Monday August 1

0900 (W) - Welcome (John HS Lee)

0940 (1A) - Detonation - Dynamics (Sergey Mevedev)
940 Numerical Simulation of Spin Detonation in Square Tube A.K. Hayashi, K. Eto, N. Tsuboi

1005 **Propagation Mechanism and Transmission of Quasi-Detonations** *P.N. Krivosheyev, O.G. Penyazkov, S.A. Zhdanok*

1030 The Unsteady Dynamics of the Head-On Collision Between a Detonation and a Shock Wave B.B. Botros, Y. J. Zhu, H.D. Ng, J.H.S. Lee

0940 (1B) - Flames - Premixed (Makihito Nishioka)
940 Effects of Radiation Reabsorption on Flame Propagation and
Flammability Limits in CO2 Diluted Flames X. Qin, Z. Chen, Y. Ju
1005 Adiabatic Cellular Premixed Flames of Methane (Ethane, Propane),
Oxygen, and Carbon Dioxide Mixtures A. A. Konnov, I. V. Dyakov
1030 Burning Velocities of Stoichiometric Methane-Hydrogen-Air Flames at
Gasturbine Like Conditions R.T.E. Hermanns, R.J.M. Bastiaaans, L.P.H. de Goey

0940 (1C) - Droplet Combustion (Carl Knowlen)

940 Numerical Study of Fiber Influences on Droplet Flow and Vaporization D. Shringi, H.A. Dwyer, B.D. Shaw

1005 Effects of Liquid Fuel Mass Fraction and Droplet Size on Droplet Group Combustion Behavior M. Nakamura, F. Akamatsu, R. Kurose, M. Katsuki 1030 A Study of the Flow, Heat Transfer, and Mass Transfer Characteristics of Droplet Arrays H.A. Dwyer, B.D. Shaw

1055 (1PO) - Poster I - Flame (Charles Kiyanda)

1055 (B) - Break

1145 (2A) - Detonation in Flowing Systems (A. Koichi Hayashi)

1145 **Detonation Initiation in Moving Non-Premixed Flows** V.V. Golub, V.V. Volodin, T.V. Bazhenova, D.I. Baklanov, S.V. Golovastov, D.G. Lisin

1210 Detonation Waves in Supersonic Stream of Homogeneous Reacting Mixture A.A. Vasil'ev, D.G. Nalivaichenko, V.I. Zvegintsev

1235 Investigation of Transition of Deflagration to Detonation in Moving Mixtures of Combustible Gases D.I. Baklanov, S.V. Golovastov, L.G. Gvosdeva, A. Kaltayev, N.B. Scherbak, V.V. Volodin

1145 (2B) - Flames - Lifted (Habib Najm)

1145 Lift-off Stability of Hydrocarbon Jet Diffusion Flames F. Takahashi, V.R. Katta

1210 Local Flame Displacement Velocity of Hydrogen Added Methane Premixed Turbulent Flames *M. Nakahara, H. Kido, K. Nakashima, H. Takamoto* 1235 A Qualitative Study of the Effect of Asymmetric Fuel Nozzles on the Blow-Out Limits of Non- and Swirling CH4-Air Diffusion Flames *T.M. Phillips, M. Birouk*

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1145 (2C) - Kinetics - Detailed Mechanisms (Alexander Konnov)1145 Chemical Kinetic Databases for the Simulation of Hydrocarbon

Combustion Phenomena *W. Tsang*

1210 Automatic Generation of a Detailed Mechanism for the Oxidation of n-Decane G. Moreac, E.S. Blurock, F. Mauss

1235 Using Genetic Algorithms to Derive the Kinetics of Smoldering Combustion G. Rein, C. Lautenberger, A.C. Fernandez-Pello

1300 (L) - Lunch

1440 (3A) - Detonation Diffraction (Joanna Austin)

1440 **Detonation Diffraction in Regular and Irregular Mixtures** *F. Pintgen, J.E. Shepherd*

1505 Promoting Detonation Diffraction from Circular Tube to Cone by
Obstacles A. Marelli, B. Khasainov, V. Guilly, H.-N. Presles, D. Desbordes
1530 Detonation Diffraction Through Different Geometries R. Sorin, R. Zitoun, D. Desbordes

1440 (3B) - Flames - Premixed Structure (Moshe Matalon) 1440 Self-Similar Behaviour of Laminar Premixed Flames G. Ribert, O. Gicquel, N. Darabiha, D. Veynante

1505 **The Role of Explosive Modes in Homogeneous Ignition and Premixed Flames** J.C. Lee, H.N. Najm, S. Lefantzi, J. Ray, M. Frenklach, M. Valorani, D.A. Goussis

1530 Effect of Particle Morphology on the Thermophoretic Behavior of Soot Particles S. Suzuki, R. Dobashi

1440 (3C) - Turbulent Combustion I (Frank Behrendt)

1440 Laser Induced Fluorescence in High Pressure Cryogenic LOx/GCH4 and LOx/GH2 Jet Flames G. Singla, P. Scouflaire, C. Rolon, S. Candel 1505 Laser Induced Plasma Spectroscopy for Local Composition Measurements Inside a Low Swirl Burner L. Zimmer, S. Tachibana 1530 Lean Premixed Turbulent Methane Combustion with Hydrogen Additions: Burning Velocities and Emissions Measurements Y.C. Chen, S.S. Shy

1555 (B) - Break

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1620 (4A) - Detonation Simulation (Matei Radulescu)

1620 Hybrid Large-Eddy Simulation of Detonations in Reactive Mixtures B. Fryxell, F. Genin, S. Menon

1645 **The Effect of Discrete Energy Sources on Detonation Propagation** *A.J. Higgins*

1710 Multi-Processor Simulation of Forming a Detonation Wave in Shock Tube on the Molecular Process Level S.V. Kulikov

1620 (4B) - Flames - Premixed Spherical (Michael Liberman) 1620 Development of Instabilities in Closed Vessel Laminar and Turbulent Explosions A. S. Al-Shahrany, D. Bradley, M. Lawes, K. Liu, R. Woolley 1645 A Theoretical Evaluation of Turbulent Markstein Number for Expanding Spherical Flames A.N. Lipatnikov, J. Chomiak
1710 How Large Can the Rate of Expansion of a Spherical Flame Grow? V.

1/10 How Large Can the Rate of Expansion of a Spherical Flame Grow? V. Karlin, J. Mai

1620 (4C) - Shock Waves (Boris Gelfand)
1620 Mathematical Modelling of Two Problems of Wave Dynamics in Heterogeneous Media A.V. Fedorov, I.A. Fedorchenko, I.V. Leontev
1645 Blast Wave on a Parallelepipedic Obstacle S. Trelat, I. Sochet, B. Autrusson, K. Cheval, O. Loiseau
1710 Shack Wave Interpretion with a Lagas Ducty Bulk B. Fern Y. Lings

1710 Shock Wave Interaction with a Loose Dusty Bulk B. Fan, X. Jiang

Tuesday August 2

0900 (1PL) - Plenary I (Ulrich Maas)900 The Development of Hydrodynamically Unstable Flames M. Matalon

1005 (5A) - Detonation Properties (Gabrielle Dupre)
1005 Influence of the Initial Temperature on the Detonability of
CH4/H2/O2/N2 Mixtures C. Matignon, D. Desbordes, H.N. Presles
1030 Effect of Two Additives (CH3NO2 and H2O2) on the Detonation
Properties of Gaseous Stoichiometric n-C7H16/O2 Mixtures B. Imbert, L.
Catoire, N. Chaumeix, G. Dupre, C. Paillard
1055 Critical Orifice Diameter Measurements for NH3-N2O at Elevated
Pressure C. Knowlen, A.T. Mattick

1005 (5B) - Flames - Quenching (Nondas Mastorakos)
1005 Effects of Flow Rate and Kinetic Quenching on the Transition of Flame Regimes in Mesoscale Combustion Y. Ju, B. Xu
1030 Study of Laminar Flame Quenching in a Rotating Cylindrical Vessel J. Jarosinski, A. Gorczakowski
1055 Detailed Numerical Simulation of the Extinction of Lean Premixed Flames Through Parallel Plates L. Tecce, F.S. Marra, G. Continillo
1005 (5C) - Explosion - Droplets (Piotr Wolanski)

1005 (SC) - Explosion - Droplets (Flott Wolaliski)
1005 Detonation Initiation in Dispersed Fuel-Air Mixtures N.N. Smirnov, V.F. Nikitin, J. Khadem, V.M. Shevtsova, J.C.Legros
1030 A Study of Shock Wave - Hexane Droplets Interaction A. Kobiera, J. Szymczyk, P. Wolanski, A. Kuhl
1055 Observation of Microexplosion in Light Oil-Water Emulsion Spray
Flame M. Fuchihata, T. Ida

1120 (B) - Break

1145 (6A) - Detonation Applications (Anatoly Vasil'ev)

1145 Effect of Boundary Layer for Wedge-Induced Attached Oblique Detonations Y. Daimon, A. Matsuo

1210 Numerical Simulation on Two-Dimensional H2/Air Detonation Waves Propagating in a Converging-Diverging Nozzle H. Jotaki, N. Tsuboi, A. K. Hayashi

1235 An Experimental Study of Rotating Detonation Engine P. Wolanski, J. Kindracki, T. Fujiwara, Y. Oka, K. Shima-uchi

1145 (6B) - Flames - Microscale (Uwe Riedel)

1145 **Film Combustion in Small Cylinders** *T.K. Pham, D. Dunn-Rankin, W.A. Sirignano*

1210 Numerical Simulation of Hydrogen/Air Combustion Characteristics Inside a Platinum Microtube G.-B. Chen, Y.-C. Chao, C.-P. Chen, C.-Y. Wu 1235 Structure of Microjet Methane Diffusion Flames T.S. Cheng, Y.-H. Li, C.-S. Chen, C.-Y. Wu, C.-P. Chen, Y.-C. Chao

1145 (6C) - Combustor Stability (Suresh Menon)
1145 High Frequency Combustion Oscillations Induced by Transverse
Acoustic Modulations F. Richecoeur, S. Ducruix, P. Scouflaire, S. Candel
1210 Stability Analysis of Low-NOx Gas Turbine Combustors F. Di Palma, A.
Di Benedetto, F. S. Marra
1235 Effect of Swirl on the Stability of a Lifted Flame Sustained by a Low-

Swirl Burner S. Tachibana, L. Zimmer

1300 (L) - Lunch

1440 (7A) - Pulse Detonation Engines (Toshi Fujiwara)
1440 Experiments on Inter-Tube Interference in a Four-Tube Pulse Detonation
Engine T. Yatsufusa, K. Nishimura, T. Yamaguchi, K. Yoshinaga, T. Endo, S. Taki
1505 Performance of Propellant Decomposition Products as Fuel in
Airbreathing PDE B. Veyssiere, B.A.Khasainov, P.Walton, E. Daniau
1530 Detonation Initiation in Pulse Detonation Engines: Experiments and
Simulations V.E. Tangirala, P.F. Pinard, K. Hinckley, A. Rasheed, A.J. Dean

1440 (7B) - Flames - Edge (Forman Williams)

1440 Edge-Flames and Cellular Structures in Oscillatory Non-Premixed Counterflows D.A. Kessler, M. Short, J. Buckmaster
1505 Flame-Edge Dynamics in Diffusion-Flame/Vortex Interactions M. Hermanns, M. Vera, A. Linan
1530 Destabilization of Non-premixed Lifted Flames by Low Amplitude

Acoustic Perturbations D. Demare, F. Baillot, A. Wyzgolik

1440 (7C) - Turbulent Combustion II (Harry Dwyer)

1440 Relevance of Approximated PDF Shapes for Turbulent Combustion Modeling with Variable Equivalence Ratio V. Robin, A. Mura, M. Champion, P. Plion

1505 A Flame Surface Density Model Including Tabulated Chemistry and Heat Losses W. Ghedhaifi, N. Darabiha, O. Gicquel, D. Veynante, L. Pierrot
1530 Modeling Turbulent Mixing of an Evaporating Spray G. Subramanian, O.

Colin, A. Pires da cruz, L. Vervisch, G. Bruneaux

1555 (B) - Break

1620 (8A) - Detonation Structure I (Sergey Frolov)

1620 **The Hydrodynamic Structure of Detonations** *M. I. Radulescu, G. J. Sharpe, C. K. Law*

1645 **Characterizing the Fluctuations in Gaseous Detonation Fronts** *J.M. Austin, J.E. Shepherd*

1710 Photographic Study of the Two-Dimensional Dynamics of Irregular Detonation Waves C.B. Kiyanda, A.J. Higgins, J.H.S. Lee

1620 (8B) - Flames - Soot (Philippe Dagaut)

1620 Effects of Dilution on Soot Formation in Laminar C2H4 Diffusion

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Flames H. Mohammed, M. Chaos, R.H. Chen, F. Xu 1645 Detailed Kinetic Modeling of PAH Growth and Soot Formation in Shock Tube Pyrolysis of Benzene and Ethylene G.L. Agafonov, I. Naydenova, M. Nullmeier, P.A. Vlasov, J. Warnatz 1710 Aspects of Modeling Soot Formation in Turbulent Diffusion Flames F.

1/10 Aspects of Modeling Soot Formation in Turbulent Diffusion Flames F. Mauss, K. Netzell, H. Lehtiniemi

1620 (8C) - Propulsion (Bernard Veyssiere)

1620 Unsteady One-Dimensional Modeling of Ram Accelerator at Elevated Pressure in the Subdetonative Velocity Regime P.A. Bauer, Y. D'Angelo, C. Knowlen, A.P. Bruckner

1645 Development of a High Test Hydrogen Peroxide (HTP) Micro-Thruster C.-K. Kuan, G.-B. Chen, Y.-C. Chao

1710 Gasdynamic Operation of Baffled Tube Ram Accelerator in Highly Energetic Mixtures A.J. Higgins, C. Knowlen, C.B. Kiyanda

Wednesday August 3

0900 (9A) - IC Engines I (Derek Dunn-Rankin)

900 Modeling Diesel Spray Ignition Using Detailed Chemistry with a Flamelet Progress Variable Approach H. Lehtiniemi, P. Amneus, F. Mauss, M. Balthasar, A. Karlsson, I. Magnusson

925 Transient Species Analysis in Homogeneous Charge Compression of Dimethyl Ether M. Ohtomo, M. Yoshii, Y. Yamasaki, T. Yamaguchi, H. Yamada, A. Tezaki

950 **Dynamic Model of Combustion in a Piston Engine** *E.Y. Bitar, H.J. Schock, A.K. Oppenheim*

0900 (9B) - Multiphase Combustion (Rudolf Klemens)

900 Finite Rate Heat-Transfer Effects on Multiphase Burning in Confined
Porous Propellants A.M. Telengator, S.B. Margolis, F.A. Williams
925 Gasification of Single Wood Particles: Experiment and Simulation B.

Wilmes, U. Kuhlmann, F. Behrendt

950 **PDF Modeling of the Mixing Process in Turbulent Spray Flows** *H.-W. Ge*, *E. Gutheil*

0900 (9C) - Detonation Modeling (Ash Kapila)

900 **On the Inclusion of Frictional Work in Non-Ideal Detonations** *V. Tanguay, A.J. Higgins*

925 Soot Track Formation by Shock Waves and Detonations K. Inaba, A. Matsuo, J.E. Shepherd

950 Study of Detonation Sensitivity of Hydrogen-Air Mixture Using an Updated Comprehensive Chemical Kinetic Mechanism *H.D. Ng, Y. Ju, J.H.S. Lee*

1015 (2PO) - **Poster II - Detonation** (Charles Kiyanda)

1015 (B) - Break

1120 (10A) - Detonation - Past and Future - In Honor of AK

Oppenheim's 90th Birthday (John HS Lee)

1120 Detonation as a Self-Sustained or "Living" Phenomenon J.E. Shepherd

1145 Theory & Modeling of Detonation Wave Stability: A Brief Look at the Past and Toward the Future *M. Short*

1210 Computing Detonations V.N. Gamezo, E.S. Oran

1235 'Explosion in the Explosion' and the Onset of Detonation S. Dorofeev

1120 (10B) - Combustors (Gaetano Continillo)

1120 Influence of Staging Ratio on a Premixed Swirled Burner N. Dioc, S. Ducruix, F. Lacas, D. Veynante

1145 The Oxidation of Hydrogen-Enriched Natural Gas Blends: Experimental and Detailed Chemical Kinetic Modeling Study G. Dayma, A. Nicolle, P. Dagaut 1210 Efficiency of Air Injection on Stability and Emission Controls in Premixed Combustion H. Sato, C. Nishidome, I. Kajiwara, T. Nagao, A. K. Hayashi

7

and S. Ogawa

1235 Kinetic Effects of Air Contamination on the Combustion of Hydrogen G. Dayma, A. Nicolle, P. Dagaut

1120 (10C) - Kinetics - Reduced (Jurgen Warnatz)
1120 An Adaptive Reduced-Order Chemical Model J.C. Lee, H.N. Najm, S. Lefantzi, J. Ray, M. Frenklach, M. Valorani, D.A. Goussis
1145 ILDM Reduced Chemistry Tailored For Large Scale Reaction Mechanisms in Complex Reactive Flow Applications V. Reinhardt, B. Schramm, D. Lebiedz, J. Warnatz
1210 Implementation of ILDMs Based on a Representation in Generalized Coordinates J. Bauer, U. Maas
1235 Generation of Reduced Models by Decoupling of Chemical Kinetics and Convection/Diffusion Processes V. Bykov, U. Maas

1300 (L) - Lunch

Thursday August 4

0900 (2PL) - Plenary II (Luc Bauwens)
900 Fundamental and Applied Studies of Fuel-Air Detonation - A Quarter Century of Large-Scale Testing at DRDC Suffield S.B. Murray

1005 (11A) - **Detonation Initiation** (Andrew Higgins)

1005 Initiation and its Optimization A.A. Vasil'ev

1030 **Detonation Initiation by Shock Reflection from an Orifice Plate** *G. Ciccarelli, B. de Witt*

1055 Shock-Wave Initiation of Detonations in Propane/Air Mixtures O.G. Penyazkov, K.L. Sevruk, V.E. Tangirala, A.J. Dean, B. Varatharajan

1005 (11B) - Flames - Unsteady (Derek Bradley)

1005 **Pressure Wave Interactions with Rippled Premixed Flames - Effect of** Lewis Number A.C. McIntosh, J. Teerling, J. Brindley

1030 Effect of an Oscillatory Small Scale Flow on Flame Propagation J. Daou, P. Sparks

1055 Parallel Bifurcation Analysis of Discontinuous Periodically Forced Reactors A. Grabski, L. Russo, G. Continillo

1005 (11C) - Blast Waves and Hybrid Detonation (Sergey Dorofeev)
1005 Simplified Modeling of Non-Ideal Blast Waves from Metallized
Heterogeneous Explosives Z. Zarei, D.L. Frost, L. Donahue, D.R. Whitehouse
1030 Secondary Pressure Waves from Rich Fireballs F. Pintgen, J.E. Shepherd
1055 Hybrid Detonation Waves F. Zhang, S.B. Murray, K.B. Gerrard

1120 (B) - Break

1205 (12A) - Detonation Structure II (Oleg G. Penyazkov)

1205 Numerical Study of Detonation Cells Under Non-Monotonous Heat

Release V. Guilly, B. Khasainov, H.-N. Presles, D. Desbordes, P. Vidal

1230 **Detonation Wave Structure for Chain-branching Kinetics** Z. Liang, L. Bauwens

1255 Three-Dimensional Numerical Simulation of H2/Air Detonation in a Circular Tube : Structure of Spinning Mode *N. Tsuboi, K. Eto, A.K. Hayashi*

1205 (12B) - Explosions I (Kailas Kailasanath)

1205 **Biomimetic Study of Explosive Discharge of Bombardier Beetle** *N. Beheshti, A.C. McIntosh*

1230 Influence of a Multi-Source Ignition on the Kerosene Flammability in a Partitioned Tank J.M. Pascaud, P. Gillard

1255 **Detonation of Hydrogen in a Partially Filled Interconnecting Vessel Following an Initial Period of Pressure Piling** S.K. Willacy, H.N. Phylaktou, G.E. Andrews, M.C. Mkpadi

1205 (12C) - Flame Ignition (Eric Petersen)

1205 **The Role of Hydrogen Pre-Reaction for Methane Catalytic Ignition** *H.-W. Hsu, J.-Y. Chen, Y.-C. Chao*

1230 Ignition of Methanol Droplet Groups with Detailed Chemical Kinetics in Different Flow Environments H.A. Dwyer, B.D. Shaw

1255 Measurements of the Probability of Ignition and Subsequent Flame Propagation Speed in Turbulent Non-Premixed Jets S.F. Ahmed, E. Mastorakos

1300 (L) - Lunch

1440 (13A) - Detonation and Interfaces (Stephen Murray)
1440 Instability of Combustion Products Interface from Detonation of
Heterogeneous Explosives D.L. Frost, Z. Zarei, F. Zhang
1505 Shock Wave Induced Mixing and Reaction D.H. Lieberman, J.E. Shepherd
1520 An Investigation of the Conditions for Detonation Initiation et a 1D

1530 An Investigation of the Conditions for Detonation Initiation at a 1D Turbulent Mixing Interface J. Chao, J.H.S. Lee

1440 (13B) - Metal Combustion (Mel Branch)
1440 Combustion of Shock-Dispersed Flake-Aluminum in a Long Tunnel
Section P. Neuwald, H. Reichenbach, A.L. Kuhl
1505 Burning Properties of Aluminum in H2O and CO2 J.J. Lee, F. Zhang
1520 Spectral Structure of the Aluminum Dust Flame I. Manuar, S. Canachin

1530 Spectral Structure of the Aluminum Dust Flame J. Mamen, S. Goroshin, A. Higgins

1440 (13C) - Flames - Nonpremixed Simulation (Marcus Day)
1440 Large Eddy Simulations of Pool Fires at Different Cross-Wind Velocities
with a Large Adjacent Object C. B. Devaud, E. J. Weckman
1505 Comparative Study of Turbulence Modelling in Hydrogen Nonpremixed
Turbulent Flame F. Tabet-Helal, B. Sarh, I. Golkalp, A. Menou
1530 A Numerical Study on NO Formation in Counterflow n-Heptane Triple
Flames H. Guo, G.J. Smallwood

1555 (B) - Break

1620 (14A) - Detonation Structure III (Akiko Matsuo)
1620 Influence of Ar Dilution on Detonation Regime in H2-NO2/N2O4
Mixtures J. Luche, H. N. Presles and D. Desbordes
1645 Study of Overdriven Detonations of H2-NO2/N2O4 Mixtures J. Luche, D. Desbordes, H. N. Presles
1710 Argon or Nitrogen Diluted Hydrogen/Oxygen Detonation in Tube with
Obstacles A.K. Hayashi, K. Eto, Y.-F. Liu, N. Tsuboi, S. Shiokawa, H. Sato, J.H.S. Lee
1620 (14B) - Shock Ignition (Pascal Bauer)
1620 Ignition of Aviation Kerosene at High Temperatures A.J. Dean, O.G. Penyazkov, K.L. Sevruk, B. Varatharajan

1645 Acceleration of Shock-Induced Ignition in CH4/Air and CO/Air Mixtures Using Hydrogen Addition E.L. Petersen, J.M. Hall, J. de Vries, A.R. Amadio, S.D. Smith, M.W. Crofton

 $1710 \quad \textbf{Initiation of Detonations and Deflagrations by Shock Reflection and}$

Focusing S.I. Jackson, P.M. Buraczewski, J.E. Shepherd

1620 (14C) - Flames - Computation (Andy McIntosh) 1620 Computational and Experimental Study of Steady Two-Dimensional Axisymmetric Non-Premixed Methane Counterflow Flames G. Amantini, J.H. Frank, M.D. Smooke, A. Gomez

1645 **Confined Burke-Schumann Flames With Small Stoichiometric Mixture Fraction and Small Fuel Radius** *M. Sanchez-Sanz, A. Revuelta, A.L. Sanchez, A. Linan*

1710 Effect of Local Flame Stretch at the Tip of the Flame Propagating in a Vortex M. Nishioka, T. Hokazono

Friday August 5

0940 (15A) - Detonation - High Explosive (Mark Short)
940 Simulation of Detonation of Aerated Ammonium Nitrate Based Emulsion Explosives A.Yu. Reshetnyak, A.E. Medvedev, V.M. Fomin
1005 Thermodynamic Solution for Combustion of PETN/TNT Products with Air A.L. Kuhl, J.B. Bell
1030 Numerical Studies of Detonation Diffraction Using the Ignition-and-Growth Model A.K. Kapila, D.W. Schwendeman
0940 (15B) - IC Engines II (Fabian Mauss)
940 Pressure Diagnostics of HCCI Combustion Initiated by Pulsed Flame Jet K. Hotta, O. Moriue, E. Murase
1005 Numerical Study of the Influence of Hot Spot Formation and EGR on Knock Occurrence in SI-Engines M.A. Liberman, L.-E. Eriksson, M.F. Ivanov, D. Valiev
1030 Fuel Composition Influence on Auto-Ignition in 3D Engine Simulations S. Jay, O. Colin

0940 (15C) - Turbulent Combustion III (Jerry Lee)

940 **Numerical Control of 3D Turbulent Premixed Flame Simulations** *M.S. Day, J.B. Bell, J.F. Grcar, V.E. Beckner*

1005 Characteristics of Flow Field and Flame Propagation in a Vortex Ring K. Asato, A. Ogura, Y. Doi

1030 Investigations on the Flamelet Inner Structure of Turbulent Premixed Flames F. Halter, C. Chauveau, I. Gokalp

1055 (3PO) - Poster III - Explosion (Charles Kiyanda)

1055 (B) - Break

1145 (16A) - **Deflagration-to-Detonation Transition I** (Gaby Ciccarelli)

1145 **Examination of the DDT Triggering in an Obstructed Tube** *S. Medvedev, S. Khomik, H. Olivier, B. Gelfand*

1210 Effect of Boundary Layer on Flame Acceleration and DDT M. Kuznetsov, I. Matsukov, V. Alekseev, W. Breitung, S. Dorofeev

1235 **DDT Properties of Hydrocarbon-Air Mixtures with Additive of Acetylene** *K. Ishii, T. Takada, T. Akiyoshi, M. Murayama*

1145 (16B) - **Dust Explosion** (Fan Zhang)

1145 **Flame Propagation Through Cornstarch Dust-Air Mixtures in a Vertical Duct** *S. Wang, Y. Pu, F. Jia, S. Wan*

1210 **Dust Lifting Up Process From the Layer in Slow Air Flow** *R. Klemens, P. Zydak*

