRACT

The efficiency of gas turbines depends on the operating temperature. To maximize the efficiency, the operating temperature should be as high as possible. Thermal barrier coatings (TBCs) are thick or thin layers of low thermal conductivity ceramic refractory materials, which prevent the damage of the engine components that are exposed to very high temperature of the hot gases. Currently TBCs are predominantly used as thermal insulators in gas turbine applications. It allows the gas turbine to operate at higher temperature by reducing the heat transfer from hot gas to superalloy blades, and thereby improving the efficiency of the gas turbine. The current choice of material for TBC is 7-8wt% YSZ (yttria stabilized zirconia) which is stable up to 1200°C for long term operation. At a temperature above 1200°C, phase transformations occur from t'-tetragonal to tetragonal and cubic, then to monoclinic zirconia. These phase transformations are associated with a volume change which leads to the formation of crack in the coatings. This limits the application of YSZ at elevated temperatures. Increasing demand to improve the efficiency of the gas turbines leads to search for better TBCs that will allow the operating temperature to increase further. In this context, new TBC material is sought that can withstand very high temperature for longer period than the current YSZ TBCs. The objective of this study was to investigate the HfO_2 based nanostructured thermal barrier coatings in which gadolinia (Gd_2O_3) was used as a stabilizer. The coatings of different compositions, namely 4, 20 and 38 mol% Gd_2O_3 and balance HfO_2, were deposited onto various substrates (IN-738, SS-403 and Si) using RF magnetron sputtering. The thickness of the coating was ~250 nm. The crystal structure of the deposited coatings was indentified using X-ray diffraction (XRD). The crystallite size was calculated from XRD analysis as a function of Gd_2O_3 content. The combined XRD and SEM studies indicate that the effect of Gd_2O_3 is remarkable on microstructure of Gd_2O_3-HfO_2 coatings. The results obtained will be presented and discussed.

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SPECTROSCOPIC ANALYSIS OF WO_3 FOR SENSOR APPLICATIONS

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ABSTRACT

Samples of WO_3 thin films for use in gas sensors were grown using radio frequency magnetron sputtering at a number of different substrate temperatures and $Ar:O_2$ pressure ratios. The properties of the samples were spectroscopically investigated with the goal of determining how variations in the above preparation parameters effect structural changes in the sensor materials. Such structural changes are of crucial importance to the question of improving the sensitivity, specificity, and durability of WO_3 based gas sensors. Experimental characterization was performed using the techniques of confocal Raman, infrared (IR) absorption, and X-ray photoelectron spectroscopy (XPS). The results from both IR and Raman demonstrate an amorphous nature for the WO_3 sample grown at room temperature and an initial crystallization into a monoclinic WO_3 structure for samples grown at temperatures between 100 and 300 ^oC. For 400 and 500 ^oC, the existence of a strained WO_3 structure is observed together with the monoclinic one, with a distribution revealed by confocal Raman mapping. XPS indicates that the film surface maintains the stoichiometry WO_x, with a value of x slightly greater than 3 at room temperature due to oxygen contamination, which decreases with increasing temperature.

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AN EXPERIMENTAL INVESTIGATION OF CH_4-O_2 FLAME STABILITY IN A LABORATORY SCALE TUBULAR BURNER

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ABSTRACT

Oxy-fuel combustion is currently being considered by U.S Department of Energy as a promising technology for carbon capture efficiently. This technology could substantially reduce NO_x and CO_2 emissions. In addition, the implementation of oxy-fuel combustion technology in a power generation system could potentially reduce negative environmental impacts of fossil fuel use. It also encourages the use of reliable and domestic energy sources. U.S. Department of Energy has made efforts to investigate the performance of CO_2 and H_2O diluted oxy-fuel combustion system in a high pressure combustor. In an effort to better understand and characterize the fundamental flame characteristics of oxy-fuel combustion this current work presents the stability of CH_4-O_2 flames. A laboratory scale burner was designed and fabricated based on capability of withstand the higher oxy-fuel flame temperatures in order to investigate the flame stability characteristics using different diameter burners. In the burner system premixed fuel and oxidant entered from the pressurized tank into the manifold through four alternate injection holes. A bank of digital mass flow controller was used to measure mass flow rates of fuels and oxidant composition. After the premixing section the fuel and oxygen mixture was ignited with an external ignition source. The resulting flame was analyzed with the use of a high-resolution digital camera. The stability maps of CH_4-O_2 were plotted using six different tubular burner diameters, ranging from 1 to 6 mm. The flame from the 1 mm diameter burner tube tended to extinguish, even at lower mass flow rates due to a quenching effect. For larger burner diameters, 2 to 6 mm, the flames tended to flashback. It was also observed that the stability regime increased with an increase in CO_2 concentration in the fuel mixtures.

* This work has been supported by U.S. Department of Energy, under awards DE-FOA-0002402

CHARACTERIZATION OF TURBULENT FLOW FIELD OF SYNGAS FLAMES IN A LABORATORY SCALE TUBULAR BURNER

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ABSTRACT

The National Energy Technology Laboratory has made efforts for developing hydrogen based gas turbine combustor which could enhance plant efficiency and ensure low NO_x production without sacrificing operational advantages. The characteristics of turbulent premixed flames, especially hydrogen content fuel like syngas (primary constituents are H_2 and CO) are quite different from isothermal turbulent flows. Differences occur due to large difference in the densities of reactants and products resulting in phenomena like counter gradient diffusion and the large turbulence energy generated within the flame. The behavior of premixed turbulent syngas flames dictate the burning velocity that results in flame flashback. A detailed understanding of turbulent characteristics of syngas flames is necessary to develop a combustor design that can accommodate various types of syngas fuels obtained from gasification of coal. The current work aims to characterize the turbulent flow-field of both methane/air and syngas/air flames in a laboratory scale tubular burner varying different burner diameter, Reynolds numbers, and blockage ratio's in the upstream of the burner. A recent progress in high speed particle image velocimetry enables to capture the turbulent flow field with high resolution which results in better understanding of phenomena like vortex shredding at the burner exit. An experimental setup is designed to visualize the turbulent flow field of both CH_4-air and syngas-air flames varying the above parameters by using high speed particle image velocimetry. An intensified camera with OH filter cap is implemented to track the flame reaction zone. The burner used in the current study is a tubular burner with a turbulence creator positioned at a distance of 15 mm downstream from top of the burner. The blockage ratio that is considered in the present study is about 92%. The turbulence flame front of premixed CH_4/air combustion was visualized with different techniques at Reynolds numbers of 920. The turbulence flow field of CH_4/air combustion was recorded at two different locations from the burner exit using Particle Image Velocimetry (PIV) technique. The magnitude of the turbulence intensity decreased downstream of the injector exit. The magnitude of the velocity fluctuations decreased as the turbulence intensity decreased.