1235 Influence of Suspension Generation on Dust Explosion Parameters *O. Bozier, B. Veyssiere*

1145 (16C) - Catalytic Combustion (Dave Frost)
1145 Development of a Catalytic Hydrogen Micro-propulsion System Y.-C.
Chao, G.-B. Chen, C.-Y. Wu, C.-P. Chen
1210 Studies of Slip Effects on Fuel Oxidation in Microscale Catalytic
Reactors B. Xu, Y. Ju

1235 Burn Rate Sensitization of Solid Propellants Using a Nano-Titania J.L. Small, M.A. Stephens, S. Deshpande, E.L. Petersen, S. Seal

1300 (L) - Lunch

1440 (17A) - Flame Acceleration I (Nabiha Chaumeix)

1440 **Control of Flame Transmission from a Vessel to a Discharge Duct** *N*. *Henneton, B. Ponizy, B. Veyssiere*

1505 **Tube Diameter Effect on Deflagration-to-Detonation Transition of Propane-Oxygen Mixtures** *J.-M. Li, K.-M. Chung, W.-H. Lai* 1530 **Simulation and Analysis of Accelerating Flames in Tubes** *C.R.L. Bauwens,*

L. Bauwens, I. Wierzba

1440 (17B) - Explosion Hazards (Allen Kuhl)

1440 Effectiveness of Protective Covers in Case of a Detonation Wave Reflection S. Medvedev, S. Khomik, H. Olivier, B. Gelfand 1505 Flame Quenching Performance of Ceramic Foam H.I. Joo, G. Ciccarelli

1530 Direct Numerical Simulation on Hydrogen Fuel Jetting from High Pressure Tank Y.-F. Liu, N. Tsuboi, H. Sato, F. Higashino, A.K. Hayashi

1440 (17C) - Multiphase Combustion (Joe Shepherd)

1440 **Combustion of Bulk Metals in Supersonic Flow** *R. El-Saadi, V. Tanguay, A.J. Higgins*

1505 Reaction of Metal Particles in Gas-Phase Detonation Products V. Tanguay, S. Goroshin, A. Higgins, A. Yoshinaka, F. Zhang

1530 Reduction of DDT Run-Up Distance in a Two-Phase Flow by Combined Means S. M. Frolov, V. S. Aksenov, V. Ya. Basevich

1555 (B) - Break

1620 (18A) - Flame Acceleration II (Daniel Desbordes)

1620 Flame Acceleration and Detonation Transition in Narrow Tubes E.S. Oran, V.N. Gamezo

1645 Hydrodynamic Instability as a Mechanism for Deflagration-to-Detonation
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1710 H2 Gradient Effect on Premixed Flame Propagation in a Vertical

Facility: ENACCEF N. Lamoureux, F. Malet, N. Djebaili-Chaumeix, A. Bentaib, A. Bleyer, C.E. Paillard

1620 (18B) - Explosions II (Andrzej Teodorczyk)
1620 Water-Mist Mitigation of Quasi-Static Pressure Buildup in Enclosures
Subjected to an Explosion D.A. Schwer, K. Kailasanath
1645 Influence of the Chamber Volume on the Rich Explosion Limit for

Hexane-Air Mixtures M. Gieras, M. Kaluzny, R. Klemens, A. Kuhl, P. Oleszczak, W. Trzcinskio, P. Wolanski 1710 Plasma-Assisted Combustion of Propane-Air and Methane-Air Mixtures. Kinetics of Flame Acceleration E.I. Mintoussov, A.V. Krasnochub, A.Yu. Starikovskii

1620 (18C) - IC Engines III (Stephane Jay)
1620 A Study of Injection and Mixing of Gaseous Jets for Direct Injection M. Sutkowski, A. Teodorczyk, C. Xia, A. Sobiesiak
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Gases A. Ahmedi, F. Mauss, B. Sunden
1710 Spark Plug and Corona Abilities to Ignite Lean Methane/Air Mixtures M. Bellenoue, S. Labuda, B. Ruttun, J. Sotton

1735 (F) - Farewell

Poster I: Flame - 1055 Monday August 1

1055 Structure of Flame Front of Hydrogen Jet Combustion in a Supersonic Air Stream U.K. Zhapbasbayev, Z.A. Mansurov 1055 The Combustion Characteristics for CO-CH4 Blended Fuels Y.-C. Chao, C.-Y. Wu, C.-H. Tien, G.-B. Chen, C.-P. Chen 1055 The Structure of Highly Impinging Flames on a Rotating Cylinder C. Stroud, M.C. Branch, M. Strobel, M. Ulsh 1055 Characteristics of Combustion of Rich-Lean Flame Burner Under Low-Load Combustion S. Kurachi, S. Hagi, Y. Umeda, S. Mochizuki, K. Asato 1055 Experimental Observation of Different Stabilisation Regimes of Laminar Partially Premixed Flames C. Lacour, D. Honore, A. Boukhalfa, S. Carpentier, P. Meunier 1055 Flame Stretch Rate of Laminar Flame Base Just Before Flashback at Different Burner Temperatures S. Sogo, S. Yuasa 1055 Infrared Measurement of Soot Particles in a Burner Flame K. Ishii, T. Tsuboi, K. Takashi, Y. Suzukawa 1055 Gas-Expansion Influence on Turbulent-Flame Propagation R.C. Aldredge 1055 Burning Liquid Fuel Films from Flat Plates Y.-H. Li, D. Dunn-Rankin, Y.-C. Chao 1055 Experimental Study on Microexplosive Burning of Binary Fuel Droplets H. Ghassemi, S.W. Baek, Q.S. Khan 1055 Nonlinear Dynamics of an Unstable Swirl Combustor: Frequency Locking and Open Loop Control B. Bellows, A. Hreiz, T. Lieuwen 1055 Absolute Concentration Measurement of Nitrogen Oxide in Flames by LIF Standard Addition Method N. Yoshikawa, H. Saitoh, H. Suzuki, T. Sano, K. Okuno, S.Hayashi 1055 A Study of Ignition Timing of HCCI Engine S. Shiba 1055 Prediction of Flame Propagation in a Tube with Obstacles Using a Fictitious Domain Method A. Kaltayev, Z. Ualiev, U. Riedel, J. Warnatz 1055 Comparative Analysis of Three Mathematical Models for Hydrogen **Ignition** *I.A. Bedarev*, *A.V. Fedorov* 1055 Formation of PAH, Fullerenes, Nanoparticles and Soot at Combustion of Hydrocarbons in Electric Field Z.A. Mansurov, N.G. Prikhodko, T.T. Mashan, B.T. Lesbaev 1055 Primary Methods of Reduction NOx and CO Concentration in Natural Gas Flame S.S. Slupek, M.K. Poskart, L.W. Szecowka 1055 Molecular Kinetic Computation of Turbulence in a Reacting Gas Flow A. Sakurai, M. Tsukamoto, H. Homma

Poster II: Detonation - 1015 Wednesday August 3

1015 Wave Dynamic Process in Detonation Reflection from Wedges Z. Jiang, Z. Hu. J.H.S. Lee 1015 Deflagration-to-Detonation Control by Nanosecond Gas Discharge V.P. Zhukov, A.Yu. Starikovskii 1015 **Detonation Initiation by the Electrical Discharges in the Plane** Channel V.A. Levin, V.V. Markov, T.A. Zhuravskaya, S.F. Osinkin 1015 Propagation of Detonation Wave in the Encumbered Channels V.A. Levin. V.V. Markov, T.A. Zhuravskava, S.F. Osinkin 1015 Application of Direct Monte-Carlo Method for Simulation of Gaseous Detonation Z.A. Walenta, A. Teodorczyk 1015 Chemical Spike in Multiheaded Detonation A.A. Vasiliev, A.V. Trotsyuk 1015 Detonation Properties of Mixed-Fuel-and-Air Gas Mixtures A. Yoshida, Y. Okuda, T. Yatsufusa, T. Endo, S. Taki, S. Aoki, Y. Umeda 1015 Development of Shock Diffuser for Pulse Detonation Turbine Engines K. Yoshinaga, T. Ofuka, A. Ochi, T. Yatsufusa, T. Endo, S. Taki, S. Aoki, Y. Umeda 1015 Re-initiation of Detonation Waves Behind a Perforated Plate J. Sentanuhady, Y. Tsukada, T. Yoshihashi, T. Obara, S. Ohyagi 1015 Equilibrium-Chemistry Model for Multiphase Reactive Premixed and Nonpremixed Flows B. Khasainov, A. Kuhl, S. Victorov 1015 Detonation in Suspended Aluminum Particles in Tubes H. Tao, Q. Chengsen, W. Pei 1015 A Thermochemical Code to Model Detonations in Condensed Energetic Materials Using Genetic Algorithms A. Zaver, U. Riedel, J. Warnatz 1015 Numerical Simulation of the Combustion of PETN/TNT Products with Air in Closed Chambers J.B. Bell, M. Day, V. Beckner, C. Rendleman, A.L. Kuhl, P. Neuwald 1015 The Role of Turbulent Transport for Detonation Initiation at a Turbulent Interface H.D. Ng, J. Chao, J.H.S. Lee 1015 Time-Dependent Dynamics of the Reaction Front Propagation in Detonation Structure P.N. Krivosheyev, O.G. Penyazkov, K.L. Sevruk 1015 Applicability Range of Detonation Resonator S. Taki, T. Fujiwara, Y. Umeda 1015 Experimental Study on a Flow Field Behind Backward-Facing Step Using Detonation-Driven Shock Tunnel T. Obara, T.-H. Kim, S. Ohvagi

1015 Numerical Simulation of Detonation inside the Electrochemical Pulse Engine I.V. Semenov, V.V. Markov, S. Wojcicki

Poster III: Explosion - 1055 Friday August 5

1055 Mitigation of Strong Deflagrations by Water Mist M.T. Parra, F. Castro, C. Mendez, J.M. Villafruela 1055 Modeling of Turbulent Jet Nonpremixed Flames Using a Scalar Combined PDF/Moment Method S. Noda, K. Yamamuro 1055 Measurement of Local Equivalence Ratio in Partially Premixed Swirling Methane Flame Using Local Chemiluminescence T.S. Cheng, C.-Y. Wu, Y.-H. Li, Y.-C. Chao 1055 Deflagrations in Closed and Vented Pipes - An Experimental Study H. Forster, C. Kersten 1055 Thermodynamic Analysis of Closed Explosion of Hexane-Air Mixtures W.A. Trzcinski, P. Wolanski, A. Kuhl 1055 Comparison Between Two Liquid Fuels for Pulse Detonation Engines P. Gillard, X. Rocourt, I. Sochet, D. Piton, A. Prigent 1055 Experimental Study of Pulse Detonation Turbine Engine Toward Power Generator T. Sakurai, T. Obara, S. Ohyagi, M. Murayama 1055 Quantitative Analysis of Explosion of an RDF Silo T. Tsuruda 1055 Gas Explosion Simulations with Flux Limiter Centred Method K. Vaagsaether, D. Bjerketvedt 1055 Experiments With Flame Propagation in Inhomogeneous Hydrogen-Air Clouds in a Small Vessel O.K. Sommersel, R.L. Shrestha, D. Bjerketvedt 1055 Ground-Based and Microgravity Study of Flame Quenching Distance in Metal Dust Suspensions S. Goroshin, J. Mamen, J.H.S. Lee, K. Sacksteder 1055 Hazard Evaluation of Hydrogen-Air Deflagrations Using Latex Balloons H. Saitoh, N. Uesaka, T. Ohtsuka, T. Mizutani, Y. Morisaki, H. Matsui, N. Yoshikawa 1055 Simple Analytical Model for Metal Particle Ignition in Condensed Explosive V. Tanguay, A.J. Higgins 1055 Plasma-Wave Initiation of Supersonic Combustion at Low Electric Energy Deposition A. Dovbnva, K. Korvtchenko, Yu. Volkolupov, A. Kosov 1055 Simulating the Influence of Obstacles on Accelerating Dust and Gas Flames T. Skiold, Y.K. Pu, B.J. Arntzen, O.R. Hansen, I.E. Storvik, O.J. Taraldset, R.K. Eckhoff 1055 Formation of SnO2 Nanoparticles from {SnCl4 + H2O} Reactive System at 30 MPa and 415oC Z. Fang, H. Assaaoudi, I.S. Butler, J.A. Kozinski 1055 Temperature Dependence of the Lower Explosion Limits of Pure

Components and Mixtures E. Brandes, M. Mitu, D. Pawel

1055 Explosions in the Courts: The Intersection of Law and Science B.A. Davis

Monday August 1

0900 (W) - Welcome (John HS Lee)

0940 (1A) - Detonation - Dynamics (Sergey Mevedev)

940 **Numerical Simulation of Spin Detonation in Square Tube** *A.K. Hayashi, K. Eto, N. Tsuboi; Aoyama Gakuin University* Spin detonation in a square tube is studied numerically using 3D compressible Euler equations with the Petersen-Hanson H2/air detailed reaction mechanism. A non-MUSCL modified-flux TVD scheme by Harten-Yee is used to integrate the governing equations. The grid size is 5 micron which equals 24 Million grid points. The results reveal that the detonation spins clockwise with a CJ speed of 1970 m/s. The numerical smoked foil pattern agrees with the experimental smoked foil records. In the present conditions, there is no tailing effect.

1005 **Propagation Mechanism and Transmission of Quasi-Detonations** *P.N. Krivosheyev, O.G. Penyazkov, S.A. Zhdanok; Heat and Mass Transfer Institute, National Academy of Sciences of Belarus* The propagation of quasi-detonations in a porous packed bed comprised of 5.5-mm steel balls and a subsequent transmission into smooth tubes has been studied experimentally. The necessary requirements for direct detonation initiation behind a regular porous bed comprised of spherical particles were determined. It was shown that the normal shock reflection mechanism itself cannot produce the successive auto-ignition of the mixture at real length scale in a porous bed and ensure the self-sustained propagation of quasi-detonation in a porous bed near the limits.

1030 The Unsteady Dynamics of the Head-On Collision Between a Detonation and a Shock Wave B.B. Botros, Y. J. Zhu, H.D. Ng, J.H.S. Lee; McGill University Recent advances in detonation theory suggest that the dynamic parameters of a detonation (e.g. detonation limits, critical tube diameter, etc.) should depend on an effective thickness or hydrodynamic thickness of the detonation in the direction of propagation. Although various methods have been tried to determine an effective thickness of a cellular detonation, they have all met with limited success. It is thus of interest to devise a more global method to determine the effective thickness of a detonation. The present study investigates the head-on collision between a detonation and a shock wave. The idea is to use the shock wave as a perturbation to investigate the dynamic behavior of a detonation wave. By analyzing more carefully the response to perturbation created by the shock and measuring the time or length required for which a steady-state detonation is re-established after the interaction, i.e. a transient relaxation length scale, the present study attempts to shed light on the structure of a detonation wave. Specifically, the ultimate goal is to achieve a means to relate the effective thickness of a cellular detonation from the characteristic features such as relaxation length scale of the transient processes of the interaction.

0940 (1B) - Flames - Premixed (Makihito Nishioka)

940 Effects of Radiation Reabsorption on Flame Propagation and Flammability Limits in CO2 Diluted Flames X. Oin, Z. Chen, Y. Ju; Princeton University Premixed flames in CO2 diluted CH4-O2-He mixtures were studied both experimentally and numerically to investigate the effects of spectral dependent radiation reabsorption on the flame propagation and flammability limit. Laminar burning velocities of CH4-O2-He-CO2 mixtures at both normal and elevated pressures up to 5 atm were measured by using a pressure-release type spherical bomb. The measured data were compared with the results from computations performed with and without spectral radiation absorption. It was found that the spectral radiation reabsorption results in higher burning velocities of CH4-O2-He-CO2 mixtures and wider flammability limits than predictions using the optically thin model. Furthermore, the enhancement becomes more significant at higher pressures. The results demonstrated that reabsorption effects must be considered to correctly predict flame speeds and extinction limits in flammability limit and burning properties of mixtures with CO2 addition.

1005 Adiabatic Cellular Premixed Flames of Methane (Ethane, Propane), Oxygen, and Carbon Dioxide Mixtures A. A. Konnov, I. V. Dyakov; Vrije Universiteit Brussel Experimental studies of adiabatic cellular flames of CH4 + O2 + CO2, C2H6 + O2 + CO2, and C3H8 + O2 + CO2 are presented. Visual and photographic observations of the flames were performed to quantify their cellular structure. Non-stretched flames of methane and propane were stabilized at atmospheric pressure on a perforated plate burner of improved design. New measurements are compared with recent results from this group. A Heat Flux method was used to determine propagation speeds under conditions when the net heat loss of the flame is zero. Under specific experimental conditions, the flames become cellular; this leads to significant modification of the flame propagation speed. The onset of cellularity was observed throughout the stoichiometric range of the mixtures studied. Cellularity disappeared when the flames became only slightly sub-adiabatic. Increasing the oxygen content in the artificial air and increasing the temperature of the burner plate led to an increase of the number of cells observed. No direct proportionality between the number of cells and propagation speeds in CH4 + O2 + CO2 flames was observed. Dependence of the number of cells as a function of equivalence ratio clearly showed a local minimum in the stoichiometric mixtures.

1030 **Burning Velocities of Stoichiometric Methane-Hydrogen-Air Flames at Gasturbine Like Conditions** *R.T.E. Hermanns, R.J.M. Bastiaaans, L.P.H. de Goey; Technische Universiteit Eindhoven* De Goey et al. recently extended the asymptotic theory for methane-air flames of Peters and Williams to methane-hydrogen-air flames. In this paper, the asymptotic theory will be verified (numerically and experimentally) at higher gas inlet pressures and higher pressures up to gasturbine like conditions with increasing hydrogen contents.

0940 (1C) - Droplet Combustion (Carl Knowlen)

940 **Numerical Study of Fiber Influences on Droplet Flow and Vaporization** *D. Shringi, H.A. Dwyer, B.D. Shaw; University of California, Davis* Results of numerical computations of time histories of supported and unsupported droplets held in a cross flow of air are presented for different fiber and droplet relative diameters for a large range of pressures, temperatures, and flow Reynolds numbers. These computations have been carried out for two fuels, methanol and octane. Full effects of thermal surface tension have been considered in these calculations. For 1000 K, 10 atm air, and initial Re=50, both methanol and octane show a trend of reduced vaporization rates with increasing fiber diameter. This is largely due to reduced circulation velocities and heat transfer from the gas phase, while the effects of increased heat transfer from the fiber are more than compensated. Large surface tension gradients generated on the droplet surface near the fiber have small effects on global circulation inside the liquid for most cases. Both octane and methanol show similar trends as regards fiber heating, surface temperatures and vaporization rates for the case considered even though internal heating characteristics are different for these droplets.

1005 Effects of Liquid Fuel Mass Fraction and Droplet Size on Droplet Group Combustion Behavior M. Nakamura, F. Akamatsu, R. Kurose, M. Katsuki; Osaka University Two-dimensional DNS is applied to spray flames formed in a laminar counterflow, and the detailed behavior is studied in terms of the droplet group combustion theory. The stretch ratio of the laminar counterflow is 40 1/s. N-decane (C10H22) is used as a liquid spray fuel, and for the combustion reaction model, a one-step global reaction is employed. The results show that with increasing the issued droplet mass flow rate, two types of spray combustions, i.e. 'premixed-like combustion' and 'diffusion-like combustion', appear in the front and inside the high gaseous temperature regions, respectively. The droplet group combustion behavior is observed in the 'diffusion-like combustion' region. The 'diffusion-like combustion' carrying the droplet combustion behavior, however, disappears when the issued droplet size is small because the droplets complete their evaporation before entering into the high gaseous temperature region. The droplet group combustion tends to reduce the gaseous temperature. This is caused mainly by the suppression of combustion reaction due to the lack of oxygen.

1030 A Study of the Flow, Heat Transfer, and Mass Transfer Characteristics of Droplet Arrays *H.A. Dwyer, B.D. Shaw; University of California, Davis* Over the last decades, there has been extensive research on droplet arrays and this research has been extremely important for understanding combustion physics and chemistry as well as understanding practical flows. At the present time, there is a serious gap between completely unsteady models and models with a fixed geometry. For example, the stability of droplet arrays has exhibited a wide distribution of both stable and unstable configurations, and it is very difficult to know in advance what conditions will produce a stable array configuration. The present research is an attempt to bridge the gap in our understanding with detailed solutions of the Navier-Stokes equations under realistic IC engine conditions. We will present detailed and time-dependent results for the flow in single and droplet arrays of methanol droplets.

1055 (1PO) - **Poster I - Flame** (Charles Kiyanda)

1055 (B) - Break

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1145 (2A) - Detonation in Flowing Systems (A. Koichi Hayashi)

1145 Detonation Initiation in Moving Non-Premixed Flows V.V. Golub, V.V. Volodin, T.V. Bazhenova, D.I. Baklanov, S.V. Golovastov, D.G. Lisin; Institute for High Energy Densities RAS In detonation devices used for practical purposes such as evaporation, cleaning of heat-receiving surfaces, crushing of scrap tires, and pulse detonation engines (PDE), it is necessary to mix the fuel components directly in the detonation combustion chamber for safety considerations. The fuel components are provided to the detonation combustion chamber (DCC) by fast acting valves or a valveless system. This may cause a mass flow variation during DCC filling. As a result, the mixture composition and turbulence characteristics will vary at the ignition location. These factors can substantially affect the DDT process. It is shown that the fuel components' mass flow rate and mixture composition are in general not constant for PDE. The fuel components' mass flow and mixture composition are strongly affected by DDT. Turbulization of the fuel components' flow by means of the resonator mounted on the injector decreases the ignition delay influence on the DDT. As the Reynolds number increases from 5000 to 55,000, the amount of the air enrichment with oxygen needed for DDT reduces from 65% to 30%. As the distance between the tube closed end and spark plug location was reduced from 1.8 to 0.3 tube diameters, the DDT length was reduced from 3.3 to 1.6 tube diameters.

1210 Detonation Waves in Supersonic Stream of Homogeneous Reacting Mixture A.A. Vasil'ev, D.G. Nalivaichenko, V.I. Zvegintsev; Lavrentyev Institute of Hydrodynamics In the supersonic stream of Mach numbers M=4.0 and 5.0, the profiles of pressure, flow velocity, and concentration are tested carefully in different cross-sections. Investigations of detonation waves (DW) in hydrogen-air mixtures, propagated upstream, are carried out. It was established that experimental values of the DW-velocity exceed the calculated values of the Chapman-Jouguet DW for the entire range of investigated values of excess air coefficients.

1235 **Investigation of Transition of Deflagration to Detonation in Moving Mixtures of Combustible Gases** *D.I. Baklanov, S.V. Golovastov, L.G. Gvosdeva, A. Kaltayev, N.B. Scherbak, V.V. Volodin; Institute for High Energy Densities RAS* In this report, new experimental data about the essential reduction of predetonation distance are given in the case of the formation of a detonation from an electric discharge in a driving gas. Experiments were done at the device which allows to model one cycle of operation of a pulse detonation engine. The experimental data are compared to the results of numerical calculations. The good agreement with experiments demonstrates the feasibility of the offered methods of calculations and allows us to give an explanation of the observed experimental effects. The results seem to be of practical application to the control of detonation process in PDE.

1145 (2B) - Flames - Lifted (Habib Najm)

1145 **Lift-off Stability of Hydrocarbon Jet Diffusion Flames** *F. Takahashi, V.R. Katta; National Center for Microgravity Research* The structure and lift-off stability of laminar jet diffusion flames of gaseous hydrocarbon fuels in coflowing air at normal earth gravity have been investigated experimentally and computationally. Measurements of the critical mean jet velocity of methane at lifting were made as a function of the coflowing air velocity. Computations with 33 species and 112 elementary steps revealed the internal structures of the stabilizing region of methane

and propane flames. The simulated flame base moved downstream toward lift-off under flow conditions close to the measured lifting limit. A peak reactivity spot (i.e., reaction kernel) formed in the stabilizing region is responsible for the flame attachment and lift-off processes.

1210 Local Flame Displacement Velocity of Hydrogen Added Methane Premixed Turbulent Flames M. Nakahara, H. Kido, K. Nakashima, H. Takamoto: Kyushu University The present study is performed to investigate directly the local flame properties of turbulent propagating flames for lean and rich hydrogen added methane mixtures as two-component fuel mixtures at the weak turbulence condition in order to clarify the influence of the hydrogen addition to hydrocarbon mixtures on its local burning velocity and turbulent burning velocity. Hydrogen added methane mixtures having nearly the same laminar burning velocity with different rates of hydrogen addition are prepared. A two-dimensional sequential laser tomography technique is used to obtain the relationship between the flame shape and the flame displacement. The local flame displacement velocity SF is quantitatively obtained as the key parameters of the turbulent combustion. It is found that the obtained SF plays an important role in the turbulent burning velocity. An attempt is also made to estimate the change in the local burning velocity at the convex part of turbulent flames toward the unburned mixture caused by the Markstein number SLt. A quantitative relationship between SF and SLt can be observed only for rich mixtures.

1235 A Qualitative Study of the Effect of Asymmetric Fuel Nozzles on the Blow-Out Limits of Non- and Swirling CH4-Air Diffusion Flames *T.M. Phillips, M. Birouk; The University of Manitoba* The research program launched at the University of Manitoba aims at participating in the international effort to help better understand non-premixed turbulent flame phenomena. The preliminary results presented in this paper determine qualitatively the effect of asymmetric nozzles on the characteristics of various swirling and non-swirling turbulent diffusion flames. The novelty of the present research resides in the combination of swirling combustion air and asymmetrical fuel nozzles to generate stable turbulent diffusion flames, where circular, rectangular, square, and triangular nozzles were used to determine their effect on flame blow-out and blow-off (lift-off extinction). The main findings here are that the flame shape is mostly dependant on swirl strength and not on nozzle geometry. In addition, asymmetric nozzles increase the stability of attached flames but do not enhance stability for lifted flames.