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EXPERIMENTAL MEASUREMENT OF RADIATIVE HEAT RELEASE RATES OF CH_4-O_2 AND CH_4-CO_2-O_2 FLAMES FOR ADVANCED COMBUSTORS

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ABSTRACT

Oxy-fuel combustion technology is inherently designed for carbon capture. This technology offers the potential to make coal burning power plants more efficient and cleaner. Department of Energy has made efforts to design an oxy-fuel based combustor that captures CO_2 which has potential to reduce green house gas emissions substantially. The inherent changes of oxy-fuel combustion properties such as: flame behavior, heat transfer, and combustion gas chemistry become major considerations for the designing of a combustor system capable of using oxy-fuel mixtures. However, higher heat output from oxy-fuel combustion needs a different design or operating approach. The oxy-fuel flame properties and heat transfer rates deviate from established models based on hydrocarbon/air combustion and has limited data available for modeling. This current work aims to measure radiative heat release rates of CH_4-O_2 flames in a laboratory scale tubular burner. The effect of CO_2 and H_2O diluents in the feed stream on radiative heat release rates is presented in order to provide information for designing advanced combustors. An experimental setup incorporated with a Mark-IV series radiometer and solar radiometer is designed to measure heat release rates of CH_4-O_2 flames. A tubular burner system that consists of three primary components: (a) platform, (b) mixing manifold and (c) burner tube assembly was designed and developed. The tube assembly section merges with the adapters to accommodate tubes of different diameters. Radiative heat release rate was plotted against equivalence ratio (φ). It was observed that the radiative heat release rate of CH_4-O_2 flame is almost constant for the lean flames, yielding F values 4.1% and 8.9% by using the solar radiometer and Mark IV radiometer, respectively. In addition, the radiative heat release rates of 75%CH_4-25%CO_2-O_2 and CH_4-O_2 flames were not significantly different at a constant fuel firing input.

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HYDRODYNAMIC ANALYSIS OF A FLUIDIZED BED OPERATING WITH SPHERICAL AND NON-SPHERICAL PARTICLES

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ABSTRACT

Gasification offers a promising solution to producing fuels effectively in the coming years. This technology provides a low-cost energy system, clean environmental performance, and reliability. This system uses heat, pressure, and steam to convert feedstock into a gaseous mixture, composed primarily of carbon monoxide (CO) and hydrogen (H_2), named as syngas. The feedstock is prepared and fed to gasifier in either a dry form or as slurry (mixed with water). One type of gasifier currently available for commercial use is the fluidized bed reactor. The 2006 Multiphase Workshop organized by the National Energy Technology Laboratory (NETL) identified several issues, and postulated a set of near-midterm, mid-term, and long-term research needs in order to attain a significant development in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants by the year 2015. A novel diagnostic technique was used in this work to generate engineering data useful for design processes for non-spherical particle based solid-fluid system. Pressure fluctuations and high speed imaging analysis using MatPIV were utilized to characterize the hydrodynamic behavior of a gas-solid based fluidized bed for spherical and non-spherical particles in semi-dilute (volume fractions of 10 or 15%). Flows with static bed height of 5 cm were used for this study. A plexiglass tube with an outside diameter of 3.8cm and a wall thickness of 0.318cm was used as the fluidized bed. 1mm borosilicate glass beads with sphericity variation of ±10% were used as the solid spherical particles. As solid phase non-spherical particles, borosilicate glass particles in the range of 600-850 µm with mean particle size of 717.57 µm, and sphericity in the range of 0.61 to 0.88. Rice particles were also used with mean equatorial diameter along x-axis 6.76 mm; mean equatorial diameter along y-axis 2.076 mm, and polar diameter along the z-axis 1.72 mm and sphericity in the range of 0.39 to 0.46. Compressed air supplied from a screw type compressor was used to fluidize the particles. Mapping of bed pressure drop with superficial gas velocity across the bed was done showing the minimum fluidization and terminal conditions for the specified fluidized bed and particles. MatPIV analysis of high speed images, captured at 500 frames per second, showing the flow field vectors, magnitude of velocity, vorticity, and streamlines for both spherical and non-spherical particles, is presented.

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A STUDY OF WO_3 AND $W_{0.95}Ti_{0.05}O_3$ THIN FILMS USING COMPARATIVE SPECTROSCOPY

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ABSTRACT

Tungsten oxide (WO_3) is important and well-studied in materials science, particularly for gas sensor applications. In this study, we consider the innovation of adding Ti to thin films of this material. Using Raman and X-ray photoelectron spectroscopy (XPS), we compare the morphology and composition of WO_3 and $W_{0.95}Ti_{0.05}O_3$ thin films, grown by radio frequency magnetron reactive sputtering at substrate temperatures varied from room temperature (RT) to 500 ºC. In the $W_{0.95}Ti_{0.05}O_3$ thin films, our Raman data reveal a phase transformation from a monoclinic WO_3 structure to an orthorhombic or tetragonal configuration, based on peak shifts of WO_3 W-O-W stretching modes from 806 and 711 cm^{-1}, to 793 and 690 cm^{-1}, respectively. In addition, Ti-doped WO_3 films require higher growth temperatures to attain crystalline microstructure than do pure WO_3 films. XPS data indicate a reduced WO_{3-x} stoichiometry at the surface of the doped material, with W^{+6} and W^{+5} tungsten oxidation states present. This observation could easily be related to the existence of a different structural phase of this material, corroborating the Raman measurements.

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THERMAL BARRIER COATINGS (TBC's) of HIGH HEAT FLUX THRUST CHAMBERS

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ABSTRACT

Thermal barrier coatings (TBC's) are ceramic coatings that are used extensively on turbine components to protect the components from the harsh service environments. Current TBC's that are used in industry are comprised of 8% yttria-stabilized zirconia (YSZ). Advanced turbine technology is pushing for higher temperatures to increase efficiency and the current TBC technology also needs to be modified. Yttria-stabilized hafnia (YSH) is being researched to compensate for the increase in high temperatures while being able to provide the same protection as current TBCs. In current thrust chambers there is no protective coating that insulates the inner lining of the chamber. Thrust chambers are being researched as potential candidates for TBC's in order to increase efficiency, increase heat transfer properties and to increase service life and burn times. Industrial grade YSZ and optimized research grade YSH will both be deposited using magnetron sputtering and pulsed-laser deposition (PLD) processes. These deposition processes will be optimized through variances in temperature and pressure to determine the best microstructure and bond between the substrate and TBC. TBC's will be deposited and analyzed on copper and silver substrates. Analysis will be performed using scanning electron microscopy (SEM) and x-ray diffraction (XRD) to characterize the microstructure, coating thickness and TBC/substrate bond, and crystal structure. Once deposition processes are optimized then deposition will then be performed on Cu/Ag/Zr substrates to simulate the material used in thrust chambers. Thermal mechanical analysis will be performed using a thermal cycling furnace to observe microstructural and mechanical behavior of the TBC's on the substrates. A select set of substrates with optimized TBC deposition will be subjected to accelerated mission testing (AMT) to save time and money to get quick and reliable results. This research should aid in engineering decisions involving the use of YSH for TBC's on thrust chambers to increase efficiency, improve regenerative cooling mechanisms and increase service life.

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HIGH TEMPERATURE TOLERANCE AND CHEMICAL STABILITY OF YTTRIS-STABILIZED HAFNIA

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ABSTRACT

Thermal barrier coatings (TBC) are used to protect the metallic surface from high temperature exposure for long time in advanced turbines. The coating is usually made of ceramic materials and applied as a very thin layer over the metallic surface which makes insulation between the components and very high temperature environment. By this way, TBCs help use high operating temperature which subsequently increases the efficiency of gas turbine power plants operating in diversified fuel environment. In this work, we investigate the high temperature tolerance and stability of yttria stabilized hafnia coatings for possible TBC application in hydrogen turbine technology. The temperature tolerance and stability of ytrria (Y_2O_3)-stabilized hafnia (HfO_2) and ytrria-stabilized hafnia-zirconia (ZrO_2) coatings named hereafter as YSH and YSHZ respectively were studied in detail. YSH and YSHZ coatings have been produced by magnetron sputtering onto 403-stainless steel and Inconel-738 substrates at various temperatures. Structural characterization performed by X-ray diffraction (XRD) indicates the stabilization of the cubic phase with a lattice parameter, a = 0.52 nm. The surface and cross-sectional imaging analysis performed by scanning electron microscopy indicate the dense morphology along with a columnar structure. High-temperature XRD measurements demonstrate the tolerance and stability of the coatings to a temperature of 1300 °C. Thermo-chemical analysis indicates the overall stoichiometry has been retained in the coatings upon exposure to 1300 °C.

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BIOLEACHING OF ILMENITE AND BASALT IN THE PRESENCE OF IRON-OXIDIZING AND IRON-SCAVENGING BACTERIA

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ABSTRACT

Understanding the biogeochemical processes that control mineral weathering rates is not only important for Earth systems, but may be a useful for developing technologies for the in-situ utilization of resources from other planets, moons, and asteroids. Traditional techniques that may be used to extract metals like iron, titanium, and aluminum from planetary rocks have large energy and/or hardware requirements that may not always be feasible. In this study, we performed biotic and abiotic leaching experiments with basalt and ilmenite ($FeTiO_3$) to determine whether bacteria increased elemental leaching rates. Our secondary objectives were (1) to determine whether *Acidithiobacillus ferrooxidans,* an Fe-oxidizing bacterial strain, could grow on the low concentrations of ferrous Fe generated by the available substrates, and (2) to determine whether *Pseudomonas mendocina,* a heterotrophic Fe-scavenging bacteria, could grow on the low concentrations of nutrient elements generated by the available substrates. Experimental results demonstrate that the Fe(II) leached from ilmenite was rapidly depleted and replaced by Fe(III) in the presence of the Fe-oxidizing bacteria. The Fe in the abiotic control system remained as Fe(II) over the entire duration of the experiment. This suggests that the bacteria were able to grow using the Fe(II) from ilmenite (and the metal-free growth media) as a substrate. The iron-oxidizing bacteria were also able to grow in the presence of basaltic rock types; however the elemental release rates of Si, Ca, and Al in the presence of *A. ferrooxidans* were actually the same or lower than those from the abiotic control experiments. This may be attributable to the metabolically active bacteria creating a thick altered layer at the mineral surface that decreased the rate of diffusion or it may be caused in part by adsorption or precipitation of Fe(III) onto the existing mineral surfaces. Blending of the basaltic rock with ilmenite to further stimulate the bacterial metabolisms by providing additional Fe(II) resulted in a slight increase in Si, Ca, and Al release rates. For example, Si was released at an initial rate of $6.6e^{-12}$ mol/m^2*s in the biotic experiments, while Si leached from the abiotic control at a rate of $4.0e^{-12}$mol/m^2*s. Additional experiments utilizing *P. mendocina*, a heterotrophic organism capable of using siderophores to scavenge Fe from refractory minerals, are underway. Results from these experiments will be presented and compared to the results obtained for the iron-oxidizing systems.

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EFFECT OF GROWTH TEMPERATURE ON OPTICAL, STRUCTURAL AND ELECTRICAL CHARACTERISTICS OF Y2O3 FILMS

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ABSTRACT

Yttrium Oxide (Y2¬O3) is a versatile material for a diverse range of applications. Its high dielectric constant (14-18) compared to that of SiO2 (3.9), high resistivity, high breakdown field strength and low leakage currents has attracted the interests of researchers working towards finding alternatives for SiO2 as a gate insulator. It has been use to stabilize the high-temperature phases of refractory ceramics, such as zirconia and hafnia, for their utilization in energy storage and conversion technologies. For instance, Y2O3-stabilized zirconia (YSZ) materials have been in use in fuel cells. In addition, YSZ coatings have been used as thermal barrier coatings in advanced turbine technology for power generation. Understanding the microstructure and properties of thin Y2O3 films is, therefore, important in order to further explore their technological applications.