1145 (2C) - Kinetics - Detailed Mechanisms (Alexander Konnov)

1145 **Chemical Kinetic Databases for the Simulation of Hydrocarbon Combustion Phenomena** *W. Tsang; National Institute of Standards and Technology* This presentation reports on current work at the National Institute of Standards and Technology aimed at improving the chemical kinetic databases used in the computer simulation of combustion related phenomenon. The work has its impetus from advances in computational fluid dynamics codes that can take an increasing amount of chemistry. Particular attention is paid to heptane combustion databases with special emphasis on the elementary reactions involved in pyrolytic decomposition. This is intended to complement existing databases that concentrate on purely oxidative phenomena and is therefore deficient for rich mixtures and the

prediction of PAH/Soot yields. The approach is systematic in the sense of beginning with reactions that create alkyl radicals, follows their decomposition to smaller alkyls and 1-olefins, the formation of 1-olefinyl radicals, and their subsequent decomposition to form dienes. The last sets of processes are particularly pertinent since they have been cursorily treated in earlier databases. The implications of these studies on the databases dealing with oxidative processes will be discussed and some of the problems outlined. Extensions to cover more complex fuels will be considered

1210 Automatic Generation of a Detailed Mechanism for the Oxidation of n-Decane G. Moreac, E.S. Blurock, F. Mauss; Lund University A detailed kinetic mechanism for the oxidation and combustion of n-decane has been written by means of an automatic mechanism generator (REACTION) developed in our laboratory. It has been validated against a wide range of experimental data and shows a good prediction of the ignition delay time versus temperature for the oxidation of n-decane at 13 and 50 bar for different equivalence ratios. The different reaction classes defined in this tool allow the automatic generation of detailed kinetic mechanisms for modeling the oxidation of alkanes at low and high temperatures. The n-decane mechanism is based on a validated and recently published C1-C4 mechanism produced manually and a generated C5-C10 sub-mechanism. This mechanism has a reasonable size, 485 species and 3684 reactions, but, nevertheless, it has an extensive range of chemistry.

1235 Using Genetic Algorithms to Derive the Kinetics of Smoldering **Combustion** G. Rein, C. Lautenberger, A.C. Fernandez-Pello; University of California, Berkeley Modeling of smoldering can lead to a better understanding of its controlling mechanisms and the strategies for the prevention and mitigation of smolder fires. Smolder models take into account the heterogeneous surface-reactions that drive the smolder process. However, the kinetics of the fuel decomposition and oxidation processes that take place during smolder are generally not well-known. In this work the kinetic parameters relevant to smoldering of polyurethane foam (PU) are derived for their application in models of its smolder combustion. Thermogravimetric experiments are used together with a new reduced mechanism of PU inert and oxidative pyrolysis to derive its smolder kinetics. The reduced decomposition mechanism is used with a simple mathematical model to simulate the thermogravimetic experiments, and optimization tools of Genetic Algorithms are used to identify the kinetic parameters that best reproduce the experimental observations. The derived kinetic and stoichiometric parameters are applied in a 1-D model simulating a steady state propagating smolder front. The results show that the model satisfactorily captures the chemical structure of the smolder front and that the kinetic constants obtained can be used to model smoldering.

1300 (L) - Lunch

1440 (3A) - Detonation Diffraction (Joanna Austin)

1440 **Detonation Diffraction in Regular and Irregular Mixtures** *F. Pintgen, J.E. Shepherd; California Institute of Technology* Diffraction of a gaseous detonation has been widely studied in the context of both applications and as a scientific experiment that provides insight into the interaction between the combustion processes at the

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wavefront and the fluid motion induced by the diffraction process. For detonation propagation in tubes and channels, it is established that there are reasonably well-defined critical conditions (e.g., critical diameter). The empirical correlation of the critical diameter being 13 times the cellsize holds for many common fuel-oxygen or - air mixtures but breaks down for mixtures with a large amount of argon dilution. The objective of the present study is to provide quantitative data to test the various theories about detonation diffraction in mixtures with very different degrees of cellular regularity. To do this we used simultaneously schlieren photography, multiple-exposure chemiluminescence imaging and planar laser-induced fluorescence (PLIF) of the OH-radical. Striking differences are seen in the failure mechanisms for the regular (70% Ar-diluted H2-O2) and the highly irregular (H2-N2O) mixtures. In the critical regime, the coupling between shock and reaction front persists significantly longer for the regular mixture. This is clearly evident on overlays of schlieren and PLIF images and the velocity profiles of the reaction front.

1505 **Promoting Detonation Diffraction from Circular Tube to Cone by Obstacles** *A. Marelli, B. Khasainov, V. Guilly, H.-N. Presles, D. Desbordes; Laboratoire de Combustion et de Détonique, CNRS, ENSMA* We have carried out an experimental study of the detonation diffraction into a cone with a diverging angle of 70°, placed at the end of a 52-mm inner diameter shock tube. It is shown that the presence of obstacles of suitable form at the cone wall can favour detonation transmission by decreasing the critical transmission pressure. Soot-covered plates used to record diffraction phenomena display that shock-wave interaction with the obstacle gives rise to a super-detonation propagating from the cone wall towards the axis. Preliminary numerical two-dimensional simulations give reasonable agreement with experimental data and lead to a few ideas on promoting detonation diffraction.

1530 Detonation Diffraction Through Different Geometries R. Sorin, R. Zitoun, D. Desbordes; Laboratoire de Combustion et de Détonique CNRS In the field of research on air breathing PDEs, the detonation diffraction is studied. The aim of this paper is to study the influence of confinement (by shock reflection and focalization) on the detonation diffraction in order to improve its transmission. We have designed two experimental devices. The first one consists of a brutal opening from a cylindrical tube i.d. d to another of larger diameter D (D/d = 1.5 and 2). The second one is an original device consisting of a reversed intermediate closed tube (of varying diameter D) between the initiator tube and the tranquilization chamber such that the diffracted shock undergoes two successive reflections. For a mixture obeying the dc = 13 λ law, the results for the brutal opening show that when 1 < D/d < 2.5, the critical value of dc to have a wall re-ignition varies from $\lambda/\pi < dc < 13\lambda$. For the double reflection configuration, we show that the transmission happens up to dc =4.3 λ through one reflection and up to dc = 2.2 λ for transmission through the two successive reflections from d = 26 mm to Dch = 200 mm. This result represents a significant improvement of the detonation transmission.

1440 (3B) - Flames - Premixed Structure (Moshe Matalon)

1440 **Self-Similar Behaviour of Laminar Premixed Flames** *G. Ribert, O. Gicquel, N. Darabiha, D. Veynante; EM2C Laboratory, CNRS-Ecole Centrale Paris* Complex chemistry features should be incorporated in simulations of turbulent

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flames to predict, for example, pollutant formation. Unfortunately, complex chemical schemes are too large to be handled in industrial calculations. A convenient approach is to use tabulation methods such as ILDM, FPI, or FGM. However, practical implementation, especially on parallel machines, may be a problem both in terms of memory requirements and computational times. This study proposes a new technique to tabulate complex chemistry, taking advantage of self-similar behaviour of laminar premixed flames, with respect to the equivalence ratio. The theoretical basis of this approach is presented and it is validated numerically by comparison with complex chemistry calculations of a CH4-air laminar premixed flame. Only the chemical source terms of O2 and CO2+CO under stoichiometric conditions have been tabulated together with similarity rules. Both for lean and rich conditions, results match very well, thus validating the new approach.

1505 **The Role of Explosive Modes in Homogeneous Ignition and Premixed Flames** *J.C. Lee, H.N. Najm, S. Lefantzi, J. Ray, M. Frenklach, M. Valorani, D.A. Goussis; Sandia National Laboratories CRF* We performed calculations to investigate the classical theories of chain branching and thermal--run--away that lead to the rapid oxidation of fuels. Mathematically, both theories infer the existence of eigenvalues with positive real parts i.e., explosive modes. We found in studies of homogeneous hydrogen--air and the methane--air mixtures that when ignition is initiated by a sufficiently high initial temperature, the transient response of the system exhibits two stages. The first stage is characterized by the existence of explosive modes. The ensuing second stage consists of fast exponential decay modes that bring the system to its equilibrium point. We demonstrated with two examples that the existence of explosive modes is not a necessary condition for the existence of a premixed flame. Homogeneous ignition calculations for mixtures with an initial concentration of radical species suggest that the diffusive transport of radical species is probably responsible for the lack of explosive modes in premixed flames.

1530 Effect of Particle Morphology on the Thermophoretic Behavior of Soot Particles S. Suzuki, R. Dobashi; The University of Tokyo In a field with a temperature gradient, small particles experience a force toward the colder region. Soot is a very small particle formed near the combustion field, where a very steep temperature gradient exists. Therefore, appropriate understanding of the thermophoretic effect is indispensable to understand the behavior of soot particles near combustion fields. In this study, simultaneous measurements of the velocity and size of aggregated soot particles were performed to examine the effect of particle morphology on the thermophoretic velocity. As the sample particle of soot, carbon black was used, which consists of primary particles of almost uniform size (about 24 nm). The measured thermophoretic velocities were much larger than expected by their aggregate size. The measured velocities are about 0.01-0.14mm/s in the temperature gradient from 2 to 20 K/mm and almost the same as the velocity evaluated by the formula for the free-molecular regime proposed by Waldmann even if the aggregate size is very large (300 µm). The distinct dependence of the themophoretic velocity on the size of aggregated particles was not found in this study. This result suggests that there should be other morphological factors than the sizes of the aggregate and primary particle, which govern the thermophoretic velocity of the aggregated particle.

1440 (3C) - Turbulent Combustion I (Frank Behrendt)

1440 Laser Induced Fluorescence in High Pressure Cryogenic LOx/GCH4 and LOx/GH2 Jet Flames G. Singla, P. Scouflaire, C. Rolon, S. Candel; EM2C Laboratory, CNRS and Ecole Centrale Paris This article deals with the application of OH PLIF to the study of high pressure cryogenic flames. Elevated pressure conditions require a careful choice of the excitation wavelength based on a detailed analysis of the absorption dependence with respect to pressure and temperature. OH PLIF is used to examine jet flames formed by a single coaxial injector fed by liquid oxygen and gaseous methane in subcritical and transcritical regimes. Below 3 MPa, the PLIF system provides good quality data. Above that pressure, in addition to OH fluorescence, a nonresonant fluorescence interference is detected and the corresponding signal increases rapidly with pressure. It is shown that this interference does not arise in high pressure LOx/GH2 experiments which provide high quality PLIF images at pressures up to 6.3 MPa. This indicates that the fluorescence signal detected with methane fuel originates from PAH generated by fuel oxidation at high pressure. This limits the application of OH-PLIF to the moderate pressure range. In the injector nearfield, instantaneous PLIF images indicate that the flame thickness often exceeds the transverse wake size and this implies that the flame will be quite sensitive to the high speed annular stream and that the stabilization point will fluctuate.

1505 Laser Induced Plasma Spectroscopy for Local Composition Measurements Inside a Low Swirl Burner L. Zimmer, S. Tachibana; Japan Aerospace Exploration Agency In Laser Induced Plasma Spectroscopy, plasma is created by focusing a laser in order to achieve breakdown. The typical size of the induced plasma is well defined in space. The ratio of atomic emission lines can describe the local composition of the gas. The amount of fuel is induced by the emission of hydrogen (or carbon) atoms whereas the oxidizer is obtained using either nitrogen or oxygen emission. Applying this technique to combustion, it is possible to measure the local equivalence ratio with a spatial resolution of the order of 1mm. To illustrate the potential of the technique, the target chosen is the Low Swirl Burner. This burner uses secondary air jets to stabilize the flame. The LIPS technique shows that the core of the burner is indeed well premixed whereas the local mixture fraction in the outer part of the burner is influenced by the mixing process with the secondary air injection. The size of the well-premixed zone is a function of swirl number and mixing length. Those measurements show that LIPS can detect gradients in mixture fraction and may be applied to other practical combustors, like those prone to thermo-acoustics oscillations, performing phase-locked measurements.

1530 Lean Premixed Turbulent Methane Combustion with Hydrogen Additions: Burning Velocities and Emissions Measurements *Y.C. Chen, S.S. Shy; National Central University* This paper investigates experimentally lean premixed methane-air turbulent combustion with various hydrogen additions. We focus on measurements of turbulent burning velocities ST and variations of NOx and CO emissions for these methane/hydrogen/air flames in a large cruciform fan-stirred burner. Results reveal that a small hydrogen addition can not only slightly expand the lean flammability limit of CH4/air mixtures, but can also significantly increase values of ST. Turbulence cannot increase values of ST continuously, and the slope of

ST/SL vs. u'/SL is found to bend towards the horizontal when values of u'/SL are greater than approximately 4. This is the so-called bending effect, as is also observed in burning CH4/air mixtures with hydrogen addition. All the present ST data of lean methane/hydrogen/air flames can be correlated with an empirical relation as a function of a turbulent Damköhler number. The use of hydrogen as an additive to natural gas should be an attractive solution both at present and in the near future for the energy problems of our society.

1555 (B) - Break

1620 (4A) - Detonation Simulation (Matei Radulescu)

1620 Hybrid Large-Eddy Simulation of Detonations in Reactive Mixtures B. Fryxell, F. Genin, S. Menon; School of Aerospace Engineering, Georgia Institute of Technology We report on a new hybrid method for performing Large-Eddy Simulations of explosions and detonations. The method combines a high-resolution shock-capturing scheme with a high-order finite-volume method. The shockcapturing method computes only those portions of the flow near shocks and contact discontinuities, while the smooth-flow solver computes the remainder of the flow. The baseline code, LESLIE3D, is a well-established solver used for LES and DNS studies of turbulent reacting single and two-phase flows. This study extends the capabilites of the code to handle strong shocks and detonations. For LES applications, it employs a localized dynamics model for the subgrid kinetic energy. Reaction-diffusion processes are modeled with many approaches (depending upon applications), including a new subgrid simulation approach called linear-eddy mixing (LEM) modeling. For multi-phase flows, the particle phase is included using a Lagrangian tracking scheme that tracks either individual particles or groups of particles. We report the results of a number of test calculations of detonations and explosions to illustrate the properties of the new method. The final paper will report on more complex applications, including the propagation of a strong shock through a reactive two-phase mixture.

1645 **The Effect of Discrete Energy Sources on Detonation Propagation** *A.J. Higgins; McGill University* The propagation of a detonation through a system of discrete energy sources that are triggered by the passage of the shock front is considered. Such a system may be sheets of energetic material separated by gaps of inert medium. This system can be compared to the corresponding homogeneous system, for which the Chapman-Jouguet solution is well-defined. For a system governed by the Euler equations, it is shown that the average propagation velocity for the discrete source system has the same functional dependence as the homogeneous CJ detonation. In order to solve the interacting ensemble of blast waves, the model system proposed by Fickett, consisting of the inviscid Burgers equation with a source term, is used. It is shown that, for a regularly spaced array of sources, the average propagation speed in the discrete source system. This result may suggest an alternative formulation of the Chapman Jouguet criterion.

1710 Multi-Processor Simulation of Forming a Detonation Wave in Shock Tube on the Molecular Process Level S.V. Kulikov; Institute of Problems of

Chemical Physics RAS The Monte Carlo nonstationary method of statistical simulation (MCNMSS) (also called DSMC) with weight factors was used in these calculations. It takes into account all processes of heat-mass transfer automatically. Simulation was carried out in the one-dimensional coordinate space and in the threedimensional velocity space. At an initial moment, the low-pressure channel (LPC) was filled with gas A and the high-pressure chamber (HPC) of a shock tube was filled with gas C. The simulation started after removing a diaphragm between the HPC and the LPC. It was supposed that chemical B+M (M=A,B and C) took place. The ratio of molecular masses→reaction A+M (mi) of gases A, B, and C was :20:20:1. The threshold of the reaction QAB was equal to 25kT1 (T1 is the temperature in LPC and HPC at the initial moment of time). The energy release in reaction Q was equal to 402.6 kT1. All considered molecules were treated as hard spheres with equal diameters without internal structure. Parallel calculations were carried out by means of a multi-processor computer. Domain decomposition of a simulation region was performed. Standard Message Passage Interface (MPI) was used to communicate data between processors, and 176 processors were used.

1620 (4B) - Flames - Premixed Spherical (Michael Liberman)

1620 Development of Instabilities in Closed Vessel Laminar and Turbulent Explosions A. S. Al-Shahrany, D. Bradley, M. Lawes, K. Liu, R. Woolley; University of Leeds The development of explosion flame instabilities, which are most marked at high pressures and very negative Markstein numbers, was observed through central windows of a spherical bomb at the high pressures attained in the later stages. This was achieved by igniting the mixture simultaneously with two diametrically opposite sparks close to the wall. In this way, two near-identical imploding flames, at significantly higher pressures than the initial value, came into the field of view of a window and their burning velocity was measured. The bomb was equipped with four fans close to the wall to generate turbulence. This technique was used to study instabilities in both laminar and turbulent rich iso-octane-air flames. With initially quiescent mixtures, burning velocities were enhanced progressively, to well beyond the laminar values at the particular temperatures and pressures, by Darrieus-Landau (D-L) instabilities. Eventually, provided the Markstein number was negative enough, at a sufficiently high pressure and rate of change of reaction rate, Taylor instabilities also were observed. A feed-back mechanism further enhanced the burning rate. In turbulent flames, no marked Taylor instabilities were observed and the D-L instabilities enhanced the turbulent burning velocity only at low levels of turbulence.

1645 **A Theoretical Evaluation of Turbulent Markstein Number for Expanding Spherical Flames** *A.N. Lipatnikov, J. Chomiak; Chalmers University of Technology* In the combustion literature, the Markstein number is commonly used to characterize the effects of weak external perturbations on a laminar flame speed. To parameterize effects of large-scale stretching of premixed turbulent flames by mean flow on the flame speed, a turbulent Markstein number is introduced in the present paper via analogy with laminar flames. For expanding, statistically spherical, premixed flames, the turbulent Markstein number regarding the burning velocity is analytically determined by invoking recent theoretical studies of self-similar developing flames. The determined turbulent Markstein number grows with the density ratio but depends neither on turbulence characteristics nor on other mixture properties.

1710 **How Large Can the Rate of Expansion of a Spherical Flame Grow?** *V. Karlin, J. Mai; University of Central Lancashire* In this paper, we are interested in acceleration of hydrodynamically unstable expanding spherical flames. In particular, we are studying the possibility of stabilization of the expansion rate for large enough time intervals, when the flame size grows sufficiently large. The investigation is based on numerical simulations of two- and three-dimensional nonlinear models of flame dynamics.

1620 (4C) - Shock Waves (Boris Gelfand)

1620 Mathematical Modelling of Two Problems of Wave Dynamics in Heterogeneous Media A.V. Fedorov, I.A. Fedorchenko, I.V. Leontev; Institute of Theoretical and Applied Mechanics SD RAS The numerical simulation results are presented describing: (1) dust lifting behind a traveling shock wave and (2) Riemann problem for a layered heterogeneous system in a frame of an equilibrium model of heterogeneous mechanics. In the case of problem 1, the differences of flow schemes in cases of the different layer edge geometries and shock shapes are shown. It has been cleared up that if the turbulence of the mixture is taken into account, the highspeed dust jet appears near the wall and the height of dust lifting is increasing. The intense interest in problem 2 is determined by the problem of estimating accidental explosion consequences. This problem was investigated both theoretically and experimentally in the paper of Gelfand et al. (1987). In their theoretical description, the volume concentration of particles had, however, a value characteristic of rarefied gas-particle mixtures (of the order 0.001), which differed significantly from actual values (0.28 for acrylic plastic and 0.72 for sand). The main goal of the paper is to present and verify the mathematical models to describe these problems.

1645 **Blast Wave on a Parallelepipedic Obstacle** *S. Trelat, I. Sochet, B. Autrusson, K. Cheval, O. Loiseau; Laboratoire Energetique Explosions Structures* The purpose of this paper is to report the blast loading characteristics resulting from the detonation of a propane-oxygen stoichiometric mixture, and to validate the approach which consists of simulating TNT explosions at large scale by small scale experiments of gaseous explosions. Several adimensional laws are expressed and validated by experiments. These relationships allow to determine the propagation of a blast wave and its interaction on a structure by the function of the position of the explosive charge in different configurations. Simulations are achieved with the Autodyn code, and a good correlation with experimental results is obtained. The blast wave's characteristics can be predicted at large scale by applying the Hopkinson law.

1710 Shock Wave Interaction with a Loose Dusty Bulk *B. Fan, X. Jiang; Nanjing University of Science and Technology* Experiments on shock waves interacting with a loose particle bulk were conducted in a shock tube. The incident shock velocity and particle diameters were measured by pressure transducers and a Malvern particle sizer, respectively. The flowfields in both the gas and granular phases induced by shock waves were recorded by means of shadow graphs and pulsed X-ray shadow graphs with trace particles. The particle motion is strongly controlled by particle-particle collision which is associated with the fluctuation kinetic energy of the particle. On the basis of the kinetic theory of granular flow, introducing 'granular temperature', the conservation and constitutive equations for a dense two-phase flow were derived and then numerical simulations were performed by using ASUM schemes with the advantages of combining the efficiency of Flux-vector splitting and the accuracy of Flux-difference splitting. Measured and calculated results were in good agreement.

Tuesday August 2

0900 (1PL) - Plenary I (Ulrich Maas)

900 **The Development of Hydrodynamically Unstable Flames** *M. Matalon; Northwestern University* The hydrodynamic instability, discovered independently by Darrieus and Landau over half a century ago, has many ramifications in combustion. The appearance of sharp folds and creases in the flame front of freely propagating flames, and the wrinkling observed over the surface of large spherically expanding flames are direct manifestations of this instability. In this presentation we discuss theoretical advances towards understanding the development of hydrodynamically unstable premixed flames. A brief account of the linear stability results for planar and spherical flames will be given, followed by results of a weakly-nonlinear theory restricted to small density changes, and finally by more recent numerical results that fully account for density variations thus elucidate the role of thermal expansion on the evolution of wrinkled flames.

1005 (5A) - Detonation Properties (Gabrielle Dupre)

1005 Influence of the Initial Temperature on the Detonability of CH4/H2/O2/N2 Mixtures *C. Matignon, D. Desbordes, H.N. Presles; CEA* The detonability of (CH4-H2) fuel mixtures, stoichiometric with O2 and diluted by N2, is studied with respect to: 1. the molar ratio of H2 for three values of the nitrogen dilution β =N2/O2 (β =0 (oxygen); 2; 3.76 (air)) and 2. the initial temperature. The results show that the detonability of the (CH4-H2) mixtures is mainly controlled by the heavier fuel, i.e. CH4, and, for instance, replacing 20% of the CH4 volume by H2 in the CH4-based mixture has nearly no effect on its detonability. The influence of the initial temperature on the detonability is strongly dependent on the dilution β and, for $\beta \ge 2$, on the preponderant fuel.

1030 Effect of Two Additives (CH3NO2 and H2O2) on the Detonation Properties of Gaseous Stoichiometric n-C7H16/O2 Mixtures *B. Imbert, L. Catoire, N. Chaumeix, G. Dupre, C. Paillard; LCSR / CNRS* Pulsed detonation engines rely on a detonation operating cycle, which requires a rapid Deflagration-to-Detonation Transition (DDT) once the medium has ignited. A previous experimental study has shown that mixtures based on n-heptane (the liquid hydrocarbon potentially interesting for this kind of application) are as sensitive as those based on light alkenes. These mixtures in air require a critical initiation energy of hundreds of kiloJoules. Since direct initiation can not be considered for a repeated use on long distance flights, it appears necessary to use DDT and to promote it in order to reduce both "run up" transition distance and time. This work presents, as an alternative to the traditional mechanical systems intended for this goal, combustion kinetics

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promotion by the effect of two chemical additives (CH3NO2 or H2O2). An experimental study in a shock tube proves that CH3NO2 appears to have very little effect, as an additive, on the thermodynamic and kinetic detonation characteristics of stoichiometric C7H16/O2 mixtures. On the other hand, numerical simulation shows encouraging results for the use of H2O2 as a sensitizer to DDT, since it efficiently shortens the ignition delays and the cell width.

1055 **Critical Orifice Diameter Measurements for NH3-N2O at Elevated Pressure** *C. Knowlen, A.T. Mattick; University of Washington* Experiments are in progress to determine the minimum inner diameter of a tube in which a Chapman-Jouguet detonation wave can propagate in NH3-N2O mixtures at pressures in the range of 0.1-5.0 MPa, to provide a data base which will facilitate the design of potential micro-spacecraft propulsion systems. The immediate goal is to determine the detonation cell width as a function of equivalence ratio and fill pressure. Direct detonation cell width measurements via soot foils are feasible at relatively low pressures; however, once the pressure exceeds ~1 MPa, it is anticipated that the characteristic dimensions of the detonation cells will become too small for the use of soot-foils to be practical. To attain data at elevated pressures (i.e., up to 5 MPa), the potential of using flush mounted sensors on the tube wall downstream of an orifice plate to determine critical orifice diameter, and hence cell width, is being investigated.

1005 (5B) - Flames - Quenching (Nondas Mastorakos)

1005 Effects of Flow Rate and Kinetic Ouenching on the Transition of Flame Regimes in Mesoscale Combustion Y. Ju, B. Xu; Princeton University The effects of channel width, flow velocity, and radical quenching on the transition between flame regimes in mesoscale combustion are numerically investigated. The twodimensional flame bifurcations are successfully predicted by a newly developed twoeigenvalue method. The results showed that channel width has a significant effect on the flame geometry, velocity, and bifurcations (Fig. 1). At a large channel width, it is shown that the flame is negatively stretched and flame velocity increases dramatically with the increase of the channel width. Furthermore, it is shown that a large channel yields a smooth transition from the fast flame regime to the slow flame regime. However, at a small channel width, it is shown that the flame is often positively stretched. In addition, a decrease of the channel width or fuel concentration results in either a flame extinction or a transition to a new flame branch. Furthermore, the results demonstrate that flow velocity has a significant impact on the flame propagation speed and bifurcations. In addition, it is shown that radical quenching greatly accelerates the quenching of the fast flame.

1030 **Study of Laminar Flame Quenching in a Rotating Cylindrical Vessel** *J. Jarosinski, A. Gorczakowski; Department of Heat Technology and Refrigeration, Technical University of Lodz* The experiments were conducted in an open cylindrical combustion vessel of 90 mm and 140 mm inner diameter and 20 mm length, made of Plexiglas. The front wall of each vessel was equipped with a central venting orifice of 15 mm in diameter. The chamber was horizontally mounted on the axis of an electric motor. It was supplied with a propane-air mixture of a required composition from a special reservoir. In the next step, the vessel was rotated at a desired speed for about one minute to establish rigid-body rotation of the mixture. After ignition, the flame propagates freely in a radial direction, preserving its regular cylindrical surface parallel to the rotation axis. During its propagation in the field of increasing radial acceleration, at a certain time, the cylindrical flame is locally quenched near the front walls, and the extinction wave gradually reduces its surface. Propagation velocity gradually decreases and, finally, the flame disappears. The higher the rotation rate, the smaller the radius of the local flame extinction rcr. The flame quenching always starts at the contact line of the flame with the walls normal to the axis of rotation.

1055 Detailed Numerical Simulation of the Extinction of Lean Premixed Flames Through Parallel Plates *L. Tecce, F.S. Marra, G. Continillo; Universita del Sannio* This work attempts to reproduce experimental results (Mihalik et al, 2000) and understand predominant extinction mechanisms. Simulations are conducted as a lean propane-air flame approaches parallel plates in a tube. Twodimensional simulations of flame propagation at near–extinction conditions are conducted with an industrial CFD code. The computational domain is discretised by means of a structured mesh with over 23,000 nodes. Simulation results are postprocessed and evaluation of heat fluxes and strain rate for three cases are considered: "real", "adiabatic", and "free–slip" at the plate boundaries, to elucidate the mechanism of flame extinction. All reported results indicate that heat transfer to the wall is the main mechanism leading to extinction.