In this work, the effect of temperature on the optical, electrical & structural properties of Y2O3 thin films has been analyzed. The increase in substrate temperature improved the structural order and cubic phase of the Y2O3 thin films. The samples grown with substrate temperature variations in the Room-Temperature (RT) to 100 º C were virtually amorphous. Analysis of XRD data indicates a preference in growth orientation along the 222 plane whilst remaining generally polycrystalline in nature in the 200 - 500 ºC range for the in-situ growth substrate temperature variations. RHEED analysis offers excellent corroboration for the observed XRD patterns in the respective ranges of substrate temperature variations, with distinctive fringe patterns for the 300 - 500 ºC range indicating the presence of dense Crystalline nanoparticles. The surface morphology analysis is further backed by the observed SEM imagery of the dense nanoparticle formations. Grain size was found to be increasing as a function of increased substrate temperatures exhibiting exponential growth patterns.

THERMAL STRESS ANALYSIS OF TITANIUM NITRIDE COATING ON SILICON UTILIZING A COMBINED ANALYTICAL MODEL

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ABSTRACT

Titanium nitride (TiN) coatings have been in use as protective and wear and corrosion resistant coatings for industrial machinery tools due to their excellent physical and mechanical properties. Controlled growth, texturing, stress and composition of the TiN layers can significantly influence their properties, phenomena and performance. The present work was, therefore, performed to elucidate the effects of thermal residual stress during a sputtering or deposition process for titanium nitride coatings on silicon (Si) substrates using analytical modelling. Analyses were performed considering Si temperature, Si thickness, TiN coating thickness, and modulus of elasticity of TiN.

The variable thermal stress in the TiN coatings is due to the existence of both positive and negative temperature gradients and thus the resultant existence of disparity of the coefficient of thermal expansion between the substrate and coating. Stoney's thin film formulation for coating-substrate systems in addition to the mathematical formulation for residual stress developed by Tsui and Clyne has been employed in this work. This analytical model is a function of several parameters, which include the effective modulus of the substrate and coating, coefficient of thermal expansions for coating-substrate system, coating and substrate thickness, and deposition or sputtering temperature and room temperature. Inherently, the effective modulus is also a function of the constituents (i.e. thin film coating and substrate) Poisson's ratios and their respective Modulus of Elasticity.

It is found from analysis, considering a two dimensional geometric setting, that the thermal stress opposed with substrate temperature from room temperature to 800 °C while holding all other parameters at fixed values increased in a linear manner as you increased the substrate temperature. However, the thermal stress, while accounting for the variable modulus of elasticity values found in the literature for TiN coatings was compared within the selected coating-substrate system, decreased in a linear fashion with increasing coating thickness from one nanometer to five microns. Additionally, the thermal stress was found to increase in an exponential decaying manner as the substrate thickness increased. Finally, utilizing the above mathematical formulation the thermal stress also increased to a higher negative value with increasing modulus of elasticity values. The examined parameters mentioned above (i.e., substrate temperature, substrate thickness, etc.) compared with thermal stress relations found in literature followed similar trends overall. The results will be presented and discussed.

GROWTH, MICROSTRUCTURE AND OPTICAL CHARACTERISTICS OF $W_{0.80}Ti_{0.20}O_3$ THIN FILMS FOR h2s SENSORS IN COAL GASIFIERS

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ABSTRACT

The search for novel materials for chemical sensors with enhanced performance has lead the scientific community that works in the field to consider ternary compounds of metal-oxide semiconductors as potential candidates. A leading criterion would be starting with a metal-oxide semiconductor that has already proven sensing capability, such as WO_3 in this case, and adding another properly chosen metal. Searching for new materials should be accompanied by a thorough study of the microstructural and electronic properties of the material under consideration. In the context of the effort described herein, the present work was performed on the Ti-doping effects in a small and controlled amount into WO_3 to produce $W_{0.80}Ti_{0.20}O_3$ for their utilization in H_2S sensors in coal gasifiers. The focus of the investigation was to explore the effects of Ti and temperature on the growth behavior, microstructure and optical characteristics. $W_{0.80}Ti_{0.20}O_3$ films were fabricated using sputter-deposition onto Si(100) wafers in a wide growth temperature range, room temperature (RT)–500 ^{o}C. X-ray diffraction (XRD), high-resolution scanning electron microscopy (SEM) and Optical spectrophotometery were performed to investigate the effect of temperature on the growth behavior, crystal structure, texturing, surface morphology, and optical properties of $W_{0.80}Ti_{0.20}O_3$ films. The results indicate that the effect of temperature is significant on the growth and microstructure of $W_{0.80}Ti_{0.20}O_3$ films. XRD results indicate that the $W_{0.80}Ti_{0.20}O_3$ films grown at temperatures <400 ^{o}C are amorphous.. Phase transformation is induced in $W_{0.80}Ti_{0.20}O_3$ resulting in tetragonal structure at 500 ^{o}C. The SEM imaging analysis indicates that the phase transformations are accompanied by a characteristic change in surface morphology. Optical band gap (E_g) is found to decrease from 3.37 to 3.64 eV with increasing substrate temperature, suggest that tuning optical properties can be achieved by controlling the size and phase. The effect of ultra-microstructure and grain-size was significant on the electronic properties of $W_{0.80}Ti_{0.20}O_3$ films.

CRYOGENIC FEED SYSTEM DEVELOPOMENT AND CONDENSATION FOR LOX/HYDROCARBON PROPULSION RESEARCH

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ABSTRACT

The Center for Space Exploration Technology Research (cSETR) is designing a cryogenic system to facilitate research efforts on non-toxic propulsion research. Current experimentation demands require the use of liquid oxygen (LOx) and liquid methane (LCH_4). The cryogen system will serve a two fold purpose, deliver respective cryogens to test set ups, and condense methane to a liquid state for propulsion testing efforts while adhering to budgetary constraints. The system is being designed based on a 15 pound (lb) thruster with line pressures up to 195 pounds per square inch (psi) at an assumed specific impulse (Isp) of 310 seconds (s). The system requirements for the delivery system are: (1) flexibility to provide different propellant mass flow rates, (2) controlled delivery and metering of propellants, (3) real time data acquisition, (4) conduct at least 10 successive tests at the highest propellant max flow rate, (5) flexibility to perform under several experimental conditions, and (6) comply with university safety regulations. The initial main function of the delivery system will be to handle LOx and LCH_4 safely and deliver it to an altitude simulation chamber while maintaining cryogenic properties of the propellants. This was accomplished by determining experimenftal test matrices and total propellant need for all testing on any particular test series day. The secondary portion of the cryogenic system requires that the methane condensation system operate safely, as efficiently as possible, and within a reasonable production time. LCH_4 condensation is necessary for laboratory experimentation due to the quantities needed in comparison to the costs and lead time from industry vendors. The unit designed to accomplish this will produce 25 L of LCH_4 in approximately 3-4 hours at 1 mega Pascal (MPa) tank pressure. The main condensate function is natural convection of flowing liquid nitrogen inside a coil inside a vacuum insulated tank holding gaseous methane. Once produced the LCH_4 will be transferred to a testing tank residing in the delivery system discussed above. The two system described above will allow for specific propellant quantities to be used for any one experiment and ensure the safety and reliablilty of cSTER research efforts.

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DEVELOPMENT OF A HEAT FLUX TEST RIG TO STUDY CRYOGENIC HEAT TRANSFER CHARACTERISTICS

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ABSTRACT

The development of a heat transfer test rig is being developed at Center for Space Exploration Technology Research (cSETR) at the University of Texas at El Paso (UTEP) for the purpose of testing liquid methane ((L) CH_4) and regenerative cooling applications in rocket engines. The rig is designed for working temperatures of up to 650 °C. The system is designed such that the maximum fluid flow rate is 180 g/s with a maximum operating pressure of 290 psi. In addition, experimentation is performed under vacuum conditions. A temperature profile is taken with each respective flow rate to attain a relation between the heat transfer and flow characteristics. This relation will be used to determine thermal diffusivity of the fluid thus finding the density, thermal conductivity, and specific heat capacity. The rig is also designed to test various non-toxic fuels that offer increased weight efficiency, an improvement in the overall performance of the propulsion system, and material compatibility. These fuels have been implemented in current rocket engine research programs by entities such as NASA and XCOR. However, data for thermodynamic fluid properties of (L) CH_4 are proprietary, thus unavailable. Research and industry laboratories have designed various thermal rigs to simulate a regenerative cooling channel on a rocket at operating conditions. However, the thermal rigs were not designed for interchangeable cooling geometries to be applied in the experiments. After reviewing several experimentation techniques, it was determined that conductive heating is the optimal method to create an environment that simulates real rocket engine chamber conditions for the cooling channels. The test rig design uses a copper block that geometrically focuses thermal energy onto a 1 inch by 2 inch test section with minimum complexity and maximum flexibility. The block allows 25 electrical cartridge heaters to be placed within it providing 5000 (W/in^2) constant heat flux. The parameters of the performed experiment are channel wall temperatures up to 650 °C, 30-200 second tests, and fully developed turbulent flow.

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MODAL ANALYSIS OF A LOW THRUST TORSIONAL THRUST BALANCE FOR THE PERFORMANACE EVALUATION OF 5N CLASS THRUSTERS

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ABSTRACT

The improvement of accurate and reliable thrust stands for the research and analysis of rocket engines is a necessity to the improvement of high performance micropropulsion technologies. Miniature satellites, multiple kill vehicles and interceptors are constrained in mass, envelope and electrical power, therefore, require the need to have the propulsion subsystems reduced in size. These propulsion systems often have intricate thrust profiles that must be fully characterized with accurate performance evaluation. As a result, the development of low thrust measurement technologies that possess the required accuracy under a variety of thrust profiles is crucial for the aerospace industry to continue this line of research. This paper presents methodology to fully describe both the dynamic characteristics and restrictions of a thrust stand based on a modal analysis of an existing torsional thrust balance (TTB) stand. The modal analysis of the TTB stand will first be computer simulated in NASTRAN to find all of modes of vibration from 0 to 150 Hz, given the geometry and the materials. The computational analysis will be compared with experimental data gathered from the actual thrust stand using 6 accelerometers and a modally tuned auto hammer. A summary of the modal analysis will include modal frequencies, modal damping, mode shapes, location of nodes and anti-nodes. The information recorded was utilized to determine the maximum thrust input at various pulsing frequencies based on material stresses, and the pulsing frequencies at which unacceptable thrust data is generated. This study will aid in establishing a “performance window” for the TTB stand, and will outline and document the procedure for the design criteria applicable to new systems or the characterization of existing ones.

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EXPLOSIVE CONSOLIDATION OF THERMOELECTRIC MATERIALS

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ABSTRACT

One of the challenges facing researchers of thermoelectric materials is turning a powder precursor material into a solid piece without destroying some of the desirable properties of said powder. One method capable of consolidating powders without excessive heat buildup is explosive consolidation. In this talk, we give an overview of the process and the results of consolidating thermoelectric nanopowders via explosive shockwaves.

DEVELOPMENT OF A TORSIONAL THRUST BALANCE FOR THE PERFORMANCE EVALUATION OF 5N CLASS THRUSTERS

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ABSTRACT

Micropropulsion technology has become a vital part of space and military operations, through utilization in both pico/microsatellites and next generation interceptors. Microsatellite (space based radar formation) and miniature interceptor applications (multiple kill vehicles, RPG countermeasures, etc.) require a high standard of performance while strictly adhering to reduced weight, size, and power consumption constraints. As a result, all subsystems within these devices, including those for propulsion (attitude control, orbital maneuvering, and station keeping) must be likewise scaled down. Improvements in the propulsion systems of newton-class thrusters is contingent upon the ability to accurately measure and characterize low thrust values and necessitates the development of measurement devices with such capabilities. This work presents the design, development, preliminary testing, and optimization of a Torsional Thrust Balance (TTB) for the performance evaluation of newton-class thrusters with a measurement range of 25 mN to 4.5 N. Although currently configured for steady state firing, it can also be configured for pulsing operations. A mass counterbalance system build into the TTB facilitates the variation of thruster weights through the adjustment of the moment arm length. A triangulated laser positioning system is used to collect displacement measurements which are then correlated to thrust values through a weighted calibration technique. The TTB system improves upon prior low thrust measurement systems through the use of the aforementioned counterbalance system, frictionless pivots, and overall design to limit and reduce the influence of sources of measurement error such as natural vibrational frequencies of the system and its components, environmental interference, and tare inducing forces. Currently, this system operates at atmospheric pressure firing conditions utilizing standard cold gas pressurization. The gasses currently utilized include Carbon Dioxide, ultra high purity Nitrogen, and Helium. This work will be expanded to include test firings with other cold gasses at working altitudes and in pulsed firing conditions. Pulsed firing tests will require the inclusion of a dampening system to ensure uniformity in the reference positioning of the thruster and a limit sensor to trigger the thruster firing once it has returned to the reference position. A 0.5 N cold gas thruster was used as the reference propulsion system within this investigation. Through analysis of the calibration and firing results, the thrust measurements taken were proven to be both accurate and repeatable.