1005 (5C) - Explosion - Droplets (Piotr Wolanski)

1005 **Detonation Initiation in Dispersed Fuel-Air Mixtures** *N.N. Smirnov, V.F. Nikitin, J. Khadem, V.M. Shevtsova, J.C.Legros; Moscow State University* This paper presents the results of theoretical and experimental investigations of the detonation initiation in heterogeneous polydispersed mixtures of liquid hydrocarbon fuels with air. Mathematical models able to predict the onset of detonation in turbulized polydispersed and homogeneous mixtures were developed. The problems of fuel droplets atomization, evaporation, and combustion are the key factors for ignition delays and shock waves attenuation evaluation in heterogeneous mixtures, and the non-equilibrium effects in droplets atomization and phase transitions were taken into account. Experimental investigations were carried out using diesel oil or vaporized gasoline as fuel and using air as an oxidant. Two types of initiation, initiation by a shock wave and by a spark ignition, were investigated.

1030 **A Study of Shock Wave - Hexane Droplets Interaction** *A. Kobiera, J. Szymczyk, P. Wolanski, A. Kuhl; Warsaw University of Technology* An experimental study of the interaction between hexane droplets and shock waves is presented. The main goals of the experiments were recording an image of the process and measuring basic parameters describing movement, dispersion, and evaporation of the droplets hit by the shock wave propagating in air. A shock tube with avisualization section was used for this research. Pictures allowed measuring positions, velocities, and sizes of clouds of mist created from dispersed droplets. Analysis of the pictures shows that there is no qualitative difference between cases of different droplet sizes. More significant differences are for cases with different Mach number of the shock wave. Quantitative analysis shows that, in such conditions, the shear breakup mechanism of dispersion was probably dominating. The droplets are broken and almost completely

dispersed into a mist cloud before they achieve mechanical equilibrium with the surrounding gas. The approximate time of the complete dispersion and acceleration of the fuel droplet varies from 300 to over 500 micro s and depends on both the diameter of the droplet and the speed of the shock. The diameter of the cloud during dispersion is controlled by the Weber number although the dispersion time is strongly related to the diameter of droplet and less to the Mach number of the shock.

1055 Observation of Microexplosion in Light Oil-Water Emulsion Spray Flame M. Fuchihata, T. Ida; Kinki University Microexplosion of light oil-water emulsified fuel droplets was successfully documented using a high-speed video camera with laser illumination. The temperature profile and the local frequency of the explosion occurrence were estimated in open spray flames of a water-in-oil type emulsion formed using an air-assist atomizer with a ring pilot burner. The estimates of the local frequency of the explosion occurrence were taken at the near nozzle region of the spray flame, since its temperature profile indicated that the reaction rate was accelerated in the upstream region from the nozzle tip to a height of 60 mm. Many microexplosions were observed in the near nozzle region, and all of those had very small spatial scale and short temporal scale. It is probable that the main factor affecting the reaction rate of the emulsion spray flame is not microexplosions of large droplets, as established theory says, but those of small droplets. We, furthermore, observed the microexplosions of small droplets using an ultra high-speed camera. It appears that small droplets whose diameters are less than 25µm explode in the spray flame and their temporal and spatial scale are around 10us and 200-300um. respectively.

1120 (B) - Break

1145 (6A) - Detonation Applications (Anatoly Vasil'ev)

1145 Effect of Boundary Layer for Wedge-Induced Attached Oblique Detonations *Y. Daimon, A. Matsuo; Keio University* Effects of the boundary layer on wedge-induced attached oblique detonations are investigated. The simulations are carried out with the two-dimensional Navier-Stokes equations with a one-step chemical reaction model. The each type of wave structure are compared with the results of simulations using the two-dimensional Euler Equations. The wave structures are basically the same except for the existence of the boundary layer, and the induction length in the Navier-Stokes simulation is shorter than that of the Euler simulation. Furthermore, the analogy with one-dimensional unsteady piston-supported detonation agrees well with that of the piston-supported detonation. The effect of the boundary layer is the shortening of the induction length due to the shock strengthening.

1210 Numerical Simulation on Two-Dimensional H2/Air Detonation Waves Propagating in a Converging-Diverging Nozzle H. Jotaki, N. Tsuboi, A. K. Hayashi; Institute of Space and Astronautical Science, Japan Aerospace Exploration Egency Unsteady two-dimensional simulations were performed for hydrogen/air detonations in a converging-diverging nozzle. Governing equations are the Euler equations, and the chemical reaction model uses the Petersen and Hanson model recently proposed. The detonation cell is the only one in the present case because high resolution should be maintained. The detonation wave for the present cases propagates successfully; however, the interaction between the transverse waves and the nozzle wall play a significantly important role in the generation of the high pressure areas in the converging section.

1235 An Experimental Study of Rotating Detonation Engine P. Wolanski, J. Kindracki, T. Fujiwara, Y. Oka, K. Shima-uchi; Warsaw University of Technology Research into the development of a pulsed detonation engine (PDE) was initiated by J.A. Nicholls et al. from the University of Michigan; however, only recently, more research has been focused on this kind of engine. Also, in the early the 1960s. Voyevodckii, Metrofanov, and Topchian performed experiments on continuously rotating detonation. More recently, Wolanski, Fujiwara, and Mitsubishi applied for a patent on the Rotating Detonation Engine (RDE). In this paper, the basic principles of the RDE are described and initial laboratory experiments of this engine are presented. The principal of the RDE is based on the creation of a large centrifugal force, resulting from the spinning detonation propagating in a disk-like chamber. For testing the idea of the RDE, a special experimental test stand was build at the Institute of Heat Engineering of Warsaw University of Technology. The stand consist of a cylindrical chamber connected on one side to the supply system and, on the other side, to a dump tank. An oxy-acetylene mixture was used as the combustible mixture. Many experiments were conducted using various mixture compositions and different pressures. A typical test lasted about 0.5 s, and many rotating detonation waves inside the chamber were recorded.

1145 (6B) - Flames - Microscale (Uwe Riedel)

1145 **Film Combustion in Small Cylinders** *T.K. Pham, D. Dunn-Rankin, W.A. Sirignano; University of California, Irvine* Small-scale devices that require tens to thousands of watts of power to operate need energy sources that possess high specific power. This demand can be met by combining the high energy per mass contained in liquid hydrocarbon fuels with the fast energy release of combustion processes. Additionally, for systems with sizes within the millimeter to centimeter range, employing liquid films is advantageous over more traditional forms of fuel injection since they provide large surface areas for vaporization and serve as buffer zones between the flame and the combustor walls. Using swirling airflow for heptane film generation and flame stabilization in a tubular chamber, study of the resulting flames has illustrated that flame ignition and stability are dependent upon the balance of several factors, including air speed, fueling method, vaporization, mixing, and film and wall temperatures.

1210 Numerical Simulation of Hydrogen/Air Combustion Characteristics Inside a Platinum Microtube G.-B. Chen, Y.-C. Chao, C.-P. Chen, C.-Y. Wu; Diwan College of Management and National Cheng Kung University A numerical simulation of H2/air mixture reaction in a Pt catalytic micro tube is performed. We identify the effects of different operational parameters on the interaction of gas phase and surface reactions inside the tube. When the flow is dominated by surface reaction, different parameters affect the transition from the kinetic control region to the diffusion control region. At high temperatures, when gas phase reaction can occur

inside the tube, variation of the operational parameters will affect the light-off location of the gas phase reaction. The location of the gas phase reaction will shift downstream with decreasing equivalence ratio or increasing inlet velocity until the gas phase reaction can not be maintained at the exit. During this process, the surface reaction dominates the upstream flow region and extends downstream with increasing the inlet velocity and finally all over the tube. Decreasing the tube diameter will enhance the fuel diffusion and heat loss and inhibit the gas phase reaction to near-stoichiometric conditions and very high wall temperatures.

1235 Structure of Microjet Methane Diffusion Flames T.S. Cheng, Y.-H. Li, C.-S. Chen, C.-Y. Wu, C.-P. Chen, Y.-C. Chao: Chung Hua University Characteristics of microjet methane diffusion flames stabilized on vertical straight stainless-steel tubes with nominal diameter ranging from 150 to 770 micron are investigated. These flames are potential energy sources for future micro power generators. Of particular interest are the flame shape, flame length, and quenching limit, as they have direct bearing on the minimum size and power of the devices in which such flames would be used. Experimental measurements of flame shape, flame length, and quenching velocity are compared with theoretical predictions. Comparisons of the flame shape indicate that the axial diffusion becomes effective when the flame is in a spherical shape. When the axial diffusion terms are included in the governing equations, the calculated flame shape is in better agreement with the experimental measurement. Using a simple jet flame model, the calculated flame lengths are also in excellent agreement with the measured data and scale well with the Revnolds number. Comparisons of predicted quenching velocity with measured results indicate that quenching occurs when the flame length equals the standoff distance.

1145 (6C) - Combustor Stability (Suresh Menon)

1145 High Frequency Combustion Oscillations Induced by Transverse Acoustic Modulations F. Richecoeur, S. Ducruix, P. Scouflaire, S. Candel; EM2C Laboratory, CNRS-Ecole Centrale Paris High frequency acoustic instabilities observed in liquid rocket engines are studied in a laboratory scale cryogenic experiment at 0.9 MPa. Three vertically aligned coaxial injectors allow to stabilize three LOx/Methane flames. Two lateral quartz windows allow to set up high speed cameras, intensified cameras, and photo-multipliers to investigate the flame's behavior. External modulation is generated by a rotating toothed wheel periodically blocking a secondary nozzle. The eigenfrequencies of the combustion chamber are experimentally determined using a frequency linear sweep and flame structure is observed with and without external modulation. Pressure fluctuations reach 10% of the mean chamber pressure developing an oscillating motion of the fluids and the reactive zones. Collective interactions are observed and proved to be a fundamental mechanism in the oscillation amplification.

1210 **Stability Analysis of Low-NOx Gas Turbine Combustors** *F. Di Palma, A. Di Benedetto, F. S. Marra; Istituto di Ricerche sulla Combustione - CNR* A mathematical model of a gas turbine combustor has been developed, suitable to be investigated in the framework of the bifurcation theory. A non-linear stability analysis has been performed with the help of the continuation method. The stability map in the operating condition typical of Low-NOx lean gas turbine combustors has

been computed, showing the role played by heat losses and burnt gas recycling in the occurrence of stable oscillations usually referred to as combustor instabilities. The possible occurrence of stable oscillations from the interaction of heat losses and recycling is demonstrated. The reported oscillating solutions have features at least in qualitative agreement with the oscillations experimentally observed in real gas turbine combustors.

1235 Effect of Swirl on the Stability of a Lifted Flame Sustained by a Low-Swirl Burner S. Tachibana, L. Zimmer; Japan Aerospace Exploration Agency, Aeroengine Testing Technology Center The low-swirl burner (LSB), which was originally developed for fundamental research on turbulent premixed flames, in recent years, has begun to attract attention for the possibility of practical applications due to its robust stability over a wide range of operating conditions. One important aspect of the LSB flame is its stability in the lean operating condition. Since the flame stability is closely linked with the swirl strength, the effects of swirl on the flame properties were investigated. A series of OH-PLIF measurements was carried out. By using OH-PLIF intensity as an indicator for the position of flame fronts, the PLIF images were binarized into unburnt and burnt states. The Reynolds mean progress variable was calculated from the binary images. Then, flame lift-off height and turbulent flame brush thickness were determined from the distribution of the progress variable. The effects of the swirl number on those properties were discussed in detail.

1300 (L) - Lunch

1440 (7A) - Pulse Detonation Engines (Toshi Fujiwara)

1440 **Experiments on Inter-Tube Interference in a Four-Tube Pulse Detonation Engine** *T. Yatsufusa, K. Nishimura, T. Yamaguchi, K. Yoshinaga, T. Endo, S. Taki; Hiroshima University* A Four-Tube PDE has been developed to study the interference of shock waves between tubes. An H2-air mixture was chosen and Shchelkin spirals were installed in the tubes to avoid the difficulty of initiating detonation. In this extended abstract, the details about the arrangement of the fourtube PDE are mentioned. We started the test run using one of four tubes and multicycle tests with a single tube were carried out after confirming the detonation was initiated in the single-cycle test. Detonation initiation was observed in a series of experiments including multi-cycle tests with 10 and 20Hz. We plan to investigate a method for scavenging burnt gas to realize operation with much higher frequency. In addition, studies on the interference of exhaust and shock waves at the collecting duct will be carried out in order to optimize the performance.

1505 **Performance of Propellant Decomposition Products as Fuel in Airbreathing PDE** *B. Veyssiere, B.A.Khasainov, P.Walton, E. Daniau; ENSMA, Université de Poitiers* Decomposition products of a solid propellant can be considered as one alternative solution for the fuel used in an airbreathing PDE. However, they may contain an important amount of solid carbon particles. Here, it is predicted that these carbon particles may be used to improve the performance of the engine by introducing an adequate quantity of air into the chamber to allow complete burning of particles. An increase of 25% of the pressure impulse can be obtained

with sufficiently small particles (diameter less than $10 \ \mu m$).

1530 **Detonation Initiation in Pulse Detonation Engines: Experiments and Simulations** *V.E. Tangirala, P.F. Pinard, K. Hinckley, A. Rasheed, A.J. Dean; General Electric Global Research Center* For propulsion systems, DDT optimization is a trade-off between minimizing run-up distance via more obstacles or higher blockage ratio per obstacle, and minimizing performance losses via fewer obstacles. In the present study, the effect of key parameters namely fuel fill, operating pressure, spark energy, number of sparks, and their arrangement on detonation initiation in a tube-PDE is investigated. The present 3D CFD predictions of the run-up distance are in better agreement with test measurements than the predictions of 2D axisymmetric simulations.

1440 (7B) - Flames - Edge (Forman Williams)

1440 Edge-Flames and Cellular Structures in Oscillatory Non-Premixed Counterflows D.A. Kessler, M. Short, J. Buckmaster; University of Illinois We examine the dynamics of non-premixed edge-flames in an unsteady counterflow configuration. The Lewis number of the deficient fuel component is taken to be 0.3. For steady counterflows, the edge can trail a stable one-dimensional strong burning solution, or a sequence of stationary or drifting flame strings. In other cases, stationary isolated flame-strings or dual interacting flame strings can be formed. We examine how these structures evolve when the strain rate associated with the underlying counterflow field oscillates in time, which is of much relevance to turbulent flow field configurations. The resulting evolution is sensitive to the amplitude and frequency of the oscillation. In particular, we identify a number of structures that are observed in the steady counterflow situation, including the stretching and splitting of isolated flame strings. We also present results for different Lewis numbers and initial mixture fractions.

1505 **Flame-Edge Dynamics in Diffusion-Flame/Vortex Interactions** *M. Hermanns, M. Vera, A. Linan; Universidad Politecnica de Madrid* We present a simple model for the dynamics of the flame-edges that form after the local extinction by a vortex ring of a diffusion flame between two counterflowing gaseous fuel and air streams of the same density. The analysis is confined to the near-stagnation point region, where the strain rate of the unperturbed velocity field is constant. We restrict our attention to cases where the typical vortex ring radius is large compared to both the size of the vorticity core and the characteristic thickness of the mixing layer. The dynamics of the flame-edges are modeled using previous numerical results, where heat release effects are fully taken into account, which provide the propagation velocity of triple- and edge-flames in mixing layers in terms of the local Damkohler number based on the local thickness. The results agree qualitatively well with experimental observations in the same parameter range.

1530 **Destabilization of Non-premixed Lifted Flames by Low Amplitude Acoustic Perturbations** *D. Demare, F. Baillot, A. Wyzgolik; CORIA-UMR 6614, CNRS-Université et INSA de Rouen, France* Non-premixed lifted flames, commonly used in many combustion processes, present problems of stability. They are sensitive

to the ambient noise able to modify the jet eddy structures. Here, experiments are performed in an organized free jet of methane in order to characterize and interpret the coupling between the flame and vortical structures resulting from aerodynamic instabilities. The lifted flame in its hysteresis zone, stabilizes on the streamwise vortices (filaments) induced by secondary instabilities. Mixture fraction and velocity measurements show that the flame is preferentially located at a distance where filaments begin to connect each other and to form long transverse ejections of matter. By means of a sine-wave acoustic modulation at high frequencies (greater than frequencies of the spectral jet broadband) and low amplitudes (same order of magnitude than the unexcited jet turbulence intensity), a non-linear coupling between forced and natural jet modulations induces an irregular development of the primary structures which disturbs streamwise vortex formation in return. As the stabilization with acoustics is still ensured by streamwise vortices, the deterioration in their formation can induce the flame reattachment definitively. Even driven by low amplitude perturbations, the jet is sufficiently modified for the lifted flame to lose its stability.

1440 (7C) - Turbulent Combustion II (Harry Dwyer)

1440 Relevance of Approximated PDF Shapes for Turbulent Combustion Modeling with Variable Equivalence Ratio V. Robin. A. Mura. M. Champion, P. Plion; LCD UPR9028 CNRS The present paper is devoted to the numerical modeling of turbulent reactive flows in situations where reactants are not ideally premixed. In this case, the description of the local thermochemistry requires at least two variables. Here, we chose the mixture fraction to describe the local composition of the fresh mixture and the fuel mass fraction to evaluate the progress of the chemical reaction. The numerical model is based on the analysis made by Libby and Williams that led eventually to the LW-P model. A two-scalar Probability Density Function (PDF) made of two or four Dirac delta functions is used to evaluate the mean chemical rate. In LW-P, the parameters of the PDF describing the magnitudes and locations of these Dirac delta functions are determined solely from the mean and variance of the two variables. The model is applied to the calculation of a turbulent reactive flow of propane and air stabilized by a plane sudden expansion of a 2-D channel. The reaction zone is fed by two streams with different equivalence ratio. In the present work, the results obtained using either a two Dirac delta functions PDF or a four Dirac delta functions PDF are compared.

1505 A Flame Surface Density Model Including Tabulated Chemistry and Heat Losses W. Ghedhaifi, N. Darabiha, O. Gicquel, D. Veynante, L. Pierrot; CNRS -Laboratoire EM2C, Ch,tenay-Malabry, France A model is derived to perform RANS (Reynolds Averaged Navier-Stockes) simulations of non-adiabatic turbulent combustion. The turbulent combustion model, based on the Coherent Flame Model (CFM), solves balance equations for the progress variable, the mixture fraction, and the flame surface density. Detailed chemistry features are included using a tabulation method (FPI). The chemical database is built from a set of laminar premixed flames with different values of equivalence ratio and enthalpy (FPI). This tabulated chemistry allows the estimation of any variables such as the species and energy chemical source terms, species mass fractions or the laminar flame speed for any values of the progress variable, the mixture fraction and the enthalpy. The model is

implemented in the commercial CFD code, FLUENT, via User-Defined Functions (UDF). A two-dimensional configuration, representative of simplified industrial burners, is considered. The results confirm the ability of the model to produce relevant qualitative and quantitative results for premixed combustion.

1530 Modeling Turbulent Mixing of an Evaporating Spray G. Subramanian, O. Colin, A. Pires da cruz, L. Vervisch, G. Bruneaux; Institut Français du Pétrole Closures for the balance equation of the mixture fraction variance with liquid spray evaporation are tested against LIEF visualizations. Experimental conditions are close to those found inside a Diesel engine with high pressure injection. Special attention is given to the source term due to evaporation. Two different models are tested for this term, which rely on different assumptions. Hollmann and Gutheil (HG) have assumed a linear relation between mixture fraction and source fluctuations, while Demoulin and Borghi (DB) argue that the source of variance is active only under the conditions at saturation. Other contributions, such as production by mean gradients and dissipation rate, are also analyzed. The global structure of the fuel fluctuations field is well reproduced. However, the variance is over-estimated near the injector by all models, even though the HG model performs better than the DB closure for the present experimental conditions. One major conclusion is that the scalar fluctuations evaporation source term cannot be neglected. Inside the core of the spray, its order of magnitude is close to variance production and dissipation terms. Moreover, its influence is mainly limited to a zone close to the liquid jet and, further downstream, fluctuations are controlled by production and dissipation terms.

1555 (B) - Break

1620 (8A) - Detonation Structure I (Sergey Frolov)

1620 **The Hydrodynamic Structure of Detonations** *M. I. Radulescu, G. J. Sharpe, C. K. Law; Princeton University* The present work treats the detonation wave structure in a probabilistic sense. In this framework, the detonation structure is of the eigenvalue type, the turbulent source terms competing with the exothermicity. One can thus define the location of the average sonic surface as the information boundary between the statistically steady detonation structure and the following expansion waves. Two-dimensional numerical simulations are used to verify the consequences of the model and measure the magnitude of the various closure terms necessary in the stochastic formulation.

1645 **Characterizing the Fluctuations in Gaseous Detonation Fronts** *J.M. Austin, J.E. Shepherd; University of Illinois at Urbana-Champaign* We propose a map of possible combustion regimes within detonation fronts, analagous to the Borghi diagram in turbulent combustion.

1710 **Photographic Study of the Two-Dimensional Dynamics of Irregular Detonation Waves** *C.B. Kiyanda, A.J. Higgins, J.H.S. Lee; McGill University* Irregular detonation waves of a stoichiometric mixture of methane and oxygen at an initial pressure of 3.4 kPa are visualized in a thin channel of 100mm by 25 mm crosssection. Schlieren visualization allows the observation of gas dynamic features, and photographs of the self-emitted light give a qualitative measure of the location of reaction within the detonation waves. The images reveal large unburned pockets created as a result of decoupling of the lead shock and the reaction front through the latter part of the cell. Evidence suggesting two different modes of combustion in these unburned pockets is shown. The interaction of this unburned pocket with the decoupled reaction front is suggested as a possible mechanism for the onset of the next cycle.

1620 (8B) - Flames - Soot (Philippe Dagaut)

1620 Effects of Dilution on Soot Formation in Laminar C2H4 Diffusion Flames *H. Mohammed, M. Chaos, R.H. Chen, F. Xu; University of Central Florida* The effects of CO2, N2, He, and Ar addition on soot formation in laminar C2H4 diffusion flames were studied at atmospheric pressure. The following properties were measured along the axes of the flames: soot concentrations, flame temperatures, and concentrations of major gas species. Results showed that larger thermal diffusivity and larger mass diffusivity between the diluting gases and C2H2 both contributed to the increase of the observed soot yields. There was a substantial chemical effect of CO2 addition on soot formation due to CO2 dissociation reactions. Reaction CO2+H=CO+OH increased the amount of CO, increased the soot oxidation by producing oxidizing species OH, and decreased the concentration of soot growth species H according to the Hydrogen-Abstraction/Carbon-Addition (HACA) mechanism.

1645 Detailed Kinetic Modeling of PAH Growth and Soot Formation in Shock **Tube Pyrolysis of Benzene and Ethylene** G.L. Agafonov, I. Navdenova, M. Nullmeier, P.A. Vlasov, J. Warnatz; Semenov Institute of Chemical Physics, RAS The new detailed kinetic model of soot formation in shock tube pyrolysis of aliphatic and aromatic hydrocarbons is proposed. The model is based on the comprehensive kinetic model of PAH formation and growth, which incorporates several pathways such as the alternating H-abstraction/C2H2 addition (HACA) route, resulting in a successive growth of PAHs, the combination reactions of phenyl with C6H6, the cyclopentadienyl recombination, the ring closure reactions of aliphatic hydrocarbons, and the combination reaction of resonantly stabilized propargyl radicals. Soot precursors are formed in the reactions of polyaromatic molecules with polyaromatic radicals (starting from biphenyl up to coronene) and in the reactions of polyaromatic radicals only (starting from cyclopentaphenanthrene and up to coronene radicals). The new pathways of PAH formation introduced into the gas-phase kinetic mechanism of the soot formation model and the new concepts of soot nucleation and soot surface growth implemented in the new model made it possible to demonstrate a decisive role of PAHs in the soot inception and soot growth and to improve considerably the agreement between the results of calculations and experimental measurements.

1710 **Aspects of Modeling Soot Formation in Turbulent Diffusion Flames** *F*. *Mauss, K. Netzell, H. Lehtiniemi; Lund University* The formation of soot in turbulent diffusion flames is a problem in combustion that is still not understood. In the past, there have been two approaches to model this process using the laminar flamelet concept: the flamelet library method and the interactive flamelet method. In this work, the representative interactive flamelet approach is chosen to provide a

reference case for further validation of the flamelet library based soot model. We found that the predicted profile for the soot volume fraction is very sensitive on a number of parameters not investigated in previous studies. The parameters we investigate are the choice of the dependence of the scalar dissipation rate on the mixture fraction and the influence of agglomeration processes. We found good agreement between calculation and experiment without assuming preferential diffusion of soot, and that there is a permanent loss of soot in the instationary flamelet model if the decrease of the maximum mixture fraction, needed in the formulation of the scalar dissipation rate, is not considered.

1620 (8C) - Propulsion (Bernard Veyssiere)

1620 Unsteady One-Dimensional Modeling of Ram Accelerator at Elevated Pressure in the Subdetonative Velocity Regime P.A. Bauer, Y. D'Angelo, C. Knowlen, A.P. Bruckner; Laboratoire de Combustion et Détonique (UPR 9028 CNRS) - ENSMA In the thermally choked operation of a ram accelerator at fill pressure beyond the range of 10 to 12 MPa, the ratio of propellant to projectile density is sufficient to generate acceleration exceeding 30,000 g. In this specific case, an unsteady analysis is required. A more accurate prediction of the thrust at high acceleration was obtained by accounting for the unsteady flow effects that are disregarded in the quasi-steady control volume model. The aim of the present study is to examine the influence of these unsteady effects in this one-dimensional modeling in combination with the use of a real gas equation of state in order to calculate the thrust characteristics of the thermally choked ram accelerator. The main basis of this model is to describe the effects of the flow around the projectile as a global process between the state of the propellant entering the control volume and the state of the thermally choked exit flow. The model is based on the standard set of onedimensional conservation equations. The flow properties are modified through a control volume by the rate of accumulation of mass, momentum, and energy in the control volume between the entrance and exit planes.

1645 **Development of a High Test Hydrogen Peroxide (HTP) Micro-Thruster** *C.-K. Kuan, G.-B. Chen, Y.-C. Chao; National Cheng Kung University and Diwan College of Management* In the design of a micro-propulsion system using HTP, the latent heat thresholds of water and HTP impede the decomposition rate and significantly degrade the performance. Lower decomposition efficiency than normal also originates from shorter resident time and enhanced heat loss when reducing the size of the reactor down to sub-meso-scales. If we want to achieve a short response of pulse thrust, an additional heat supply is needed. For the improvement of instability due to flow rate flogging and pressure feedback, a fine spray atomization system may be the solution. The design of the catalytic reactor with a higher surface area to volume ratio is a key point to accelerate the decomposition rate for a micro-thruster.

1710 **Gasdynamic Operation of Baffled Tube Ram Accelerator in Highly Energetic Mixtures** *A.J. Higgins, C. Knowlen, C.B. Kiyanda; University of Washington* A novel baffled-tube concept for enabling unlimited energy addition behind the ram accelerator projectile has been proposed and tested. Experiments have shown that the projectile is able to pass through the baffles at supersonic velocity without generating an unstart. Combustion was successfully initiated behind an axisymmetric, full-bore projectile that was launched without an obturator. Positive acceleration has been demonstrated.

Wednesday August 3

0900 (9A) - IC Engines I (Derek Dunn-Rankin)

900 Modeling Diesel Spray Ignition Using Detailed Chemistry with a Flamelet Progress Variable Approach *H. Lehtiniemi, P. Amneus, F. Mauss, M. Balthasar, A. Karlsson, I. Magnusson; Lund University* In this work, an unsteady flamelet library for a flamelet progress variable, based on sensible enthalpy, is used to model autoignition under Diesel engine relevant conditions. An unsteady flamelet library containing the source term for the progress variable and an expression for enthalpy as a function of temperature and mixture fraction, and the other parameters of the flamelet library, is coupled to a commercial CFD code. Using this approach, we are able to resolve local effects such as local turbulence and heat losses to the walls on a CFD grid-cell level. The results obtained using the unsteady flamelet library are compared to results obtained using the representative interactive flamelet (RIF) method. We see that after autoignition, the results using the unsteady library approach and the RIF method are virtually identical.

925 Transient Species Analysis in Homogeneous Charge Compression of Dimethyl Ether M. Ohtomo, M. Yoshii, Y. Yamasaki, T. Yamaguchi, H. Yamada, A. Tezaki; The University of Tokyo A number of species detection methods have been applied to further clarify the autoignition process of premixed dimethyl ether (DME) taking place in an externally motored single cylinder piston engine. As a crank angle resolved measurement, pulse valve sampling with in vacuo quadrupole massspectrometric (QMS) detection method was developed. It was successful to improve time resolution of the sampling by eliminating dead volume and boundary layer contributions with an open time differentiation scheme so that profiles of formaldehyde and hydrogen peroxide between cool and hot ignition stages were obtained. The formaldehyde profile was consistent with that obtained with in situ laser-induced fluorescence (LIF) monitoring. In hot ignition suppressed conditions, exhaust gas analysis is also useful to elucidate the cool ignition chemistry. FT-IR and OMS are complementary methods that were used to detect a variety of species. It was found that formic acid is formed in cool ignitions with a yield at a fraction of formaldehyde, as proposed in the 2000 version of the Curran et al. detailed DME oxidation model. In the chain reaction system of cool ignition, formic acid acts as an inert species whereas the chain terminating effect of formaldehyde determines the fuel consumption of cool ignition.

950 **Dynamic Model of Combustion in a Piston Engine** *E.Y. Bitar, H.J. Schock, A.K. Oppenheim; University of California, Berkeley* The sole purpose of combustion in a piston engine is to raise pressure. Hence, the recorded pressure profile provides a measure of its effective productivity. Provided by it, moreover, is the input to a model expressing the performance of combustion as that of a dynamic object. Furnished for this purpose is an algorithm for a micro-electronic control system for optimization of the service provided by the combustion system. The output of the algorithm is made out of time profiles of the mass averaged thermodynamic

parameters tracing the evolution of the combustion field, as well as of the effective product of the consumed fuel expressed in terms of analytic functions. On this basis, gains in the reduction of fuel consumption are evaluated, bearing directly upon the minimization of pollutant formation, achievable by modulating the exothermic process of combustion by means of a micro-electronic control system.

0900 (9B) - Multiphase Combustion (Rudolf Klemens)

900 Finite Rate Heat-Transfer Effects on Multiphase Burning in Confined Porous Propellants A.M. Telengator, S.B. Margolis, F.A. Williams; University of California at San Diego Combustion in porous solid propellants is often affected by an increasing pressure difference (overpressure) between the burned-gas region and the gas deep within the pores of the material. In the limit of an infinitely large rate of heat exchange between coexisting phases, a single-temperature model is obtained. However, increasing convective-gas velocities in the two-phase regions reduce the degree of thermal equilibration between the coexisting phases. As a result, finite heat-transfer effects begin to play an increasingly important role. Inclusion of twotemperature effects considerably complicates the analysis of the problem in the chemical boundary layer and, as the rate of interphase heat transfer decreases, temperature nonequilibrium eventually spreads into the preheat region, thus requiring a separate analysis. In the present work, we investigate analytically and numerically the finite heat-transfer effects for the regime in which temperature nonequilibrium is confined to the reaction zone, for varying levels of a scaled interphase heat-transfer parameter. Increasing burned-gas pressure is shown to result in a higher burning rate, increasing temperature-nonequilibrium effects and, ultimately, a transition from conductive to convective burning. This transition has been observed even in the limit of thermal equilibrium; however, it is significantly sharpened when finite heattransfer effects are taken into account.

925 **Gasification of Single Wood Particles: Experiment and Simulation** *B. Wilmes, U. Kuhlmann, F. Behrendt; Berlin University of Technology* The aim of this work is a detailed understanding of all physical and chemical effects involved in the gasification of wood. Experimental and simulation investigations are carried out. We examined spherical wood particles (16 mm dia.) during pyrolysis over the flame of a flat-flame burner (McKenna, stoichiometric methane-air mixture). By Raman spectroscopy, we monitored the exhaust gases near the stagnation point of the hot gas flow around the sphere. A transient one-dimensional mathematical model which simulates the gasification of a single wood particle is set up. Balance equations for mass, species, momentum, and energy are developed for all phases (solid, liquid, and gas). Proper boundary conditions at the border of the particle are given by the results of a stagnation-point flow delivering real conditions in the surroundings of the particle.

950 **PDF Modeling of the Mixing Process in Turbulent Spray Flows** *H.-W. Ge, E. Gutheil; IWR, Heidelberg University* A probability density function (PDF) method is developed to simulate the mixing in turbulent spray flows. The PDF transport equation of the gas-phase mixture fraction for turbulent spray flows is deduced, modeled, and solved. The numerical results of the methanol vapor mass fraction for a non-reacting spray, which are obtained using the PDF method, are in good agreement with experimental data and improve the ones from the finite-volume method. Furthermore, the shapes of the PDF of the mixture fraction at different positions, which are computed by the Monte-Carlo method, are presented and analyzed. It appears that the spray source changes the value of the mean mixture fraction, but it does not change the shape of its PDF. A comparison of the Monte-Carlo PDF with the standard beta-PDF shows the beta function to fail to describe the shape of the PDF. With the definition of appropriate local maximum and minimum values of the mixture fraction, a modified formulation of the b PDF is suitable to reflect the shape of the Monte-Carlo PDF very well.

0900 (9C) - Detonation Modeling (Ash Kapila)

900 **On the Inclusion of Frictional Work in Non-Ideal Detonations** *V. Tanguay, A.J. Higgins; McGill University* Different researchers have treated non-ideal detonations (detonations with friction) in different ways in the recent literature. Some authors include a source term in the conservation of energy equation, taking into account the work done by friction, while others do not. This difference is addressed here and it is concluded that the work term should be included in the analysis. The conservation laws are integrated with and without the frictional work term to evaluate the magnitude of the term. It is found that the qualitative nature of the solution is not changed but the inclusion of the work term significantly increases the detonation velocity as compared with the case without a work term.

925 Soot Track Formation by Shock Waves and Detonations K. Inaba, A. Matsuo, J.E. Shepherd; Keio University The purpose of this paper is to explore an explanation of soot track formation by shock waves and detonations. Focusing on the role of shear stress in transporting soot along the surface, we investigated the non-reactive Mach reflections experimentally with soot foil records and numerically with three-dimensional compressible Navier-Stokes simulations and two-dimensional soot simulations. Numerical trajectory angles of triple points are compared with experimental and numerical soot track angles to interpret the effect of shear stress spatial and temporal variations on soot redistributions. We propose that features of the soot tracks in experiments depend largely on the shear stress variations in direction and magnitude created by the boundary layer adjacent to the soot foil. The motions of soot due to surface shear stress in gas phase flow are computed with treating soot as both fine particles and fluid parcel. Redistributed soot thicknesses are examined to verify our proposal, and it is suggested that the same mechanism would also explain the soot track formation in detonation.

950 Study of Detonation Sensitivity of Hydrogen-Air Mixture Using an Updated Comprehensive Chemical Kinetic Mechanism *H.D.* N_g , *Y. Ju, J.H.S. Lee; McGill University* Hydrogen economy has been recognized as an ideal long-term solution to energy related problems. However, the wide-spread use of hydrogen creates public concern because of its high sensitivity to detonation. A common accident scenario is when high-pressure hydrogen storage facilities are contaminated with air. For most hydrocarbon mixtures, the detonation sensitivity increases for increasing pressure. However, hydrogen may not have this behavior at elevated pressure because of the chain-termination step that leads to the second explosion limit. With recent kinetic data of hydrogen oxidation, it is of interest to re-examine

the detonation sensitivity of hydrogen-air mixtures at high-pressure conditions. The dynamic detonation parameters provide an indication of detonation sensitivity. Correlation with chemical length scales is commonly used for estimating these parameters. However, results depend strongly on the kinetic model. In this study, we explore the validity of a recently updated comprehensive kinetic mechanism of hydrogen combustion by Li et al. (2004) for detonation studies. Performing ZND analyses with this mechanism and using semi-empirical models, various dynamic parameters for hydrogen-air detonations are estimated and compared with experimental data. Results obtained using this mechanism for the study of the hydrogen-air detonation sensitivity at elevated pressure are then reported.

1015 (2PO) - Poster II - Detonation (Charles Kiyanda)

1015 (B) - Break

1120 (10A) - Detonation - Past and Future - In Honor of AK Oppenheim's 90th Birthday (John HS Lee)

1120 **Detonation as a Self-Sustained or "Living" Phenomenon** *J.E. Shepherd; California Institute of Technology* The structure of detonation waves was recognized as a central problem in the Gasdynamics of Explosions by Oppenheim. He immediately grasped the significance of the observations of "turbulent" detonation by White and wrote in 1961: "...the detonation may form an essentially non-steady, non-uniform regime so that, in order to explain its precise nature, multidimensional effects in space as well as its irregular behavior in time have to be taken into account." Since that time, researchers worldwide have being working toward an explanation of this "precise nature". For example, in Oppenheim's laboratory during the 1960s and 1970s, there were experimental observations with the laser schlieren method, analyses of wave interactions, and the study of exothermic centers. Despite substantial efforts, the precise nature of detonation fronts still eludes us. I will discuss some recent contributions to our imprecise knowledge, emphasizing the coupling between physical and chemical processes that occurs in highly unstable waves.

1145 Theory & Modeling of Detonation Wave Stability: A Brief Look at the Past and Toward the Future M. Short; University of Illinois, Urbana and Los Alamos National Laboratory Drawing on pioneering work conducted in the 1960's, a large number of papers have been written recently that concern the theoretical analysis of detonation wave stability. The purpose of this talk is to give a basic overview of our current state of knowledge in the area of detonation wave stability theory, what we have learned from these studies, and a personal opinion as to where the direction of this field should be heading in the future. I will briefly review results from: formal linear stability theory for gas phase detonations with simple and multistep reaction kinetics; asymptotic studies on the linear and nonlinear evolution of unstable detonation fronts based on various limiting cases (including slowly evolving, weakly curved approximations, and high-overdrive and weak heat release limits); and relationships between predictions of linear stability analysis and direct numerical simulation of detonation wave evolution for pulsating and cellular instabilities. Finally, I will highlight some future challenges for detonation wave stability theory, including the need for different asymptotic approaches for resolving the practical issue of the evolution of Chapman-Jouguet detonations, analyzes of detonation stability for full reaction chemistry, and the study of detonation in condensed-phase (high-explosive) systems.

1210 **Computing Detonations** *V.N. Gamezo, E.S. Oran; Naval Research Laboratory* This presentation will summarize key historical results of detonation modeling and overview current research in this field. We will focus on multidimensional numerical simulations of cellular detonations in gases, in particular considering the development of detonation cells from small fluctuations, formation of unreacted pockets, regular, irregular, and secondary cellular structures, detonation diffraction, and effects of chemical kinetics. Condensed-phase and astrophysical detonations will also be considered. We will discuss connections between theoretical, numerical, and experimental results, and outline unsolved problems.

1235 'Explosion in the Explosion' and the Onset of Detonation S. Dorofeev: FM Global The processes of deflagration to detonation transition (DDT) in gaseous mixtures have attracted intense interest for a considerable time due to both their fundamental and practical importance. Since the invention of the rotating mirror camera in 1920th, studies of DDT have revealed a puzzling complexity of the wave interaction processes leading to the onset of detonation. Further improvements in experimental techniques and analysis efforts culminated in 1960s with the classical studies of A. K. Oppenheim, who introduced the concept of 'explosion in the explosion' as a final event in DDT that actually results in the onset of detonation. Since that time processes of the onset of detonations were studied by many researchers in smooth tubes, in channels with repeated obstacles, and in other experimental situations, including photochemical systems, hot turbulent jets, and shock-flame interactions. Mechanisms involved in the processes of the onset of detonations were analyzed analytically and numerically. This presentation intends to review the progress in our understanding of the onset of detonation since the 'explosion in the explosion' event has been introduced by A. K. Oppenheim. What is the nature of the final stages of the transition process? What is modern understanding of 'explosion in the explosion' event? Why do certain critical conditions exist in the onset of detonation? These and other important questions that are related to fundamental aspects of the transition to detonation are discussed in the presentation.

1120 (10B) - Combustors (Gaetano Continillo)

1120 **Influence of Staging Ratio on a Premixed Swirled Burner** *N. Dioc, S. Ducruix, F. Lacas, D. Veynante; CNRS - Laboratoire EM2C* The recent technology of two-staged fuel distribution for gas turbines is implemented in a lean-premixed, swirl-stabilized burner. The proportion of propane in each stage is a fundamental parameter of the burner behaviour. It controls flame structure, NOx emissions, and pressure fluctuations. Analysis of the flame structure (using Laser Induced Fluorescence and chemiluminescence) enables us to explain the influence of staging on stabilization and position of the flame. As more fuel is injected in the upstream stage, the large central recirculation zone stabilizing the flame enters in the premixing tube. The mixing between the two stages and the composition of the flame in terms of burnt gases properties and acoustic coupling. We show that staging

has a different effect on pollutant emissions and acoustic fluctuations so that a robust control algorithm is required to operate in optimal conditions.

1145 The Oxidation of Hydrogen-Enriched Natural Gas Blends: Experimental and Detailed Chemical Kinetic Modeling Study G. Davma, A. Nicolle, P. Dagaut; CNRS-LCSR The kinetics of hydrogen-hydrocarbons mixtures is interesting to study since the combustion of hydrogen-enriched fuels under fuel-lean conditions in gas turbines could reduce the emissions of CO, CO2, and NOx. Experimental results were obtained for the kinetic of oxidation of hydrogen-natural gas mixtures in a fused silica jet-stirred reactor operating at 1 to 10 atm over the temperature range 900-1300 K. Probe sampling followed by on-line FTIR analyses and off-line GC-TCD/FID analyses were used to measure the concentration profiles of the reactants, stable intermediates, and the final products. The addition of hydrogen in variable concentrations significantly increases the reactivity of the natural gas blend used (methane-ethane and methane-ethane-propane), particularly in fuel-lean conditions. The present experiments were modeled by means of a detailed chemical kinetic reaction mechanism. We obtained an overall good agreement between the present data and the modeling. According to the proposed kinetic scheme, the enhanced oxidation of methane by hydrogen proceeds through an increased production of OH. The increase in hydrogen initial concentration increases the formation of HO2 radicals at low temperature, yielding, in turn, higher concentrations of H2O2 and OH. Since the oxidation of hydrogen, methane, ethane, and propane mostly proceeds via reaction with OH, they react faster.

1210 Efficiency of Air Injection on Stability and Emission Controls in Premixed Combustion H. Sato, C. Nishidome, I. Kajiwara, T. Nagao, A. K. Hayashi and S. Ogawa; Aoyama Gakuin University In this investigation, we show the performance of air-jet injection through outer injection nozzles, which are set around the flame holder, for reducing the combustion instability without modification of the major geometric design of the flame holder. Particularly, we show the results of the ACC system established by the air-jet injection using a H ∞ /H2 hybrid mixturecontroller. Methane, hydrogen, and air injections are carried out to reduce the pressure fluctuation and to improve the flame structure. A small amount of additional air-jet with periodic injection yield good performance for suppressing the pressure fluctuations and furthermore, it can effectively improve the flame structure. As for the emissions control, NOx reduction is achieved with the additional air-jet.

1235 **Kinetic Effects of Air Contamination on the Combustion of Hydrogen** *G. Dayma, A. Nicolle, P. Dagaut; CNRS-LCSR* Besides the possible future switch to a hydrogen-based economy, there are many interests in studying the kinetic of combustion, oxidation, and ignition of hydrogen, particularly in relation to the development of advanced air-breathing propulsion systems. A better knowledge of the kinetic of hydrogen oxidation in the presence of NOx (NO and NO2) is of particular importance since these species are present in vitiated air streams used for supersonic combustion tests. We present new kinetic results for the oxidation of hydrogen perturbed by the addition of NO or NO2 in a JSR (700-1150K,1 to 10atm, equivalence ratio of 0.1-2.5. The experiments were performed at fixed residence time and variable temperature. Sonic probe sampling at low pressure followed by on-line and off-line analyses (GC, FTIR) was used to follow the reaction. A detailed kinetic modelling of the present data was performed using several kinetic schemes taken from the literature and that proposed here. Further model validations were performed simulating the ignition of hydrogen-air and hydrogen-NOx-air mixtures, and the burning velocities of hydrogen-air mixtures. A good agreement between the data and the present modeling was observed. The present results confirm the lower literature value of the rate constant for the reaction of NO2 with H2.

1120 (10C) - Kinetics - Reduced (Jurgen Warnatz)

1120 An Adaptive Reduced-Order Chemical Model J.C. Lee, H.N. Najm, S. Lefantzi, J. Ray, M. Frenklach, M. Valorani, D.A. Goussis; Sandia National Laboratories We demonstrate a new strategy for construction of an adaptive chemistry model. The technique is based on a slow manifold projection scheme derived from computational singular perturbation (CSP) combined with the Piecewise Reusable Implementation of Solution Mapping (PRISM). PRISM is used to tabulate the response surfaces of the CSP tensors. We examine the effectiveness of this scheme by considering a model problem with variable stiffness. We find that, while the degradation in accuracy is minimal, the CPU-cost of the CSP projection method can potentially be reduced substantially using this tabulation strategy, which bypasses the CPU-intensive CSP analysis. Furthermore, we find that the size of the hypercubes used to build the PRISM tabulation can be very large and their dimensionality can be reduced. The dimensionality reduction is achieved by collapsing the dimensions corresponding to the CSP-radicals. This reduction in the hypercubes' dimensionality is a key aspect of the new strategy.

1145 **ILDM Reduced Chemistry Tailored For Large Scale Reaction Mechanisms in Complex Reactive Flow Applications** *V. Reinhardt, B. Schramm, D. Lebiedz, J. Warnatz; IWR, University of Heidelberg* We present some new developments in ILDM-based model reduction of detailed chemistry. These developments cover the fields of computational time (parallelisation), model consistency (dimension switching, adaptive coordinate stepsize), and efficient data handling (AVL trees). With this, ILDM reduced chemistry becomes more applicable even for CFD simulations of complex technical combustion processes with large scale mechanisms. These developments are implemented in an existing ILDM code and tested for the case of a 1-D laminar flame.

1210 **Implementation of ILDMs Based on a Representation in Generalized Coordinates** *J. Bauer, U. Maas; Universität Karlsruhe (TH)* In this paper, we discuss an implementation of ILDM (Intrinsic Low-Dimensional Manifolds) in terms of generalized coordinates. In contrast to the standard implementation scheme of ILDM, it does not use chemical species concentrations to parametrize the ILDM, but generalized coordinates which offer many advantages concerning the robustness of the method. It is based on two steps: 1) the generation of ILDMs using a multidimensional continuation method and 2) the direct implementation of the results in CFD codes. All necessary data (thermokinetic state, reduced reaction rates, diffusion matrices, projection matrices) for the projection of the governing equation system onto the system of generalized coordinates (grid indices of the ILDM mesh) are precalculated and stored during the identification of the ILDM. Examples of laminar flame calculations verify the approach.

1235 Generation of Reduced Models by Decoupling of Chemical Kinetics and Convection/Diffusion Processes V. Bykov, U. Maas; Institute of Thermodynamics, Karlsruhe University This work focuses on the construction of low dimensional manifolds representing the slow system dynamics in the state space. The technique is based on decoupling of the chemical and convection/diffusion processes. This idea is widely exploited in combustion theory in both analytical and numerical aspects due to the strongly non-linear and singular structure of combustion models. The method of Intrinsic Low Dimensional Manifolds (ILDM) is used for the decomposition of detailed chemical kinetics and for the approximation of the system dynamics on the intrinsic manifold in the domain of the fast chemistry. In the domain of the slow chemistry, the low dimensional linear manifold is used to approximate the system dynamics. The matching/projecting procedure can be treated as a projection of the system dynamics onto a linear manifold containing an initial point and an intersection of the boundary of the fast chemistry domain with the slow manifold. A simple example is presented to verify the approach, but an extension to more complex systems is possible without major difficulties.

1300 (L) - Lunch

Thursday August 4

0900 (2PL) - Plenary II (Luc Bauwens)

900 **Fundamental and Applied Studies of Fuel-Air Detonation - A Quarter Century of Large-Scale Testing at DRDC Suffield** *S.B. Murray; DRDC Suffield* When the Fuel-Air Explosives (FAE) program at DRDC Suffield (formerly the Defence Research Establishment Suffield, DRES) began in the late 1970s, scientific investigations of gaseous detonation generally fell into two broad categories: (i) those dealing with the 'microscopic' features of detonation or the structure of the wave front, and (ii) those concerning the 'macroscopic' aspects of detonation or the gross dynamic behaviour of the wave. Large-scale experiments were carried out at Suffield to quantify the effect of confinement on detonation propagation, the critical tube diameter for detonation transmission, and the critical energy for direct initiation of detonation. DRDC Suffield has also studied many detonation applications to technological issues such as FAE weapons effects, mine clearing, hazard analyses for petrochemical industries, and propulsion.

1005 (11A) - **Detonation Initiation** (Andrew Higgins)

1005 **Initiation and its Optimization** *A.A. Vasil'ev; Lavrentyev Institute of Hydrodynamics* The critical initiation energy E* for a detonation wave (DW) is used as the base parameter of detonation hazards. The spatial–time history of initiator energy–release is required for correct experimental determination of critical initiation energy. An influence of the spatial factor of initiator energy–release is not similar to the time factor; the optimal configuration exists when initiation is more effective. The blast explosion approximation is preferable for correct experimental determination of E*. A similar method is identically suitable both to the various initiators with large distinctions in the spatial–time characteristics of energy-input (flame igniters, electrical or laser spark, exploding wire, high explosive, high-speed bullet...) and to various mixtures. The methods of optimisation of critical energy are discussed. Code SAFETY was used for calculation of cell size, critical initiation energy, critical diameter, etc. Calculated results are well correlated with experimental data.

1030 **Detonation Initiation by Shock Reflection from an Orifice Plate** *G. Ciccarelli, B. de Witt; Queen's University* This paper reports on the investigation of detonation initiation by shock reflection off an obstacle where the shock wave is produced by an accelerating flame in an obstacle field. The shock wave is made to interact with a single orifice plate in order to determine the critical mixture composition required for successful detonation initiation. Using this technique, the non-ideal aspects of the shock front which exist ahead of the fast flame propagating in an obstacle field is preserved for the interaction with the obstacle.

1055 **Shock-Wave Initiation of Detonations in Propane/Air Mixtures** *O.G. Penyazkov, K.L. Sevruk, V.E. Tangirala, A.J. Dean, B. Varatharajan; Heat and Mass Transfer Institute, National Academy of Sciences of Belarus* The auto-ignition and initiation domains in stoichiometric propane-air mixtures at post shock pressures of P = 3.2 + 0.5 atm were determined at shock-wave focusing in 1)hemi-spherical and hemi-cylindrical reflectors with radii R= 38 mm; 2) wedge and cone reflectors with apex angles of 900; 3) parabolic and paraboloidal reflectors. Experimental results are compared with multidimensional (2D axisymmetric and 3D) computational simulations for two specific cases: strong initiation and transient initiation for the case of a cone reflector. Comparisons of predicted and measured pressure-time traces show reasonable agreement

1005 (11B) - Flames - Unsteady (Derek Bradley)

1005 **Pressure Wave Interactions with Rippled Premixed Flames - Effect of Lewis Number** *A.C. McIntosh, J. Teerling, J. Brindley; University of Leeds* In this paper, we consider the effect of Lewis number on the interaction of an oscillatory pressure disturbance with a rippled premixed flame. There are two main effects. Firstly, at large Lewis numbers representing a fuel lean hydrocarbon, there are clear cases where the pressure wave causes holes to develop in the flame where effectively the reaction rate in those locations has been made to slow down. At Lewis numbers greater than unity, we encounter (as expected) the thermal-diffusion instability, and the growth of the overall mass burning flux is appreciably greater.

1030 **Effect of an Oscillatory Small Scale Flow on Flame Propagation** *J. Daou, P. Sparks; Department of Mathematics, University of Manchester* The present investigation describes new results addressing the validity of Damkohler's second hypothesis in parallel small scale flows. Two main contributions have been made. The first is analytical based on matched asymptotics, and leads to a formula for the effective speed of a premixed flame in the presence of an oscillatory parallel flow, valid when the flow scale is much smaller than the laminar flame thickness. The second contribution, which is numerical, provides a significant set of two-dimensional calculations aimed at assessing the range of validity of the asymptotic findings. The calculations are based on a finite-volume multigrid approach and

account, in particular, for volumetric heat-loss and differential diffusion effects. A good agreement between the numerics and asymptotics is found in all cases, both for steady and oscillatory flows, at least in the expected range of validity of the asymptotics. Additional related aspects such as the difference in the response of thin and thick flames to the combined effect of heat-loss and fluid flow are also discussed.