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SHORT TERM ELECTRIC POWER CONSUMPTION FORECASTING USING LINEAR PROGRAMMING SUPPORT VECTOR REGRESSION

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ABSTRACT

Accurate forecasting of electric power consumption by the national electric power grid is critical for short term operations and long term utilities planning. The power load prediction impacts a number of decisions (e.g., which generators to commit for a given period of time) and broadly affects wholesale electricity market prices. Load prediction algorithms also feature prominently in reduced-form hybrid models for electricity pricing which are some of the most accurate models for simulating markets and modeling energy derivatives. Within the realm of short term power load prediction, we propose a large-scale linear programming support vector regression (LP-SVR) model. The LP-SVR is compared with other two non-linear regression models: Feed Forward Neural Networks (FFNN) and Bagged Regression Trees (BRT). The three models are trained to predict hourly day-ahead loads given temperature predictions, holiday information and historical loads. The models are trained on hourly data from the New England Power Pool (NEPOOL) region (courtesy ISO New England) from 2004 to 2007 and tested on out-of-sample data from 2008. Experimental results indicate that the proposed LP-SVR method gives the smallest error when compared against the other approaches. The LP-SVR shows a mean absolute percent error of 1.58% while the FFNN approach has a 1.61%. Similarly, the FFNN method shows a 330MWh (Megawatts-hour) mean absolute error, whereas the LP-SVR approach gives a 238MWh mean absolute error. This is a significant difference in terms of the extra power that would need to be produced if FFNN was used. The proposed LP-SVR model can be utilized for predicting power loads to a very low error, and it is comparable to FFNN and over-performs other state of the art methods such as: Bagged Regression Trees, and Large-Scale SVRs.

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A FINITE ELEMENT DAMAGE MODEL FOR ADHESIVE FAILURE OF MASTIC-AGGREGATE INTERFACES

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ABSTRACT

The adhesive damage initiation and progression criteria at mastic-aggregate interfaces can be predicted using Finite Element Models (FEM). Under both dry and wet condition; the rheological properties of mastic have been determined by Dynamic Shear Rheometer (DSR) and the mastic-aggregate interface strength parameters have been determined from aggregate pull-off test in the laboratory. The surface based traction-separation damage law has been used to define the adhesive damage at the interfaces using ABAQUS. A finite element model consists of aggregate surrounded by mastic has been developed. Three different load patterns, which represent the speed of traffic, have been used to predict the adhesive damages. In addition three different types of load magnitude is used to observe the severity of damages along the interfaces. The result shows that the interface failed under both dry and wet status in particular locations under prescribed loading conditions. Vehicles with stop and go phenomena show higher damages than faster moving vehicles. The wet interfaces of mastic-aggregate show higher damages than the dry interfaces under similar loading and boundary conditions. For both fast and slow moving vehicles; wet interfaces show de-bonding between mastic and aggregate but dry interface shows surface damages but no de-bonding have been observed.

EFFECT OF DWELL TIME, LOADING RATE AND UNLOADING RATE ON VISCOELASTIC MATERIAL IN NANOINDENTATION TEST

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ABSTRACT

A nanoindentation test results in load versus indentation depth plot, which is typically analyzed by the Oliver-Pharr method. Specifically, this method uses positive slope of the unloading curve to determine elastic modulus and hardness of the indented materials. If the slope of the unloading curve is negative, which is the most frequent case for viscous materials, the Oliver-Pharr method is not applicable. Traditionally, such negative of slope of unloading curve from viscoelastic materials are avoided by applying a dwell time when materials flow without any applied load. In this study, attempts are made to examine and analyze the effect of dwell time on the slope of the unloading curve for indenting asphalt binders. In addition, the effect of loading rate and unloading rate are also examined by conducting nanoindentation test on aged and unaged asphalt binder samples. It is shown that the effects of dwell time, loading rate, and unloading rate are significant for successful analysis of nanoindentation data using Oliver and Pharr method. As the dwell time increases the bowing out or nose effect of the unloading portion of the force displacement curve decreases. At a very low unloading rate and small dwell time, the unloading portion of the force displacement curve becomes negative.

DEVELOPMENT OF AN OPTICALLY ACCESSIBLE HIGH PRESSURE TURBINE COMBUSTOR

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ABSTRACT

Future generation gas turbine combustors for power production are expected to have the capability of operating on high hydrogen content fuels. The high-pressure combustor facility allows for the observing of combustion processes under realistic gas turbine conditions. This process can provide the realistic data to promote the development of fuel flexible combustors. This current work presents a design of a high pressure combustor facility based on 500 kW power and 15 bar pressure. A finite element analysis of the designed burner, under thermal stress and 15 bar pressure, is carried out using NASTRAN 6.1. The purpose of this numerical analysis is to observe combustor behavior and ensure safety of experiments and personnel. The apparatus is comprised of two chambers: (1) an outer chamber made of stainless steel whose inner diameter is 700 mm (2) an inner chamber made of high temperature resistant quartz having 130mm inner diameter and 700 mm length. The cylindrical test section has optical access from three sides using rectangular windows whose side walls are made up of 85 x 700 mm2 quartz glass in the combustion zone. The test chamber is also fitted with a variable area flow restrictor to control the pressure drop across the burner and can be flexible with a range of chamber operating conditions. Two different cooling systems are also included in the design to extract heat and avoid structural failure. The outer test section is equipped with copper coiling using cooling water as a driving fluid. The inner coolant system is designed to circulate nitrogen around the inner quartz tube**.** This facility will allow the analyzing of the flame structure, flow field characterization using high speed particle image velocimetry (PIV), and flash back propensity in high hydrogen content fuel combustion under high pressure typically encountered in a gas turbine environment.