1055 **Parallel Bifurcation Analysis of Discontinuous Periodically Forced Reactors** *A. Grabski, L. Russo, G. Continillo; Universita del Sannio, Italy* In this work, we propose a new approach to a parallel continuation algorithm for bifurcation analysis of periodically forced systems with time–discontinuous forcing. The approach is based on parallelising the numerical computation of the Jacobian derivatives; that is, by far, the most expensive task in the stability analysis for such systems. The approach is successfully tested on the distributed (PDE) dynamical model of a Reverse Flow catalytic combustor. The rationale of the new approach is briefly outlined, and excellent speedup results are reported regarding computation conducted on up to 8 nodes on a Linux cluster. The resulting procedure opens to detailed bifurcation analysis a class of distributed models resulting in large systems of ODEs, which could be otherwise untreatable.

1005 (11C) - Blast Waves and Hybrid Detonation (Sergey Dorofeev)

1005 Simplified Modeling of Non-Ideal Blast Waves from Metallized Heterogeneous Explosives Z. Zarei, D.L. Frost, L. Donahue, D.R. Whitehouse; McGill University, Mechanical Engineering Department In the present paper, a simplified numerical "bursting-sphere" model is used to investigate the effect of afterburning on the blast wave generated from unconfined explosives. Of particular interest is the effect of afterburning from metalized explosives that contain a large mass fraction of reactive metal powders. In this case, the afterburning is due to the oxidation of the added metal particles as well as the unreacted detonation product species, and can occur within the combustion products and in the shocked air surrounding the charge. Several afterburning scenarios are considered. If the afterburning occurs within the combustion products, the maximum diameter of the combustion products interface increases, but the blast wave overpressure and impulse decrease relative to the no-afterburn case. If the afterburning occurs immediately behind the blast wave, the blast wave pressure and velocity are augmented. The effect of variations in both the temporal and spatial history of the afterburning on the blast wave propagation are considered.

1030 Secondary Pressure Waves from Rich Fireballs F. Pintgen, J.E. Shepherd; California Institute of Technology Accidental and deliberate explosions often result in fireballs of rich products. If these products mix with the surrounding atmosphere and burn on the appropriate time scale, the resulting pressure waves may enhance the blast created by the primary explosion. We have carried out laboratory experiments on this effect and demonstrated the production of secondary pressures when rich mixtures of propane and oxygen are detonated or burned in an atmosphere of air. Pressure measurements and high speed video images of the luminosity are used to document the blast and fireball. The repeatable production of strong secondary waves is observed for equivalence ratios between two and three. An acoustic analysis of the pressure signals reveals that the secondary pressure waves are consistent with the volumetric growth of the fireball. Comparison with experiments on high explosives in scaled variables indicates that although the initial blast is substantially lower for rich propane-oxygen mixtures than for high explosives, the positive=-phase impulses are similar.

1055 Hybrid Detonation Waves F. Zhang, S.B. Murray, K.B. Gerrard; Defence Research and Development Canada - Suffield Detonation in heterogeneous mixtures of micrometric grades of aluminum and detonable fuel-air gas was studied in an 80 mm I.D., 15-m long detonation tube. Three steady hybrid detonation modes were identified, namely, a weak mode, a CJ mode, and a strong mode. The weak and CJ hybrid detonation modes are characterized by a two-shock structure where the second shock behind the gas CJ plane has a velocity less than or equal to the leading shock velocity, respectively. The strong hybrid detonation is featured by a leading shock followed by a pressure wave that penetrates the gas detonation zone. In all three modes, the secondary shock or pressure wave increases the impulse. The steady hybrid detonation waves can propagate in micrometric aluminum particles suspended in the gas detonation products with the presence of oxygen or water vapor, but propagation is unlikely in the detonation products of carbon monoxide. High initial pressure facilitates steady hybrid detonation waves. Strong initiation is required to form a two-shock detonation wave, while the fuel-air detonation alone is insufficient to initiate it. The apparent detonation cell size corresponds mainly to the gas detonation and does not vield information about the sensitivity of aluminum combustion and its initiation.

1120 (B) - Break

1205 (12A) - Detonation Structure II (Oleg G. Penyazkov)

1205 Numerical Study of Detonation Cells Under Non-Monotonous Heat Release V. Guilly, B. Khasainov, H.-N. Presles, D. Desbordes, P. Vidal; LCD, UPR 9028 CNRS, ENSMA, BP 40109, 86961 Futuroscope, France Detonation structure in the case of a simple model reaction comprising two successive exothermic steps is studied numerically under the assumption that the flow of detonation products is bidimensional. The calculated traces of maximum pressure behind the detonation wave seem quite similar to the regular double detonation structure observed in pure gaseous nitromethane and nitromethane-O2 mixtures and in H2-NO2/N2O4 mixtures. The numerical simulations shed light on the effect of the governing parameters of the simple two-step reaction on the characteristics of a two-level detonation structure.

1230 **Detonation Wave Structure for Chain-branching Kinetics** *Z. Liang, L. Bauwens; University of Calgary* We examine the detonation wave structure for a four-step chain-branching reaction model exhibiting three explosion limits, similar to hydrogen-oxygen chemistry. A perturbation analysis is used to resolve the steady wave structure, clarifying the differences between explosion and no-explosion regions and allowing for an evaluation of the reaction length. Assuming high activation energy and slow initiation, the wave structure can be resolved, and a closed form evaluation of the reaction length is obtained. Three cases are identified, respectively with post-shock pressure and temperature located (1) within the

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explosion region; (2) close to the explosion limit; (3) within the no-explosion region. As expected, the reaction length suffers significant changes as the post-shock state crosses between explosion and no-explosion regions, as the induction length is shorter and the reaction rate is larger by several orders of magnitude in the explosion region. In the no-explosion region, the reaction becomes extremely stiff. In all cases, the chain-branching zone is significantly shorter than the initiation zone, and it has a structure similar to the single step model of Buckmaster and Ludford (1987). Corresponding two-dimensional numerical simulations show different cell structures and differences in regularity in different zones.

1255 **Three-Dimensional Numerical Simulation of H2/Air Detonation in a Circular Tube : Structure of Spinning Mode** *N. Tsuboi, K. Eto, A.K. Hayashi; Institute of Space and Astronautical Science, Japan Aerospace Exploration Egency* Unsteady three-dimensional simulations were performed for hydrogen/air detonations in a circular tube. The lowest mode, namely a single spinning detonation, was simulated. One rotating transverse detonation and a long pressure trail originated from the transverse detonation appeared in the present simulation. This spinning detonation is one of an irregular spin and a Mach configuration, which consists of a Mach leg and two whiskers which periodically oscillates. The maximum pressure history shows the ratio of the pitch to the tube diameter equals 3, and it agrees well with the experimental results and theoretical prediction.

1205 (12B) - Explosions I (Kailas Kailasanath)

1205 **Biomimetic Study of Explosive Discharge of Bombardier Beetle** *N. Beheshti, A.C. McIntosh; University of Leeds* In this paper, we briefly describe the combustion mechanism of the bombardier beetle. Because application to other devices is the main motivation of this work, we then discuss the modelling of the water steam explosion in a cylindrical chamber with about the same volume as the one for the beetle. Specifically, weconduct a study of the phase change and twophase flow in the beetle's device and the effect of the exit nozzle diameter on its efficiency. Then a scaled up chamber for application to gas turbine relight is simulated with a hydrocarbon fuel (hexane) instead of water. All the CFD simulations are performed using the CFX 5.7 code. The presentation will involve showing the possible biomimetic applications of this unique combustion system to microcombustion devices.

1230 Influence of a Multi-Source Ignition on the Kerosene Flammability in a Partitioned Tank J.M. Pascaud, P. Gillard; LEES Universite d'Orleans A simple modelling initially developed as part of a novel study on ignition and combustion of classical propulsive powders has been presented in order to predict the main characteristics of these explosions in a closed or a vented vessel. A calculation methodology allows to adapt the numerical simulation to the transmission of the explosion from one compartment to another adjacent compartment by the means of the hot flow through the shared orifice and finally to generalise this methodology to a complex multipartitioned structure. The aim of this work is to study the effects induced by a multi-source ignition on the kerosene flammability in a partitioned tank and a wide energy range (Eign < 5000 J). Simulated predictions have been compared with experimental results obtained in the laboratory in a two-compartment vessel and a special kind of kerosene (F.34).

1255 Detonation of Hydrogen in a Partially Filled Interconnecting Vessel Following an Initial Period of Pressure Piling S.K. Willacy, H.N. Phylaktou, G.E. Andrews, M.C. Mkpadi; University of Leeds The focus of this paper is partially filled interconnected vessels using hydrogen-air mixtures in the lean flammable range. In this paper, the dangers of even a small leak are illustrated, where mixtures well below stoichiometric levels can produce detonation events in localised areas. The rig used consists of a small cylindrical vessel (L=0.5m, D=0.5m), connected to a dump vessel (L=2.0m, D=0.5m) through a connecting pipe (L=1.0m, D=0.162m). Measurements were made using an array of thermocouples and pressure transducers. Homogeneous hydrogen/air mixtures (10-22%) were prepared in the smaller vessel only, and end ignition. Results indicate that between 18 and 22%, the flame-speeds and pressures produced are synonymous with detonation (ranges of 900-1494 m/s and 17-36 bara, respectively), illustrating the severity of a partially-filled interconnected vessel. At low hydrogen concentrations, the mechanisms involved are comparable to those reported in literature for fully filled vessels, and at higher concentrations, the detonation mechanism is displayed. Implications that stem from this research include that an ordinarily non-flammable mixture when concentrated in a single chamber of a system, or even a gas pocket, within an interconnected vessel geometry, can produce overpressures sufficient to cause destruction to buildings and non-pressure rated equipment.

1205 (12C) - Flame Ignition (Eric Petersen)

1205 **The Role of Hydrogen Pre-Reaction for Methane Catalytic Ignition** *H.-W. Hsu, J.-Y. Chen, Y.-C. Chao; National Cheng Kung University* The role of H2 prereaction for hydrogen-assisted methane catalytic ignition is examined in this study. Transient behaviors of hydrogen-assisted methane-air catalytic combustion are explored by experimental measurements and two-dimensional numerical simulations with a multi-step gas phase mechanism and surface reaction mechanism to provide a better understanding of the catalytic ignition processes. The results suggest that in addition to thermal effects, chemical kinetics on the catalyst surface can also play an important role in hydrogen-assisted catalyst combustion. The competition between the oxidation channels between surface species H(*) and C(*) is found in the low H2 content hydrogen/methane/air mixture catalytic reaction. This is believed to be the key factor in hydrogen-assisted catalytic ignition of methane if the H2 content or the temperature are low.

1230 **Ignition of Methanol Droplet Groups with Detailed Chemical Kinetics in Different Flow Environments** *H.A. Dwyer, B.D. Shaw; University of California, Davis* At the present time, there are very few research studies where detailed chemical kinetics have been used to predict the ignition of liquid droplet groups under realistic thermodynamic conditions, Ref [1]. The majority of the previous studies have used global chemical kinetics, Ref [2], which were not developed to treat the sensitive conditions associated with ignition. This problem is quite important for modern IC engines and for understanding safety concerns with the handling of liquid fuels. At the present time, we have considered small groups of droplets, two and three, in a fully three dimensional and time-dependent environment, where the

influence of droplet relative geometry and cold walls can be brought into play, Ref. [3]. The paper shows extreme sensitivity of the ignition process to flow thermodynamics conditions as well as droplet group orientations. In general, the larger and more concentrated groups lead to a more stable ignition process.

1255 Measurements of the Probability of Ignition and Subsequent Flame Propagation Speed in Turbulent Non-Premixed Jets *S.F. Ahmed, E. Mastorakos; University of Cambridge* This paper describes an experimental investigation of the ignition probability as a function of flow velocity and of spark position, duration, size, and energy in a turbulent non-premixed jet of methane in air. The subsequent evolution of the flame is also characterised by measurements of its propagation speed by a fast digital camera. The results show that energetic sparks with long-durations or from large electrode gaps give higher probability of ignition at a given point, and the ignition probability contour is consistent with previous experiments in jets. The measured net flame speed decreases from about 0.65 m/s to 0.25 m/s for jet velocities of 12 and 25 m/s, while the corresponding estimated relative flame propagation speed along the stoichiometric contour is about 1.5 and 2.5 m/s, respectively. The measurements can assist theoretical efforts aimed at constructing models for spark ignition engines with inhomogeneous mixtures and for the performance of ignitors for aviation gas turbines.

1300 (L) - Lunch

1440 (13A) - Detonation and Interfaces (Stephen Murray)

1440 **Instability of Combustion Products Interface from Detonation of Heterogeneous Explosives** *D.L. Frost, Z. Zarei, F. Zhang; McGill University* In this paper, the instability of the combustion products interface from the detonation of metalized explosives is considered both experimentally and numerically. Experiments with homogeneous (liquid nitromethane) and heterogeneous (packed beds of metallic particles saturated with nitromethane) spherical charges show that, in both cases, instabilities develop on the combustion products' interface at early times due to the Rayleigh-Taylor instability. For the metalized explosives, the deceleration of the interface is reduced and the perturbations grow more slowly and persist for a longer time. For particle-laden explosives, in some cases, perturbations can also develop on the surface of the expanding particle cloud due to particle-flow interactions which lead to the formation of particle jets. Numerical calculations using a simplified model for the afterburning also demonstrate the influence of afterburning on the development of the interface instabilities.

1505 **Shock Wave Induced Mixing and Reaction** *D.H. Lieberman, J.E. Shepherd; California Institute of Technology* Experiments are being performed on the interaction of a shock wave and an interface between air or oxygen and partiallyoxidized detonation products. The goals of these experiments are to study the mixing and subsequent chemical reactions that result from the creation of a turbulent mixing zone (TMZ) from the interface. The experiments in the current study will greatly simplify the geometry, using a thin membrane or sliding valve to separate the interface between reactants and oxidizer. A planar detonation will be used to combust the reactants. The detonation will pass through the interface between the combustion products and oxidizer, setting the interface into motion and creating a transmitted shock wave. The interfacial acceleration caused by the incident detonation and reflected shock wave create a TMZ by the Richtmyer-Meshkov (RM) instability.

1530 An Investigation of the Conditions for Detonation Initiation at a 1D **Turbulent Mixing Interface** J. Chao, J.H.S. Lee; McGill University In the present study, an attempt is made to elucidate the turbulent mixing parameters required for direct initiation by reflecting a CJ detonation from a perforated plate. The detonation products that are transmitted through the plate mix with the downstream reactants at a quasi 1D turbulent interface. The parameters that control initiation via turbulent mixing (i.e., thermodynamic and chemical properties of the products and of the reactants, and the turbulent scales in the mixing zone) are systematically varied in order to establish the critical conditions for the onset of detonation. A detonation tube 150 mm in diameter is used. Perforated plates with different hole diameters (d = 8and 15 mm) were tested, and the hole spacing to hole diameter ratio was maintained at 0.5. The driver mixture was either fixed as stoichiometric hydrogen-oxygen or stoichiometric hydrogen-air. Downstream, different hydrogen-air mixtures were tested at normal temperature and pressure. The ratio of the turbulence scale to the cell size of the reactants provides a better correlation of the critical conditions for successful initiation. The thermodynamic state and the chemical properties of the products also play a role in the initiation process.

1440 (13B) - Metal Combustion (Mel Branch)

1440 Combustion of Shock-Dispersed Flake-Aluminum in a Long Tunnel Section P. Neuwald, H. Reichenbach, A.L. Kuhl; Ernst-Mach-Institut, Fraunhofer-Institut für Kurzzeitdynamik Laboratory experiments on SDF (Shock-Dispersed-Fuel) charges with a fill of 1 g flake-aluminum and a 0.5-g PETN booster have been performed in a small-scale model of a long tunnel section (dimensions: 8 cm x 8 cm x 300 cm). Three types of diagnostics were utilized: piezo-electric pressure gages in one tunnel side-wall and the tunnel end-wall, photo-diodes in the tunnel roof, and an electro-conductivity probe immersed into the tunnel interior at different locations. From the time histories of pressure, luminosity, and electro-conductivity, wave diagrams were constructed which present some basic characteristics of the flow field in the tunnel. The main results: initially, the reaction of the dispersed flake-aluminum is rapid enough to feed energy into the propagating blast front and to enhance its peak overpressure. Later on, the increasing gap between the faster blast front and the slower combustion zone hampers further energy coupling into the front. The main effect of the subsequent combustion phases is the built-up of additional quasi-steady overpressure in the closed tunnel segment. However, compared to the performance in geometries with a length-to-diameter ratio near one, a somewhat reduced combustion efficiency of the flake-aluminum was observed.

1505 **Burning Properties of Aluminum in H2O and CO2** *J.J. Lee, F. Zhang; DRDC* Prompted by interest in particle combustion in non-ideal explosives, the burning properties of sub-millimeter aluminum particles in quiescent combustion products are investigated. Particle ignition is initiated by injecting the particles into hot products resulting from burning gaseous mixtures of H2/O2/N2 and CO/O2/N2 in a closed spherical vessel. The ignition delay and combustion time are measured. A wide range of conditions is investigated with particles from 2-100 microns, product pressures from 10-100 atm, and temperatures from 1500-3000 K. Specific issues of interest are the oxidizing efficiency of H2O relative to CO2, the difference between results obtained in a shock tube and from particle injection into a quiescent gas, scaling effect of particle size, and the burning properties for a wide range of temperatures and pressures.

1530 **Spectral Structure of the Aluminum Dust Flame** *J. Mamen, S. Goroshin, A. Higgins; McGill University* In order to resolve the mechanism of flame propagation in suspensions of nonvolatile fuels (i.e., metal) in a gaseous oxidizer, a technique to measure the spectral emissions of a dust flame is developed. This technique uses a fiberoptic spectrometer to view an aluminum dust/air flame stabilized on a Bunsentype burner via a rotating mirror, so as to scan across the structure of the flame. An Abel transformation is then applied to the measured spectral structure in order to determine the relative intensities along a slice through the flame. Measurement of the predominate intermediate (AIO) in aluminum oxidization shows that the reaction zone thickness of the flame is of the order of 2 mm. This is comparable in thickness to the preheat zone, in contrast to gas flames where the preheat zone is typically much longer than the reaction zone.

1440 (13C) - Flames - Nonpremixed Simulation (Marcus Day)

1440 Large Eddy Simulations of Pool Fires at Different Cross-Wind Velocities with a Large Adjacent Object C. B. Devaud, E. J. Weckman; University of Waterloo The present investigation is focused on Large Eddy Simulation (LES) of a liquid-fuelled fire in the vicinity of a large object in a cross-wind. Both experimental and computational configurations are intended to reproduce the scenario of an aviation fuel spill fire that occurs close to a plane fuselage. The aim of the present study is to investigate the capabilities of an LES code for three-dimensional and time-dependent calculations of fire behaviour in the fuel spill scenario outlined above. Modelling issues are also identified in order to initiate further developments in the code for this application. The computational domain and boundary conditions are defined according to the experimental configuration used in tests run by the Fire Research Group at the University of Waterloo. This setup consists of a 2-m-diameter pool fire fuelled with kerosene and located 1-m-upstream of a 2.7-m-diameter culvert in a large enclosure. Cross-wind velocities ranging from 4 m/s to 13 m/s are imposed on the fire and culvert. Results for different fire scenarios with various cross-wind velocities are presented and compared to the experimental data for the corresponding conditions.

1505 **Comparative Study of Turbulence Modelling in Hydrogen Nonpremixed Turbulent Flame** *F. Tabet-Helal, B. Sarh, I. Golkalp, A. Menou; Laboratoire de Combustion et Systèmes Réactifs* Two turbulent models are compared in turbulent hydrogen nonpremixed flame. These are the Reynolds stress model with a value of 1.82 for the constant $c\epsilon^2$ and the k- ϵ model with a limited Pope correction. The predictions are validated against experimental data. The combustion is handled with the flamelet approach. The chemical model used for the generation of the flamelet library is Yetter's et al. (1991) mechanism. It consists of 10 chemical species and 21 reactions. The comparisons with experimental data demonstrate that predictions based on the Reynolds stress turbulence model are superior to those obtained using a limited k- ε model. Overall, profile predictions of axial velocity, turbulent kinetic energy, mixture fraction, flame temperature, and major species are in reasonable agreement with data and compare favourably with the results of earlier investigations that used both first-order conditional moment closure (CMC) and transported probability density function methods (PDF).

1530 A Numerical Study on NO Formation in Counterflow n-Heptane Triple Flames *H. Guo, G.J. Smallwood; National Research Council of Canada* The mechanism of NO formation in counterflow n-heptane triple flames was investigated by numerical simulation. Detailed chemistry and complex thermal and transport properties were used. The results indicate that a triple flame produces more NO than the corresponding premixed flames due to the appearance of the diffusion flame branch and the interaction between flame branches. The relative contributions of different routes to NO formation in the premixed flame branches change with the variation of the equivalence ratio, but the thermal mechanism always dominates in the diffusion flame branch. The interaction between flame branches is enhanced with the decrease of the distance between them. Both heat and radical exchange between flame branches contribute to the interaction.

1555 (B) - Break

1620 (14A) - Detonation Structure III (Akiko Matsuo)

1620 Influence of Ar Dilution on Detonation Regime in H2-NO2/N2O4 Mixtures J. Luche, H. N. Presles and D. Desbordes; Laboratoire de Combustion et Détonique We have studied the influence of argon dilution on the detonation of a mixture (H2-NO2/N2O4 – equivalence ratio 1.2) exhibiting a non-monotonous heat release leading to a double cellular structure. Experimental results show that: 1) in up to 25% of Ar dilution, the detonation is quasi-ideal and has a double cellular structure, 2) for Ar dilution larger than 35%, the detonation is "non-ideal", it has a simple cellular structure, and its velocity is lower by about 25% than the theoretical one, and 3) for Ar dilution in the range of 25% - 35%, both regimes can exist in the same experiment succeeding each other with abrupt bifurcations.

1645 **Study of Overdriven Detonations of H2-NO2/N2O4 Mixtures** *J. Luche, D. Desbordes, H. N. Presles; Laboratoire de Combustion et Détonique* We have studied the influence of the degree of overdrive (D/DCJ) on the detonation of a H2-NO2/N2O4 mixture at equivalence ratio 1.2. This exhibits a double cellular structure which originates in the two chemical exothermic steps during the detonation heat release process. Experimental results show that: 1) the detonation is quasi-ideal and has a double cellular structure up to an overdriven degree equal to 1.11 2) for exact exothermic steps, a good agreement of the experimental curves lambda/lambda CJ vs D/DCJ compared to a numerical ones Li/LiCJ vs D/DCJ giving activation energies related to each step. 3) the activation energy of the first exothermic step is close to the H2/O2 and the activation energy of the second is close to H2/NO.

1710 Argon or Nitrogen Diluted Hydrogen/Oxygen Detonation in Tube with Obstacles A.K. Hayashi, K. Eto, Y.-F. Liu, N. Tsuboi, S. Shiokawa, H. Sato, J.H.S.

Lee; Aoyama Gakuin University Detonation propagating in the argon or nitrogen diluted mixture through obstacles is studied experimentally and numerically to clarify the activation energy effect on detonation quenching. A particular objective is to investigate whether the use of Euler equations together with a single-step reaction mechanism causes detonation quenching or not. This objective is not attained yet but will be reached by the conference. Numerical simulation as well as experiments for argon or nitrogen diluted detonation quenching are discussed in the text. The detonation in the H2/air mixture diluted with argon is more stable than that with nitrogen although the latter has a faster detonation velocity than the former at certain mixtures. The numerical results of detonation propagation through obstacles in the H2/air mixture diluted mixture did not give such quenching results, but the higher dilution by N2 gave the detonation quenching. Further detailed analysis will be presented at the conference.

1620 (14B) - Shock Ignition (Pascal Bauer)

1620 **Ignition of Aviation Kerosene at High Temperatures** *A.J. Dean, O.G. Penyazkov, K.L. Sevruk, B. Varatharajan; Heat and Mass Transfer Institute, National Academy of Sciences of Belarus* Ignition delay times were measured behind reflected shock waves at post-shock pressure of 10 atm for lean, stoichiometric, and rich Jet-A/Air mixtures (f = 0.5, 1, 2) within the temperature range of 1000 -1700 K. An empirical correlation for ignition delay has been derived based on the experimental data. The critical post-shock temperatures required for direct initiation of detonation in Jet-A/Air mixture were determined. The obtained data can be used directly for propulsion applications, verification of kinetic mechanisms, and for analysis of detonability limits and explosion hazards of Jet-A fuel.

1645 Acceleration of Shock-Induced Ignition in CH4/Air and CO/Air Mixtures Using Hydrogen Addition *E.L. Petersen, J.M. Hall, J. de Vries, A.R. Amadio, S.D. Smith, M.W. Crofton; University of Central Florida* Hydrogen addition to fuel/air mixtures is known to accelerate the ignition process. To obtain fundamental shockinduced ignition delay times of fuel/hydrogen mixtures at elevated pressures, a series of shock-tube experiments was performed using mixtures of methane/hydrogen and CO/hydrogen at an equivalence ratio of 0.5 in air. For the methane-based tests, pressures near 20 atm were studied; both mixtures (80/20 and 60/40 methane/hydrogen) exhibited markedly decreased ignition times relative to a puremethane fuel. Two CO/hydrogen fuel mixtures were tested (60/40 and 40/60 CO/hydrogen) at pressures near one atmosphere and temperatures between 900 and 1260 K. The CO-based mixtures were highly reactive and exhibited detonation behavior at the lower temperatures.

1710 Initiation of Detonations and Deflagrations by Shock Reflection and Focusing S.I. Jackson, P.M. Buraczewski, J.E. Shepherd; California Institute of Technology Detonation initiation by shock reflection and focusing involves propagating a shock wave into a concave wall. The shock reflection from the concave wall produces a high-energy focus region with temperatures and pressures in excess of those generated by shock reflection from a flat wall. The high-energy focus promotes the initiation of detonation and deflagration. Most previous research on

detonation initiation with focusing reflectors is concerned with hydrogen-oxygennitrogen mixtures. Less work is available for hydrocarbon-oxygen-nitrogen mixtures, in spite of their appeal to pulse detonation engine technology. Initiation requirements of propane-air mixtures are of particular interest since they have similar detonation properties to heavier hydrocarbon-air mixtures such as JP10- or JetA-air. In the current study, detonations and deflagrations were initiated by shock reflection from a parabolic end wall in a tube filled with stoichiometric fuel-oxygen mixtures diluted with nitrogen. Hydrogen, ethylene, and propane were used as fuels. The results determine the critical shock strength necessary to initiate detonations and deflagrations in hydrocarbon mixtures. Mixtures using hydrogen fuel are a baseline and relate these experiments to other studies. The data also provide a comparison to other types of wave focusing schemes used to initiate detonations, such as toroidal imploding detonations and shock waves.

1620 (14C) - Flames - Computation (Andy McIntosh)

1620 Computational and Experimental Study of Steady Two-Dimensional Axisymmetric Non-Premixed Methane Counterflow Flames G. Amantini, J.H. Frank, M.D. Smooke, A. Gomez; Yale University We investigated computationally and experimentally the structure of steady axisymmetric, laminar methane/enrichedair diffusion flames. Experimentally, the forward reaction rate (RR) of the reaction CO + OH -> CO2 + H was measured by simultaneous imaging of single-photon OH LIF and two-photon CO LIF. In addition, particle image velocimetry (PIV) was used to measure velocities in the proximity of the fuel and oxidizer nozzles, providing detailed boundary conditions for the simulations. Computationally, we implicitly solved the steady-state equations in a novel vorticity-velocity formulation on a nonstaggered, non-uniform grid. Furthermore, we compared the results from twodimensional simulations along the axis of symmetry with corresponding onedimensional simulations, and we showed consistency between the two sets of data. The comparison between the experimental and computational data vielded quantitative agreement for all the measured quantities, namely the CO number density, the OH LIF, the RR, and the velocity field. The decay rate of the stoichiometric scalar dissipation rate was found to be exponential in the radial direction. Additionally, various flame observables were correlated with the mixing layer thickness, and good correlation was found only between CO2, H2O, N2 layers, and the mixing layer thickness.

1645 **Confined Burke-Schumann Flames With Small Stoichiometric Mixture Fraction and Small Fuel Radius** *M. Sanchez-Sanz, A. Revuelta, A.L. Sanchez, A. Linan; Universidad Carlos III de Madrid* The Burke-Schumann limit of infinitely fast reaction rate is used to investigate flames formed when a fuel jet of very small radius discharges into a coaxial ducted air flow of radius a. When the boundary layer aproximation is used to describe the resulting flow, the solution is seen to depend on four parameters of order unity, namely, the dimensionless temperature increases, the global equivalence ratio, the inverse of the Froude number, and the Craya-Curtet number C, defined as the square root of the ratio of the momentum flux of the air stream to that of the fuel jet. Solutions are determined numerically for parametric ranges of interest for both uniform and developed coflow velocity profiles. The analysis shows how the appearance of a toroidal region of recirculating flow for values of C smaller than a critical value Cc readily promotes mixing of the two streams. The recirculating region is affected by the thermal expansion, an effect more pronounced for underventilated conditions, when the flame extends to the confining duct.

1710 Effect of Local Flame Stretch at the Tip of the Flame Propagating in a Vortex *M. Nishioka, T. Hokazono; University of Tsukuba* The phenomenon of highspeed flame propagation along the axis of a vortex tube of methane-air premixed gas was numerically simulated, and the effects of the local flame stretch at the flame tip on the local flame structure and the local burning velocity were investigated. The contribution of the flame curvature term in the flame stretch rate was also examined. As a result, it was found that the contribution of curvature is not as large in the steadily propagating period, and the extinction at the tip occurs suddenly as the stretch rate decreases. The latter fact suggests that there exists some strong unsteady effect causing extinction of this kind of the propagating flame.

Friday August 5

0940 (15A) - Detonation - High Explosive (Mark Short)

940 Simulation of Detonation of Aerated Ammonium Nitrate Based Emulsion Explosives A.Yu. Reshetnyak, A.E. Medvedev, V.M. Fomin; Institute of Theoretical and Applied Mechanics, RAS The mathematical model is constructed assuming that the bulk emulsion matrix is non-detonating, the detonation is associated with pores, and starts from their surface and propagates into a "zone of their influence" only. Thus, heat release behind the front of the leading shock wave is determined by the total heat release in the common reacting domain. Porosity, pore size, and the size of a "zone of influence" of a pore are used as the geometric parameters of the model. The physicochemical transformations accompanying detonation of emulsion explosives are a sequence of two kinetic processes: a rapid monomolecular decomposition of ammonium nitrate and a second-order reaction of oxidation of the combustible components of an emulsion explosive (oil) by the products formed in the decomposition of ammonium nitrate. Thus, the specific heat release is represented by the sum of the heat release from the two processes. The equation of state is an empirical function of porosity. The proposed model takes into account the basic features of the detonation of emulsion explosives and exhibits good agreement with the experimental data.

1005 **Thermodynamic Solution for Combustion of PETN/TNT Products with Air** *A.L. Kuhl, J.B. Bell; Lawrence Livermore National Laboratory* We consider the explosion of a 1-g spherical TNT charge in air in a 6.6-l calorimeter. The hot detonation products are rich in fuel, and when they mix with air, they release 2,500 cal/g (in addition to the 1,100 cal/g released by the detonation) by a non-premixed turbulent combustion process. Here we trace the evolution of this combustion process in Thermodynamic State Space—to elucidate the mechanisms that control this process. Mixing and combustion in a thermodynamically isolated chamber is constrained by the initial energy in the system. It establishes not only the initial state (temperature) of the reactants and the final state (temperature) of the products, but also the locus of combustion states in thermodynamic space. The most important contribution of this paper is that we show that the gas dynamic solution of this problem, when projected from physical space to thermodynamic space, rapidly approaches the combustion locus predicted by the Thermodynamic model—thereby demonstrating that the combustion locus is a strong attractor for this reactive system. This model is especially useful in cases where the kinetics of the system is not known.

1030 Numerical Studies of Detonation Diffraction Using the Ignition-and-Growth Model A.K. Kapila, D.W. Schwendeman; Rensselaer Polytechnic Institute The focus of this work is a detailed study of detonation diffraction in twodimensional (and axisymmetric) expanding geometries using the ignition-and-growth (IG) model of condensed-phase, heterogeneous explosives. The primary interest is to determine the effects of transverse disturbances introduced into the reaction zone by area changes. In order to perform this study, we compute well-resolved numerical solutions of the governing equations of the IG model in various expanding geometries. It is found that while a local failure of the detonation may occur due to a weakening of the leading shock, the weakly-shocked explosive reignites in due course. A fully fledged detonation reappears for all calculations performed, and there remain no sustained dead zones.

0940 (15B) - IC Engines II (Fabian Mauss)

940 **Pressure Diagnostics of HCCI Combustion Initiated by Pulsed Flame Jet** *K. Hotta, O. Moriue, E. Murase; Kyushu University* Homogeneous Charge Compression Ignition (HCCI) engines with lean fuel/air mixtures have a number of advantages over conventional spark ignition and compression ignition engines. The onset of the HCCI combustion depends on the autoignition of the fuel, so it is quite difficult to control the ignition timing. On the other hand, Pulsed Flame Jet (PFJ) has a great potential to enhance ignition reliability and burning rate in lean mixtures, and we have demonstrated that PFJ has a potential for controlling the start of HCCI combustion directly. In this paper, the technique of pressure diagnostics was used in HCCI combustion with and without ignition timing control by PFJ, and it was revealed that the HCCI combustion with ignition timing control by PFJ shows higher effective use of heat released by the reactions of fuel than that without ignition timing control by PFJ.

1005 Numerical Study of the Influence of Hot Spot Formation and EGR on Knock Occurrence in SI-Engines *M.A. Liberman, L.-E. Eriksson, M.F. Ivanov, D. Valiev; Uppsala University* We present results of multidimensional numerical study of the autoignition onset in an SI engine and compare the calculations with the experimental data. Numerical modeling is performed in scope of 2D and 3D simulation of the reactive Navier-Stokes equations, including the effects of viscosity, thermal conduction, molecular diffusion, and heat losses to the cylinder walls coupled with the chemical kinetic model. Detailed analysis of the calculated temperature and pressure fields has shown that the development of the autoignition is tightly connected to the formation of hot spots that evolved from the nonuniformities caused by pressure waves emitted by the propagating flame. The influence of EGR and stoichiometry is calculated using both 2D and 3D CFD coupled with a generalized Shell model. Validation of the developed model shows that the calculated dependence of the temperature and pressure on crank angle and predicted time of the autoignition onset for different engine operation conditions, in particular, for different percentage of EGR, are in good agreement with the experimental data.

1030 **Fuel Composition Influence on Auto-Ignition in 3D Engine Simulations** *S. Jay, O. Colin; IFP* With the developments of new internal combustion engines, the necessity to suitably model low temperature processes has led to approaches using complex chemistry in 3D CFD codes. In this work, we investigate the sensitivity of the auto-ignition process to the fuel detailed kinetics for different operating conditions. A mixture composed of 70% n-decane and 30% 1-methylnaphthalene is used to describe a practical complex Diesel fuel. Firstly, this model fuel is validated against basic experiments. Secondly, we propose a delay sensitivity analysis along different initial thermodynamic conditions by comparing the mixture with n-heptane. Then it is tested in 3D simulations. Comparisons between the different fuels in homogeneous configurations and in practical engine simulations show that little difference is expected in classical Diesel direct injection cases but that the accurate description of the chemical reactions becomes essential in homogeneous charge compression ignition conditions.

0940 (15C) - Turbulent Combustion III (Jerry Lee)

940 Numerical Control of 3D Turbulent Premixed Flame Simulations M.S. Day, J.B. Bell, J.F. Grcar, V.E. Beckner; Lawrence Berkeley National Laboratory We extend to three-dimensions a feedback control algorithm that was designed originally for two-dimensional flows. The algorithm automatically stabilizes a turbulent flame by dynamically adjusting the mean inflow velocity, and produces a statistically stationary, stable flame configuration for detailed statistical flame analysis. The flame simulations are based on a low Mach number formulation for a mixture of reacting gases using a mixture-averaged model for differential species diffusion. The chemical kinetics are evaluated using the GRI-Mech 3.0 without nitrogen chemistry. The numerical discretization combines a symmetric operatorsplit coupling of chemistry and diffusion processes with a density-weighted approximate projection method to evolve the constrained advection. The discretization is embedded in a parallel block-structured adaptive grid framework which is used to concentrate grid resolution around the flame and regions of high vorticity. We demonstrate the performance of the control algorithm and show details of a representative controlled 3D flame.

1005 **Characteristics of Flow Field and Flame Propagation in a Vortex Ring** *K. Asato, A. Ogura, Y. Doi; Gifu University* The characteristics of flow field and flame propagation in a vortex ring were investigated. The flow field and the flame speed in the vortex ring were measured using PIV and a high-speed video camera. The method of obtaining the moving velocity of the vortex ring from the PIV images was proposed. The profile of the rotating velocity is in good agreement with that of Burger's vortex. The relationship between the moving velocity and the maximum rotating velocity can be predicted by the theoretical equation of Tung and Ting. The models of flame propagation in the vortex tube proposed previously cannot predict accurately the flame speed in the cases in which the maximum rotating velocity becomes large and the mixture is lean.

1030 Investigations on the Flamelet Inner Structure of Turbulent Premixed Flames F. Halter, C. Chauveau, I. Gokalp; CNRS Orléans Interactions between flame and turbulence are of primary importance to understand the combustion mechanisms in all practical combustion systems. Planar Rayleigh scattering measurements were performed to investigate the inner structure of flamelets in premixed turbulent Bunsen flames. Pressure was varied from 0.3 to 0.9 MPa for two equivalence ratios (0.6 and 0.7). Local information regarding the thickness and the curvature of the flamelets was obtained. PDFs of flame front thickness were constructed. Contrary to the laminar case, the mean thermal thickness of the flamelet is almost the same when the pressure is increased from 0.3 to 0.9 MPa. Concerning the impact of the equivalence ratio, the results are in accordance with laminar flame computations. We also investigated the impact of curvature on the flame front thickness. The curvature has the same effect on the flame front thickness when the mixture is the same, whatever the pressure. However, when we change the equivalence ratio, the impact of curvature on the flame front thickness is different. The dependence of the flamelet thickness to curvature is decreased when the equivalence ratio is increased from 0.6 to 0.7.

1055 (3PO) - **Poster III - Explosion** (Charles Kiyanda)

1055 (B) - Break

1145 (16A) - **Deflagration-to-Detonation Transition I** (Gaby Ciccarelli)

1145 Examination of the DDT Triggering in an Obstructed Tube S. Medvedev, S. Khomik, H. Olivier, B. Gelfand; Institute of Chemical Physics, RAS The process of deflagration-to-detonation transition (DDT) in gaseous mixtures of hydrogen-air and hydrogen-hydrocarbon-air was studied in the obstacle-filled 141-mm diameter detonation tube. The investigation considers what parameters of accelerating shockflame structures are relevant to the conditions of detonation triggering. The analysis was performed on the basis of pressure and flame position measurements. The conditions of self-ignition due to the reflection of a leading shock wave at the orifice ring obstacle were investigated on the basis of calculations of the induction time. Representation of the DDT/no DDT boundary in terms of the criterion of Thomas et al. (2002) and shock-flame separation distance allows to draw a line between two different modes of detonation onset. Direct initiation of detonation is associated with the reflection of a sufficiently intensive leading shock. In this case, the accelerating flame plays an auxiliary role and it simply acts as a piston supporting a shock wave. Another mode of detonation onset is observed for a weaker shock that is not capable of initiating detonation directly. In this case, DDT is caused by the reflected shockflame interaction that produces a high distortion of the flame front, and detonation is initiated in a turbulent flame brush.

1210 **Effect of Boundary Layer on Flame Acceleration and DDT** *M. Kuznetsov, I. Matsukov, V. Alekseev, W. Breitung, S. Dorofeev; FM Global* The evolution of the boundary layer ahead of accelerated flames in a relatively smooth channel and its role in the onset of detonations was studied using high speed shadow photography.

Stoichiometric hydrogen-oxygen mixtures at the initial pressures from 0.2 to 0.75 bar were used. The average visible thickness of the boundary layer at flame positions was found to be somewhat lower than the theoretical model (Kuznetsov, 2003). The data scattered in the tests due to variations of the detailed history of the flame acceleration for the same initial conditions. It was found that the model, as intended, gives a rather good estimate for the upper bound for the boundary layer thickness observed in the tests. The run-up distances appeared to be in agreement with the theoretical model, with the exception of the tests with the initial pressure of 0.2 bar, where the reflected shock wave affected the process of FA. The photos of the onset of detonations showed that detonations originated near the tube wall at a distance from the wall, which is close to the thickness of the boundary layer.

1235 DDT Properties of Hydrocarbon-Air Mixtures with Additive of Acetylene K. Ishii, T. Takada, T. Akiyoshi, M. Murayama; Yokohama National University In the present work, the DDT process of hydrocarbon-air mixtures with an additive of acetylene was experimentally studied to reveal the controlling parameters of the DDT process. The detonation tube has a total length of about 7 m and an inner diameter of 50 mm. The base mixture is a methane-air or a propane-air mixture to which acetylene is added to stimulate the detonability of the mixtures. The volumetric percentage of acetylene in the binary-fuel ranges from 0% to 100% under the condition that a total equivalence ratio of 1.0 is kept constant. To enhance the initial development from laminar to turbulent flame, a Shchelkin spiral with a length of 1.0 m or of 1.5 m was inserted into the detonation tube. The experimental results show that the initial deflagration speed increases monotonically with the volumetric percentage of acetylene for both of the base mixtures. While propane-air mixtures with the addition of 20 % or more acetylene shows DDT within 2 m from the ignition point. Methane-air mixtures show longer DDT distances or no detonation transition under the same volumetric percentage of acetylene.

1145 (16B) - **Dust Explosion** (Fan Zhang)

1145 **Flame Propagation Through Cornstarch Dust-Air Mixtures in a Vertical Duct** *S. Wang, Y. Pu, F. Jia, S. Wan; National Microgravity Laboratory, Institute of Mechanics, CAS* The flame propagation through cornstarch dust-air mixtures has been investigated in a vertical duct. The experimental apparatuses were designed based on an improved dust dispersion mechanism that could generate a uniform and repeatable dust cloud. At the same time, the turbulence level induced by the dispersion process is much lower than those obtained with previous dispersion systems. Upward propagating dust flames were recorded by a high-speed video camera. According to the ignition delay time, two kinds of flames were observed in the present study: laminar and oscillating flame, and turbulent flame. The flame speeds were measured during the propagation process.

1210 **Dust Lifting Up Process From the Layer in Slow Air Flow** *R. Klemens, P. Zydak; Warsaw University of Technology* The aim of the research was to investigate the dust lifting up process from a layer in a slow air flow. This research is closely related to the flame propagation problem in channels where the dust is not premixed with air but is deposited in the form of a layer. Most of the investigations done in this field were devoted to the problem of dust dispersion from a layer behind a

propagating shock wave. The aim of the conducted research is to extend the experiments to slow gas flows. The experiments were carried out in a tube of internal cross section 72x112 mm2 and 3,5 m long. The air flow velocity generated by the centrifugal fan was about 29 m/s. Four different dusts were chosen and three kinds of dust layer thickness were used in the experiments.

1235 Influence of Suspension Generation on Dust Explosion Parameters O. Bozier, B. Veyssiere; Laboratoire de Combustion et de Détonique, ENSMA Combustion mechanisms of a suspension of solid particles in a gaseous mixture are studied with the aim of correlating the constant volume explosion characteristics with the initial state of the suspension at ignition time. Two vessels have been specially designed for this study, with similar geometrical characteristics (cylindrical chamber, volume 20 l, L = 500 mm, D = 230 mm, and L/D \approx 2,2). The first one is completely transparent with an octagonal cross section, allowing visualization of the dispersion process in all directions. The second one is made of steel and can support 50 bar overpressures to measure the characteristics of combustion at constant volume. Particle dispersion in the chamber is achieved by means of the turbulent flow created by the discharge of pressurized air. Experiments were made with cornstarch particle suspensions. Evolution of the flowfield and dust distribution inside the chamber were recorded with high-speed imaging, LDV and PIV. The required delay to obtain an optimal mixture (minimum velocity and turbulence intensity, quasi-homogeneous concentration) is between 500 and 700ms. For stoichiometric dust-air mixtures, explosion characteristics are in satisfactory agreement with results obtained by other researchers. Theses values decrease with the initial turbulent intensity.

1145 (16C) - Catalytic Combustion (Dave Frost)

1145 **Development of a Catalytic Hydrogen Micro-propulsion System** *Y.-C. Chao, G.-B. Chen, C.-Y. Wu, C.-P. Chen; National Cheng Kung University* In this study, a platinum catalytic tube of inner diameter 500µm and length 1 cm is used as the reactor and placed inside a quartz casing with a convergent nozzle made of quartz for ease of observation. The effects of fuel/air flow rate, equivalence ratio, and nozzle contraction ratio on the thruster performance are investigated both experimentally and numerically. The results show that the maximum thrust measured is 6.8 mN and the Isp is 70 s for the hydrogen/air cases, and a much higher Isp can be reached if oxygen is used instead of air. The output of the micro-propulsion system is amply to be used in attitude control for a nano-satellite or a micro-satellite.

1210 Studies of Slip Effects on Fuel Oxidation in Microscale Catalytic Reactors *B. Xu, Y. Ju; Princeton University* In this work, the coupling between the surface catalytic reactions and the homogeneous gas phase reactions in a microscale catalytic channel is investigated. Three different types of nonequilibrium effects (temperature, velocity, and species slips) are considered at the catalytic surface. The results show that the rarefied gas effect significantly reduces the momentum, heat, and mass transfer near the wall, and thus decreases the surface reaction rate. Furthermore, it is shown that the slip effects can dramatically change some radical distributions, which will yield a strong coupling between the gas phase reaction and catalytic surface reaction in microscale reactors. It also shows that the temperature jump has an opposite effect when the gas temperature is higher or lower than the wall

temperature. Finally, there is a nonlinear distribution of surface reaction rates near the entrance of the microchannel resulting from the slip effects. Also, the surface reaction rates of major species can be reduced by the slip effects.

1235 **Burn Rate Sensitization of Solid Propellants Using a Nano-Titania** *J.L. Small, M.A. Stephens, S. Deshpande, E.L. Petersen, S. Seal; University of Central Florida* Composite solid propellant based on an Aluminum/Ammonium Perchlorate/HTPB mixture was prepared with and without the addition of titania nanoparticles. The nano-sized titania with average diameters on the order of 10 nm were manufactured using a sol-gel technique. The resulting solution was added to the other propellant ingredients, and the liquid solvent was removed by vaporization under a vacuum. This process allowed the particles to remain in intimate contact with the other ingredients, and the mass of the titania was 0.4% of the total propellant mass. After curing, samples of the propellant grain were burned in a high-pressure strand burner at pressures ranging from 43 to 250 atm. The mixture samples with the nano-titania additive produced burning rates that were nearly a factor of ten higher than the baseline mixture without nano-titania.

1300 (L) - Lunch

1440 (17A) - Flame Acceleration I (Nabiha Chaumeix)

1440 **Control of Flame Transmission from a Vessel to a Discharge Duct** *N. Henneton, B. Ponizy, B. Veyssiere; ENSMA Poitiers* A solution allowing quiet evacuation of gases in a vented explosion propagating from a vessel into a discharge duct has been studied. It consists of placing a wire-net insert at the duct entrance in order to delay flame penetration into the duct and prevent the occurrence of a secondary explosion. Experimental results demonstrate that the important pressure rise in the vessel is due to the turbulent combustion of pockets of unburned gases which are "trapped" in corners of the vessel near the duct entrance. Addition of the insert promotes slow combustion of these trapped gases, preventing the re-increase of the vessel pressure. The effect of the insert is studied by a numerical model,based on the "nodal method". The insert is treated as only a heat absorber, and its influence on the mixing process between fresh and burnt gases is not considered. Parametric study of the influence of the heat transfer coefficient h, indicates that an adequate insert is able to decrease the temperature of burnt gases to values for which flame extinction may occur.

1505 **Tube Diameter Effect on Deflagration-to-Detonation Transition of Propane-Oxygen Mixtures** *J.-M. Li, K.-M. Chung, W.-H. Lai; National Cheng Kung University* In the present study, single shot experiments were carried out with the propane-oxygen mixtures in a smooth tube. The Deflagration-to-Detonation Transition run-up distance is determined with varying equivalence ratio in three tube diameters (1, 2, 6 inches). The overdriven state of the detonation is evaluated, which is the key parameter for successful detonation diffraction. The dependence of the degree of overdriven detonation on the distance from the transition location through the DDT process was also addressed. The results show that the effect of the tube diameter on the run-up distance may depend on the mixture compositions. Overdriven detonation is observed and is decayed to the C-J state within a few tube

diameters.

1530 **Simulation and Analysis of Accelerating Flames in Tubes** *C.R.L. Bauwens, L. Bauwens, I. Wierzba; University of Calgary* A multiple time scale model is presented for the one-dimensional flow and acoustics in a tube filled with a reactive mixture, open at one end and closed at the other end, where ignition takes place. Results of that model and from numerical simulation are compared, showing a reasonably good agreement. The front oscillates and occasionally reverses its direction of propagation as it moves along the tube, although not as much as in the experiments. It is clear that a significant part of the physics of flame acceleration in tubes is multidimensional. However, the results show that it is the acoustics impulsively set in motion by ignition, which push the unburnt toward the open end, that trigger the oscillation. The key aspect still missing is the Rayleigh-Taylor instability of the front due to the acoustic acceleration. That phenomenon is inherently multidimensional and strongly nonlinear. As such, it is not amenable to simple analysis.

1440 (17B) - Explosion Hazards (Allen Kuhl)

1440 Effectiveness of Protective Covers in Case of a Detonation Wave Reflection S. Medvedev, S. Khomik, H. Olivier, B. Gelfand; Institute of Chemical Physics, RAS The investigation of interaction of a detonation wave with a rigid wall covered by porous materials was performed in the 141 mm diameter detonation tube. The porous materials consisting of compressed steel wool and metal rubber were placed onto the rigid surface (endflange) equipped with a pressure transducer. The incident detonation wave was initiated in a 30% hydrogen in air mixture at an initial pressure of 1 bar. The experiments revealed a strong dependence of the maximum overpressure (measured in the substrate) on the layer thickness. There exists a proper value of depth of the layer at which the peak overpressure attains a maximum value. This value can be three to four times higher than the maximum overpressure in the case of an uncovered surface. Therefore, depending on the covering thickness the loading can be both enhanced and weakening. It was shown that a more dense covering material is more effective for the purposes of detonation loading mitigation.

1505 **Flame Quenching Performance of Ceramic Foam** *H.I. Joo, G. Ciccarelli; Queen's University* For most industries that have vents, pipes, or ducting where flammable mixtures may be present, flame arresters are typically used to prevent flame propagation in the event of ignition. Different types of materials are used in flame arresting devices, for example, wire gauze and sintered metal is commonly used in commercial flame arresters. Ceramic "foam" represents a novel material that can be used for flame arrester applications for which there is no quenching data in the literature. The interconnectivity of the pores in the foam form a matrix of tortuous and narrow passageways that the flame is forced to pass through, where flame extinction can occur. The objective of this paper is to present experimental data on the flame quenching effectiveness of ceramic alumina foam with different pore densities. The quenching performance of the foam will be compared to that of arresters consisting of packed spheres and narrow tubes.

1530 Direct Numerical Simulation on Hydrogen Fuel Jetting from High

Pressure Tank *Y.-F. Liu, N. Tsuboi, H. Sato, F. Higashino, A.K. Hayashi; Aoyama Gakuin University and Institute of Space and Astronautical Science* In this paper, the behavior of a hydrogen jet coming from a 40Mpa high pressure tank is directly simulated by using two-dimensional Euler equations and full chemical mechanisms. The very strong jet wave creates a chemical reaction of hydrogen and oxygen at the very beginning of the contact surface. This reaction, in turn, increases the temperature, and the maximum temperature at the contact surface is 3000K. The chemical reaction has very little influence on the propagation of the jet shock wave. As the jet propagates away from the tank, its strength decreases and the chemical reaction at the contact surface finally ceases.

1440 (17C) - Multiphase Combustion (Joe Shepherd)

1440 Combustion of Bulk Metals in Supersonic Flow R. El-Saadi, V. Tanguay, A.J. Higgins: McGill University The combustion of reactive metals (aluminum. magnesium, titanium, and zirconium) in a supersonic flow of shock-heated oxygen is investigated. The material samples are cylinders of sufficiently large size (1-3 mm diameter) that the interior of the samples remain cool for the duration of the experiment. The flow of oxygen is accelerated by a strong shock wave driven by the detonation of an explosive charge at one end of a 1.2-m-long tube filled with oxygen; the samples were located at the other end of the tube. The shock Mach number ranged from Mach 5 to 9, generating supersonic (M > 2) flows with static temperatures of 1500 K to 3600 K. Intense surface luminosity was observed on the zirconium and titanium samples for even the weakest shock waves generated. Aluminum and magnesium were seen to be less reactive, requiring a stronger shock before the onset of reaction. The mass of material removed from the samples by reaction with the oxidizer was measured as a function of shock strength. The luminosity and mass removal were shown to be combustion (as opposed to conventional ablation) by performing a control experiment with pure nitrogen, in which no mass removal or luminosity was observed on the sample surfaces.