CONCEPTUAL DEVELOPMENT OF AN EXPERT SYSTEM TO AID DESIGNERS IN THE SELECTION OF SUSTAINABILITY METHODS

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ABSTRACT

The objective of this paper is to present the development of an expert system to aid designers in the selection of design methods, in particular for sustainability methods. When practicing engineers need help in their design process, they look for design methods and tools; this is a challenge especially for inexperienced engineers in the sustainability area. It is well known that engineers will stick to one or few methods during their professional life. The origin of this situation can be traced to engineering education, where it is typical that an instructor prefers one or few methods in particular, and even when he or she attempts to teach other methods, students may get confused since it is different to learn a method than learning how to select it. This paper presents a concept for an expert system has been developed by first characterizing key elements such as principles, guidelines, techniques and tools. Each element brings a vast set of variables that are not always well defined. An attempt was made to synthesize a logical model to represent the fundamental characteristics of an experienced method selection process. The result is a conceptual model that defines fundamental entities and relationships; such model can be used by engineers to select sustainability methods. Moreover, the expert system accepts the input from the designer as a series of simple questions such as: what is the design stage, the solution characteristics, among others, and the expert system filters the database to suggest matching design methods. Authors foresee that this expert system will be used by practicing design engineers. The expert system will also reveal cases for which methods do not seem to exist; these can be identified as areas of research opportunity. Finally, the characterization process for the development of the expert system has been a challenge by itself and it has improved our understanding of the methods and their application.

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COMPUTATIONAL FLUID DYNAMICS AND VEINS

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ABSTRACT

The aim of our study is to do a fluid analysis in deep veins with the help of the software provided by ANSYS. We are going to create a geometry which resembles the vein containing unidirectional venous valves and are going to create the same flow circumstances which depict the flow undergoing in the veins.

It would be interesting to see what happens to the flow when the blood flows past the valves in the veins. We could see the flow patterns in the blood veins and find where the vortices are formed when there are obstructions like the valves which are acting to stop the flow, this could be helpful in estimating if there is a chance for the clot formation in some specific areas. Also the better understanding of such complicated flow physics can be very helpful in developing artificial valves effectively.

Elderly people and pregnant women are the ones who are most likely to develop deep vein thrombosis. From previous studies it was determined that women in their postpartum period are at the highest risk of developing a DVT and even pulmonary embolism in most of the cases. The aid of computational study could help in improving the prophylaxis given to old people and pregnant women, by better understanding the physics involved in the clot formation.

FUNDAMENTAL STUDY OF A BEAM VIBRATION FREQUENCY

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ABSTRACT

Fluid mechanic problems often require of extensive analysis having to do with the flow-induced vibrations (FIV), because of a fluid flow going past them a body undergoes unsteady motion. This phenomenon can be found in different situations, such as in conductor tubes, or even in human veins. This kind of vibrations can result in fatigue failure. We approached this problem by starting with simple 2D geometries we performed a fundamental analysis on these simple geometries using beams within the cross section of subject tests. We studied several characteristics such as the fluctuating lift and drag forces exerted on the beam due to the periodic changes. To obtain a better understanding of the fundamentals of the Flow-induced vibrations, so we can later apply our knowledge in more complicated problems. We used the software ANSYS v. 12 using its dynamic mesh user defined functions to facilitate the analysis in our specific cases. We are still working in the results.

COMPUTATIONAL FLUID DYNAMICS FOR PARACHUTE ANALYSIS

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ABSTRACT

The main focus is on the Computational fluid interaction of the effect of parachutes is use on stresses and forces in the material. Constant research is being done to understand how air behaves when it interacts with parachutes. Due to the high turbulence and chaotic air behavioral it is difficult to predict the behavior of the parachute. The stresses and pressure measurements are nearly impossible to take when in actual use. By simulating such problem in a computer software major advancement is made. The measurements are now taken and the behavior of the parachute is obtained. Rather than having to physically experiment and conduct these experiments time an a large amount of money is saved.

These problems are solved with the help of computer software. The main objective is to use example problems to learn how to use LS DYNA Pre-Post and Post Processor, and learn in order to work on problems of our own. The purpose is to duplicate a army parachute and use results to create more efficient parachutes. LS DYNA only reads K files and K files are also covered in the report, these K files are automatically created when working on the Pre Post Processor. The combination of various computer software's is used to solve parachute problems. The results are analyzed interpreted and a conclusion is made. All scenarios are for actual parachutes. Parachutes include the G-12 a 64 ft diameter parachute. Also included are a T-10 personal parachute. The T-10 parachute is a 32 ft diameter parachute. All parachutes covered are those used by the ARMY.

POINT SITE SELECTION FOR SEQUESTERING CO2: DETERMINING THE IMPACT OF AN EARTHQUAKE ON SEAL INTEGRITY OF A RESERVOIR CAP-ROCK

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ABSTRACT

One of the most important steps involved in Carbon Capture and Store (CCS) is selecting a site for the CCS. Some of the most promising methods for assessing potential carbon dioxide geologic storage sites are the focus of the latest in a series of U.S. Department of Energy (DOE) CCS "best practices" manuals. One of the best practices of selecting a CCS site is to understand the sear-integrity of cap-rock formation during or after natural or induced seismic activities from an Earthquake or carbon sequestration process. Seismic activities are characterized by normal P- and shear S- wave. We perform computational analysis of multiphase fluid flow in a potential CO2 sequestration reservoir system. The normal (pressure) and shear stress at the reservoir boundaries are assumed to be varying in both space and time to simulate an Earthquake. We plan to estimate the boundary conditions from a real life Earthquake in the form of P-wave and S-wave.

COMPUTATIONAL THERMAL ANALYSIS AND MEASUREMENT OF THE SALT GRADIENT STABILITY IN A SOLAR POND

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ABSTRACT

Thermal Energy Storage (TES) systems are a group of technologies employed for the storage and reuse of energy in the form of heat. A promising technology which has proven to be efficient is the solar pond. Solar ponds combine solar energy collection with long-term storage and can provide reliable thermal energy at temperature ranges from 50 to 90°C. An extensive analysis of the stability of a small scale solar pond prototype is performed. The apparatus, which is composed of an acrylic tube with a hot plate emulating the solar thermal energy input, serves as a model to study various saltwater gradients. The Solar Pond consists of three distinct zones. The first zone, which is located at the top of the pond and contains the less dense saltwater mixture, is the absorption and transmission region, also known as the upper convective zone (UCZ). The second zone, which contains a variation of saltwater densities increasing with depth, is the gradient zone or non-convective zone (NCZ). The main purpose of this zone is to act as an insulator to prevent heat from escaping to the less dense zone, maintaining higher temperatures at deeper zones. The last zone is the storage zone or lower convective zone (LCZ). In this region, the density is uniform and near saturation. Furthermore, two-dimensional computational studies of the heat transfer phenomena using Fluent are performed utilizing user-defined parameters. The results from both the experimental setup and the computational analysis are compared and a Stability Margin criterion is established.

A VARIATIONAL APPROACH TO ONE PHASE NON-NEWTONIAN FLOW IN CIRCULAR DUCT

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ABSTRACT

Carbon capture and storage(CCS) is one of the potential ways of mitigating the contribution of fossil fuel emissions to global warming, based on capturing carbon dioxide from large point sources, storing it away from the atmosphere through a different means. The underlying physics associated with carbon dioxide sequestration can be properly described as a capturing by the pore-network modeling of permeable rocks in a reservoir. Non-Newtonian flow physics is an important study in carbon dioxide sequestration. Variational approach is a method to approximate analytical expressions for computing flow conductance through various cross section pores. We are developing a multiphase flow conductance model using variational methods for generalized pore geometries. The variational approach allows an extension at the fluid to fluid interface concerning dimple free-slip or no-slip boundary conditions that can minimize the computational effort. Test functions are used to approximate the velocity from the C^2- continuous inside the natural porous media resulting in generally unpredictable absorption kinetics and total absorption capacity for injected fluids. Based on our study in single and two phase Newtonian flow in triangular and circular ducts, the variational method was applied for a non-Newtonian fluid in circular cross section pores, which provided a good approximation for hydraulic conductance of pore throats in this study.

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A MULTIPLE OBJECTIVE APPROACH TO SOLVE THE PARALLEL-SERIES SYSTEM REDUNDANCY ALLOCATION PROBLEM WITH ENVIRONMENTAL CONSTRAINTS

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ABSTRACT

The well-known reliability optimization problem, the redundancy allocation problem (RAP) involves the simultaneous selection of system components and a design level configuration that can meet several design constraints in order to optimize the predefined objective function(s). The RAP has been predominantly solved as a single objective optimization problem with the reliability of the system to be maximized or system design cost to be minimized. When considered as a multiple objective reliability optimization problem, the system reliability is maximized and the cost and weight of the system are minimized. In this paper, the RAP was formulated as a multiple objective optimization problem with the system reliability to be maximized and the cost and environmental carbon dioxide emissions to be minimized. A well-known Multi-objective Evolutionary Algorithm (MOEA) named Non-dominated Sorting Genetic Algorithm II (NSGA-II) was used to solve this multiple objective redundancy allocation problem (MORAP).

OPTIMIZATION OF WIND TURBINE PLACEMENT USING VIRAL SYSTEM

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ABSTRACT

In the present research, a new algorithm is developed to search the optimal number and placement of wind turbines in large wind farms with the objective of minimizing the cost per unit power produced from the wind park. In this research a viral system optimization algorithm is used to find the solution that provides the optimal solution to three well known problems in literature: (a) Constant wind speed and unidirectional uniform wind, (b) Constant wind speed with variable direction, and (c) Non-uniform variable wind speed with variable direction. The distance between two wind turbines is reduced to one meter, compared to 5 rotor diameters in previous studies.

A POST-PARETO ANALYSIS TO SOLVE THE RENEWABLE ENERGY SYSTEM INTEGRATION PROBLEM CONSIDERING MULTIPLE OBJECTIVES

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ABSTRACT

In the present work, a modeling and simulation framework using a micro power optimization software (HOMER®) to solve the multi-objective renewable energy integration problem considering various renewable energy technologies is presented. The main objectives considered in the present study are the minimization of the total lifecycle cost of the system, considering the capital, replacement, operation, maintenance, fuel and interest costs and the minimization of green gas house emissions. The final solution to the multi-objective renewable energy integration problem is a set of solutions usually known as Pareto solutions. This paper shows why clustering methods such as K-means and DGSOT are not very helpful as Post-Pareto Analysis when utilizing specifically HOMER® as the basis for obtaining Multi-Objective approaches by expanding such answers, and hence the Nash-Equilibrium concept from Game Theory can be utilized to select a single solution out of the Pareto Front when a game is defined where each dimension is an agent that tries to optimize its own objective playing against the other agents which in turn represent other dimensions, thus providing an equilibrium that can be interpreted as a single final solution that simultaneously solves the different objectives.

ZERO NET CARBON STUDY

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ABSTRACT

This paper presents the status of a campus project to discover all the sources on the UTEP campus emitting carbon and greenhouse gases. The project addresses the major UTEP entities involved in emission control to quantify and model the emissions that may lead to carbon reduction programs on campus. The project is supervised by two professors from Civil Engineering and the UTEP Director of Energy Initiatives. Material on GHG and CO_2 emissions from the National Renewable Energy Laboratory (NREL) and the National Energy Technology Laboratory (NETL) is used as a guide to performing the study.

The objectives for this project are to measure the CO_2 and greenhouse gas levels on campus to quantify and establish a 2011/2012 baseline. This baseline for the UTEP campus can be used to create a plan that will include potential measurement and modeling techniques to be used by the entities emitting the gases. UTEP understands that total zero net carbon goals are unattainable; however GHG and CO_2 reduction programs are possible on campus.

This kind of study can help UTEP to decrease GHG and CO_2 emissions to understand where the sources are and what can do to decrease the emission level. Categorization and labeling of the sources on the UTEP campus needs to be the first step. Existing data from various department and entities will be examined. From the source data we identify methods measure the carbon emission at the sources of the campus. With the data, a baseline can be set for CO_2 and greenhouse gases using the modeling programs, such as ones used by the National Renewable Energy Laboratory (NREL) or National Energy Technology Laboratory (NETL). Then a goal needs to be set that UTEP wants to meet for their air quality levels. The current status of the project will be described in this presentation.

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