1505 **Reaction of Metal Particles in Gas-Phase Detonation Products** *V. Tanguay, S. Goroshin, A. Higgins, A. Yoshinaka, F. Zhang; McGill University* The reaction of metal (aluminum, zirconium, etc.) particles in gaseous detonation products is investigated. Using a detonation wave reflected from a detonation tube end wall, it is possible to expose particles to extremely large, transient convective transfer similar to that experienced by particles in condensed phase detonation. Reaction of the particles is observed via a window mounted in the end flange, permitting luminosity from the particles to pass into a fast photomultiplier which is filtered to observe the strong AlO band of aluminum oxidation. The results fail to show any correlation in the onset of reaction times to particle size. Intense luminosity is associated with the reflected shock re-crossing the cloud of particles. These results suggest that the particles react in a kinetic regime where there is no significant departure from the surrounding gas temperature.

1530 **Reduction of DDT Run-Up Distance in a Two-Phase Flow by Combined Means** S. M. Frolov, V. S. Aksenov, V. Ya. Basevich; Semenov Institute of Chemical *Physics, RAS* In view of the growing interest in the application of detonation to propulsion and power engineering, the studies of DDT enhancement in liquid-fuel drop suspensions in air are getting increasingly important. The objective of this paper is the reduction of DDT run-up distance in fuel drop suspensions by various combined means, including discharge chambers, Shchelkin spirals, transition cones, and a new element - tube coil. The tube coil introduces expansive and compressive surfaces to the propagating shock wave leading to gasdynamic "focusing" phenomena and promotion of the detonation onset. As a result of replacing a straight, smooth-walled 51-millimeter diameter tube by a 28-millimeter tube with a Shchelkin spiral, tube coil, and transition cone to the 51-millimeter tube, the initiation energy of spray n-hexane–air and n-heptane–air detonations was reduced by two orders of magnitude, i.e., from 3300 to 30 J, with the DDT run-up distance of about 1 m.

1555 (B) - Break

1620 (18A) - Flame Acceleration II (Daniel Desbordes)

1620 **Flame Acceleration and Detonation Transition in Narrow Tubes** *E.S. Oran, V.N. Gamezo; Naval Research Laboratory* The work described here arose from the confluence of two studies: one on micropropulsion for microgravity environments and another on fundamental mechanisms of deflagration-to-detonation transition. Here we present selected results of numerical simulations of flame acceleration in narrow tubes from the micropropulsion point of view. We show how, under appropriate conditions, an accelerating laminar flame in a small channel can produce significant thrust and eventually undergo a transition to detonation.

1645 Hydrodynamic Instability as a Mechanism for Deflagration-to-Detonation **Transition** M.A. Liberman, G.I. Sivashinsky, D.M. Valiev, L.-E. Eriksson; Uppsala University The purpose of the present study is to gain a better insight into the identification of the basic mechanisms controlling the spontaneous transition from deflagrative to detonative combustion. To visualize the spatial picture of the transition, a wave of premixed gas combustion spreading from the closed to the open end of a smooth-walled rectangular channel is studied by direct numerical simulation of the two-dimensional Navier-Stokes equations for a compressible reactive flow with a simplified chemical model based on single-step Arrhenius kinetics. It is, for the first time, shown that, in sufficiently wide channels subjected to free-slip and adiabatic boundary conditions, the classical Darrieus-Landau instability may bring on interaction of emitted and reflected shocks capable of nucleation of hot spots, ahead or within the folds of the corrugated flame, triggering an explosive transition from deflagration to detonation. The effect is found to be sensitive to the flame's incipient speed, the reaction rate temperature- and pressure-dependences, favoring fast flames, high activation energies, and high order reactions.

1710 **H2 Gradient Effect on Premixed Flame Propagation in a Vertical Facility: ENACCEF** *N. Lamoureux, F. Malet, N. Djebaili-Chaumeix, A. Bentaib, A. Bleyer, C.E. Paillard; CNRS - LCSR* The present work aims at providing an experimental database on flame acceleration of lean H2/air-based mixtures characterized by a hydrogen gradient. The experimental work is completed by computations using the TONUS CFD code (Rivière et al. 2004). The H2 gradient establishment is controlled using GC gas sampling analysis, and the results are compared to the modelling. Finally, the flame speed measurements in the nonuniform

mixtures are compared to those for uniform mixtures. The main results of this work are: (i) a flame of lean H2/ air , is greater than σ can be strongly accelerated if the expansion ratio, 3.75; (ii) the comparison between a flame propagating in a mixture with a negative H2 gradient and a homogeneous one showed that the maximum velocity achieved by the flame is the same although it behaves differently once in the dome; (iii) in the case of a positive gradient, the maximum flame velocity is lower than the one obtained in the homogeneous case with a hydrogen concentration corresponding to the average one. The H2 gradient effect will be discussed in the final paper.

1620 (18B) - Explosions II (Andrzej Teodorczyk)

1620 Water-Mist Mitigation of Quasi-Static Pressure Buildup in Enclosures Subjected to an Explosion D.A. Schwer, K. Kailasanath; Naval Research Lab With water-mist systems being implemented in the machinery spaces of LPD-17 and DD(x) for fire suppression, there is considerable interest in the possibility of using them in a dual-role function both for blast mitigation and fire suppression. The present research attempts to obtain a more accurate understanding of the interaction between water mists and the flow-field generated by a blast wave, and to assess the mitigation capability with water-mist systems. Unsteady, multi-dimensional, multiphase simulations were done to help study the effect of water-mist on spherically expanding blast waves and quasi-static pressure rise in enclosures subjected to blasts from explosives. The simulations found that for the configurations studied, suppression of the secondary reactions were minimal due to the water-mist being pushed towards the outer walls and the secondary reactions remaining in the interior domain. Even though suppression of the reactions was limited, overall reduction in the overpressure was found to be very good. This reduction is accomplished mainly through energy extraction from vaporization. These results are dependent on several variables, including explosive size and type, enclosure size, water-mist droplet size and mass-loading, and current simulations are attempting to understand the relationship between these different parameters.

1645 Influence of the Chamber Volume on the Rich Explosion Limit for Hexane-Air Mixtures M. Gieras, M. Kaluzny, R. Klemens, A. Kuhl, P. Oleszczak, W. Trzcinskio, P. Wolanski; Warsaw Univerity of Technology The purpose of this research was to obtain fundamental hexane vapor-air and hexane droplets-air explosibility parameters by measuring the explosion pressure variation in closed chambers of volume 5.6 dm3, 40 dm3, 150 dm3, and 1250 dm3. The influence of hexane vapor initial temperature and droplet diameter on the explosion process was also investigated. The ignition source was a single electrical spark discharge of 5 J energy or a chemical igniter of 2 kJ energy. It was found that the rich explosion limit for hexane droplets – air mixture is in the range of 1.8 to 5.5 kg/m3 and is about 30 to 40 times higher than the stoichiometric concentration and three to nine times higher than the one for hexane vapor-air mixtures. It was stated that the rich explosion limit increases along with an increase of the droplet mean diameter as well as the chamber size. For hexane vapor-air mixtures, the most significant effect on the rich explosion limit is from ignition energy. It was found that the rich explosion limit in this case, determined in a 5.6 dm3 chamber with a temperature of 363 K, for 5 J electric spark ignition is equal to 0.275 [kg hexane/kg air]. Using the chemical igniter of 2 kJ energy causes an increase of the rich explosion limit to the value of 0.5 [kg hexane/kg air].

1710 Plasma-Assisted Combustion of Propane-Air and Methane-Air Mixtures. Kinetics of Flame Acceleration *E.I. Mintoussov, A.V. Krasnochub, A.Yu. Starikovskii; Moscow Institute of Physics and Technology* The study of the nanosecond barrier discharge influence on flame propagation and flame blow-off velocity was carried out. With energy input negligible in comparison with the burner's chemical power, a double flame blow-off velocity increase was obtained. The present paper shows that, besides the proper form of energy input, proper organization of the discharge is of great importance. It was found that active particles (O and OH primarily), which are produced in the streamer head under its action, play the most significant role in the effect of combustion acceleration. The model of flame acceleration, suggested in the previous work, was confirmed by the new experimental data.

1620 (18C) - IC Engines III (Stephane Jay)

1620 A Study of Injection and Mixing of Gaseous Jets for Direct Injection M. Sutkowski, A. Teodorczyk, C. Xia, A. Sobiesiak; University of Windsor Mixture preparation in engines occurs through the interaction of two turbulent flows, a gaseous fuel jet, and combustion air flow. Questions arise regarding how the gaseous fuel injection characteristics and transient cylinder turbulence interact and affect the mixing of air and fuel, and what will be the optimal turbulence intensities and scales, within both flows, to satisfy the varying requirements for air-fuel mixture homogeneity at different engine operating conditions. In order to provide some answers to these questions, a project has been set-up to investigate the mixing and combustion processes of a directly injected jet of natural gas into a combustion chamber of fixed volume with controlled levels of nearly uniform turbulence. Concurrently, a computational fluid dynamics (CFD) modeling of the same processes was undertaken. The overall objective is to find optimal turbulence intensity and iet characteristics to satisfy the varying requirements of the fuel-air mixture for the various operating conditions of the engine. In the present study, the processes of fuel injection and flammable mixture formation were examined through physical experimentation and numerical simulation for methane and hydrogen jets spreading into air.

1645 **Analysis of an Extended Ionization Equilibrium in the Post-Flame Gases** *A. Ahmedi, F. Mauss, B. Sunden; Lund University* A zero-dimensional model that provides an engine- or reactor-like environment in which the engine simulations allow for a variable system volume and heat transfer both to and from the system has been used [3]. Equilibrium assumptions have been adopted for the modeling of the thermal ionization, in which Saha's equation was derived for single ionized molecules. The investigation is focused on the thermal ionization and electron attachment of six chemical species. The equilibrium calculation using Saha's equation is performed in a post process using the temperature and pressure history from model calculations. Existing models for the ionization current assume nitric oxide as the main electron donor in the post-flame gases [1, 8, and 9]. This is reasonable as long as NO is the species with the lowest ionization energy in the burned gas composition, and electron attachment does not influence the electron concentration. However, it has been shown before that the inclusion of alkali metals found in the environmental air have a strong influence on the calculation of ionization current. Alkali metals are present in the atmosphere at a concentration of approximately 200 [ng/m3]. In this contribution, we investigate the influence of electron attachment reactions on the calculated ionization current.

1710 Spark Plug and Corona Abilities to Ignite Lean Methane/Air Mixtures M. Bellenoue, S. Labuda, B. Ruttun, J. Sotton; LCD Futuroscope Spark plugs and pulsed coronas have been used for ignition of quiescent extremely lean fuel methane/air mixtures of equivalence ratio 0.55 and 0.517. Ignition ability and energetic efficiency have been analysed for these ignition systems at the same geometry of the electrodes and the discharge gap. Schlieren visualization of corona ignition allows registration mixture decomposition in the discharge. There probably is a spot ignition at this stage. The gas area modified by the discharge acts as an electrical conductive channel for the development of a streamer (or low current spark) passing the discharge gap and igniting the combustible mixture similar to a conventional spark. The advantage of corona ignition over spark plug ignition becomes more clearly apparent in the tests when a CH4/air mixture of equivalence ratio 0.517 has been used. In this mixture, spark plug ignition doesn't allow combustion in the entire volume of the combustion chamber; ignition occurs around the spark gap and then the flame is guenched. The use of a corona allows the ignition of this extremely lean fuel mixture and flame propagation through the combustion chamber at much less discharge energy (25-30 times). It is also shown that corona discharge ignition promotes the combustion due to generation of intensive turbulent flow around the discharge electrodes.

1735 (F) - Farewell

Poster I: Flame - 1055 Monday August 1

Structure of Flame Front of Hydrogen Jet Combustion in a Supersonic Air Stream U.K. Zhapbasbayev, Z.A. Mansurov; Al-Faraby Kazakh National University Study of the structure of combustion zones at great change of airflow temperature is of great interest. We show numerical results of the distribution of OH hydroxyl concentration at braking temperature change from 1850K up to 2600K. The ignition leads to the hydrogen jet mixing with airflow, producing a homogeneous reacting mixture, which does not ignite due to the low temperature of the hydrogen jet. As a result of mixing of the cold jet with the hot flow, the temperature of the hydrogen-air mixture increases up to 900K thus providing kinetic conditions for reacting mixture ignition. The flame-front has a complex configuration. The homogeneous reacting mixture fully burns out in the internal part of the front. The outside flame front is in the mixing layer and shows the diffusion character of the interaction between the fuel jet and the oxidizer flow. The form of the flame front is determined by the effect of disturbance waves. In rarefaction zones, the mixture accelerates and, in the compression zones, it becomes slower. The diffusion flame front has a cellular structure in accordance with the wave structure of the flow. The diffusion flame front has finite thickness; the zone of the chain reactions is not

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localized on a thin surface. The OH hydroxyl concentration has maximal value in the combustion zone.

The Combustion Characteristics for CO-CH4 Blended Fuels *Y.-C. Chao, C.-Y. Wu, C.-H. Tien, G.-B. Chen, C.-P. Chen; National Cheng Kung University* The combustion characteristics of artificially blended CO-CH4 mixtures are experimental and numerically studied in the present study. The simulations included the use of PREMIX and SPIN ChemKin packages accompanied by GRI 3.0 mechanisms for burning velocity estimation and simulation of 1-D flame spatial distribution, respectively. The results show that the burning velocity of mixtures reaches its maximum value, which is higher than the maximum burning velocity of CH4 or CO, at about 10 - 20 percent of CH4 in CO-CH4 mixtures. Results also show that the concentration of CH4 alters the reaction process, reaction rate, and flame structures.

The Structure of Highly Impinging Flames on a Rotating Cylinder C. Stroud. M.C. Branch, M. Strobel, M. Ulsh; University of Colorado at Boulder Flame treatment of polymer films involves exposing one side of a thin film to a laminar, premixed flame while cooling the opposite side with a ceramic-coated metal roller. The flame treatment results in an increase in the wettability of the surface through surface oxidation and can also make it possible to more readily perforate the film to produce film porosity. The results described in the present study focus on the role of fluid mechanics in the flame treatment process to provide a more coherent understanding of the optimum flame treatment conditions and to explain a number of anomalies that can occur. The research utilized two techniques to characterize the thermal and flow environments created in the flame treatment zone. The first technique was color schlieren imaging to visually describe the thermal gradients generated in the flame treatment zone. The second technique was temperature measurements throughout the flame environment to generate a three dimensional thermal image. These results enabled thermal and flow regime characterizations to be made for the range of experimental conditions and have been used to improve the speed of the treatment process and the uniformity of treatment.

Characteristics of Combustion of Rich-Lean Flame Burner Under Low-Load Combustion *S. Kurachi, S. Hagi, Y. Umeda, S. Mochizuki, K. Asato; Toho Gas Co., Ltd.* Development of a burner used in the domestic hot water generator with high efficiency under low-load combustion will be needed. We investigate characteristics of combustion of the conventional type of rich-lean flame burner used in the domestic hot water generator, and we propose a new type of rich-lean flame burner with high efficiency under low-load combustion. By supplying air to the boundary between the rich and lean flames, the temperature of the burned gas and the burner plate can be lowered. Even under a burner load fraction of 1/5.5 which is out of the operating range of the conventional type of burner, the burner plate temperature can be lowered below 200 . The formation of NOx in the lean flame zone is suppressed by decreasing the flame temperature, and CO generated in the rich flame zone also decreased due to improving imperfect combustion in the rich flame zone.

Experimental Observation of Different Stabilisation Regimes of Laminar Partially Premixed Flames C. Lacour, D. Honore, A. Boukhalfa, S. Carpentier, P. Meunier; CORIA - CNRS UMR6614 - INSA de Rouen Most of the domestic gas burners, such as ovens, cooking stoves, or boilers generate laminar partiallypremixed flames. Designers of gas cooking burners intend to create better performing appliances. Nevertheless, the lack of understanding of the physical phenomena involved has limited burner innovation. The aim of this study is to point out the physical phenomena responsible for partially premixed flame stabilisation of the domestic cooking gas burner. Partially premixed flames generated by a twodimensional domestic slot burner are studied. The global operating ranges have been established first and the stability limits have been defined. The flame structure has been analysed by means of OH PLIF experiments. Several combustion parameters have been modified to analyse their effects on the flame structure evolution to blowout. The bottom flame base is strongly lifted-off and the distance between the flame and the burner has been determined. The bottom edge flame position has a transition point, linked to heat exchange between the flame and the burner body. This transition corresponds to a change in the physical phenomenon leading to flame stabilisation.

Flame Stretch Rate of Laminar Flame Base Just Before Flashback at Different Burner Temperatures S. Sogo, S. Yuasa; Urban Life Research Institute, Tokyo Gas Co., Ltd., Flashback is generally attributed to the mechanism where the laminar flame propagates upstream in boundary layers when its normal velocity exceeds the local flow velocity. It is well known that increasing the burner temperature makes flashback easy to occur. At a flame base, however, the phenomenon becomes complicated because the local burning velocity is modified by the heat flux to the burner, the ambient air dilution, and the flame stretch effect. It is especially very important that all effects on flashback become clear. We measured the velocity distribution by PIV and the temperature profiles in the vicinity of the burner rim at a different burner temperature for the lean methane/air flame. The flame stretch rate was estimated by the experimental results at the flame base. The effects of flame stretch rate, heat flux to the burner, and diffusivity of the deficient reactant become clear at the flame base just before flashback. Results show that these factors have inhibitory effects on flashback for a higher burner temperature than a lower burner temperature.

Infrared Measurement of Soot Particles in a Burner Flame *K. Ishii, T. Tsuboi, K. Takashi, Y. Suzukawa; Yokohama National University* In the present work, optical measurement which is usually used in laboratory-scale experiments was applied to an industrial test burner to confirm the effectiveness of the measurement method as the first step to this goal. The measurement system was composed of thermography, multi-channel infrared spectral analysis of soot radiation, and the laser extinction method. An industrial test burner used in the present work has a cross-section of 800 mm x 800 mm and its total length is about 3300 mm. As for fuel, heavy-oil was supplied to a single-hole-nozzle placed at the burner tile. The experimental results show that the optically obtained temperature of soot particles is reasonable as compared to temperature measured with thermocouples suspended in the burner. The value of the optical thickness of the soot particles agrees well with that obtained from the combination of a narrow-band filter and a thermographic camera. Laser extinction measurement had difficulty in obtaining meaningful data, since a relatively long optical path is sensitive to temperature gradients in the burner.

Gas-Expansion Influence on Turbulent-Flame Propagation R.C. Aldredge;

University of California, Davis It is shown in the present work that the turbulentflame speed varies inversely with a power of the temperature ratio across the flame when the temperature ratio is large. This power is a function of the ratio of the integral length scale to the Taylor microscale, characterizing an initially isotropic excitation turbulence through which the flame propagates. Variations in turbulence kinetic energies and vorticity across the flame and in hydrodynamic zones upstream and downstream from the flame are evaluated also.

Burning Liquid Fuel Films from Flat Plates *Y.-H. Li, D. Dunn-Rankin, Y.-C. Chao; University of California, Irvine* This paper describes an experimental study of liquid fuel films burning off of a flat plate in a laminar flow wind tunnel. The goal is to understand the coupling between the flame and the fuel vaporizing to sustain it. This is known classically as the Emmons problem. The application of the research is in miniature combustion systems where fuel is expected to burn off of combustor surfaces.

Experimental Study on Microexplosive Burning of Binary Fuel Droplets *H. Ghassemi, S.W. Baek, Q.S. Khan; Korea Advanced Institute of Science and Technology* A comprehensive study of the combustion of multicomponent fuel droplets has been carried out. Combustion characteristics of single and multicomponent droplets hanging at the tip of a quartz fiber are studied experimentally at different environmental conditions under normal gravity. Normal Heptane and normal Hexadecane are selected as two fuels with different volatility, burning rates, and boiling temperatures. The burning rates thus calculated are then compared with evaporation rates calculated at similar conditions. It was found that the combustion also exhibits the three staged behavior. Droplet rupturing (partial microexplosion) has also been observed. The effects of component concentration, ambient temperature, and pressure on the combustion rates and disruptive burning have also been examined.

Nonlinear Dynamics of an Unstable Swirl Combustor: Frequency Locking and Open Loop Control *B. Bellows, A. Hreiz, T. Lieuwen; Georgia Institute of Technology* This paper describes the application of an open-loop control scheme on a lean, premixed combustor, resulting in effective damping of combustion instabilities. Control of the system was performed by forcing the combustor with loudspeakers operating on a frequency different from that of the instability frequency. We also investigate the nonlinear interaction, known as frequency locking, between the unstable combustor mode and the driven mode in the combustor as a function of frequency difference, driving amplitude, and other parameters. Initial results indicate that control of the instability is established with reductions in amplitudes up to 85%. Furthermore, the interaction between the unstable and driven modes has a hysteresis behavior with respect to the driving amplitude. Further results will be provided in the final paper.

Absolute Concentration Measurement of Nitrogen Oxide in Flames by LIF Standard Addition Method N. Yoshikawa, H. Saitoh, H. Suzuki, T. Sano, K. Okuno, S.Hayashi; Nagoya University The present research aims at developing a quantitative measurement technique of concentration and temperature of nitrogen oxide (NO) in practical burners used for jet engines and other energy supply systems.

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Laminar methane-air premixed flames were tested for different equivalence ratio mixtures. The distributions of fluorescence intensities along the beam of an excimerdye laser system were obtained using an image-intensified CCD camera. Temperature was determined using a two-line method. The concentration was obtained using a standard addition method of nitrogen-diluted NO gas into flames. Absolute concentrations of NO were determined through calibrating the comparison with the data of NO-doped flames. The number density of NO molecules was determined using the data of mole fractions and temperature. The results were in good agreement with the data of the time-resolved LIF method.

A Study of Ignition Timing of HCCI Engine S. Shiba; Okayama Prefectural University The investigation of HCCI Engine is becoming more developed around the world. Alcohol-based fuels and ether fuels are useful because there will be fewer changed parts on the occasion of application to the existing internal combustion engine. Non-dimensional numerical simulation of a homogeneous compression ignition engine system that uses DME as fuel was performed and the following results were obtained. DME fuel in the LLNL model starts 2-stage combustion in all the ranges of this research. Ignition times decrease with decreasing equivalence ratio in the model used for this study. Also, for the initial temperature near normal values, correct ignition timing can be obtained with a high rate of compression. It was possible to carry out stable operation over a wide range of equivalence ratio. In this study, we found that over the range of the initial temperature of 5 K and the equivalence ratio of 0.2, the ignition timing is maintained within 2-degree from TDC. The ignition temperature of the DME compression ignition engine with proper ignition timing in this research is from 690 K to 710 K. This was observed for a wide equivalence ratio range.

Prediction of Flame Propagation in a Tube with Obstacles Using a Fictitious Domain Method *A. Kaltayev, Z. Ualiev, U. Riedel, J. Warnatz; al-Farabi Kazakh National University* A fictitious domain method is extended and implemented for simulation of combustion problems in a non-regular domain. We considered the case when a 2D flame propagates in a rectangular tube with length L and a cross section of 2h x 2h. A plate obstacle with height h/2 is mounted perpendicular to the axis of the combustion vessel filled with the stoichiometric methane-air mixture. The study is based on the assumption of a low Mach number flow. A single step, global irreversible reaction of the methane-air laminar flame is used. The results of the case when a flame is travelling in a tube with obstacles at various distances x from the point of ignition are given and analyzed. Simulations of other cases will also be presented.

Comparative Analysis of Three Mathematical Models for Hydrogen Ignition *I.A. Bedarev, A.V. Fedorov; Institute of Theoretical and Applied Mechanics SD RAS* A comparative analysis of three kinetic schemes of hydrogen ignition in oxygen and three gas-dynamic models of the reactive mixture flow behind the initiating shock wave has been performed. The importance of the criterion is shown, which is used to determine the ignition delay time while comparing with experimental data. A numerical analysis of these kinetic schemes has shown that the scheme with 38 reactions of 8 components describes in the best way the experimental data in the temperature range from 900 to 2500 K. It is also shown that, at low initial concentrations of hydrogen-oxygen mixture in argon, even a simple model, which does not account for the influence of heat release on gas parameters, enables a satisfactory description of the induction period dependencies on temperature. As the initial concentration of reacting components grows, a mathematical model is to be applied, which takes into account the mixture temperature variation.

Formation of PAH, Fullerenes, Nanoparticles and Soot at Combustion of Hydrocarbons in Electric Field Z.A. Mansurov, N.G. Prikhodko, T.T. Mashan, B.T. Lesbaev; Al-Farabi Kazakh National University In the present work, the research of the influence of a constant electric field of different polarity, in the burning of benzene in an oxygen medium in C/O = 1.0 atomic ratio with the addition of 10% argon by volume at P = 40 Torr on the soot formation process, yield and structure of soot particles, yield of PAH and fullerenes in the U=0...20 kV range were investigated. Soot samples obtained undergo electron-microscopic analysis. The analysis results showed that soot particles became larger with benzene additives. Round, spherical particles of 250-350 A series are bound by a chain but, between them, empty spaces can be observed. Therefore, microscopic pictures showed that with PAH removed from the surface, soot particles more resemble graphite. Soot obtained under different conditions was extracted by a cold extraction method in C6H6. Then the extract was analyzed by the IR-spectroscopic method. The presence of fullerene is also seen from the spectra. Thus, fullerenes and PAH were identified in combustion of hydrocarbons under the conditions of low pressure.

Primary Methods of Reduction NOx and CO Concentration in Natural Gas Flame *S.S. Slupek, M.K. Poskart, L.W. Szecowka; AGH University of Science and Technology, Krakow* Reduction of emissions of gaseous pollutants, particularly NOx and CO, is necessary because it increases the efficiency of the combustion process and contributes to the environmental protection. This approach stimulates development of new combustion technologies (e.g., construction of new burners). Natural gas combustion in industrial furnaces is characterized by high temperatures existing in a flame. Such conditions intensify NOx formation. Therefore, the aim of primary methods of NOx reduction is to decrease combustion temperature. This paper describes an experimental work focused on the effect of combustion gas recirculation, staged combustion and reburning on the reduction of NOx and CO concentration in the exhaust gas.

Molecular Kinetic Computation of Turbulence in a Reacting Gas Flow *A. Sakurai, M. Tsukamoto, H. Homma; Tokyo Denki University* We consider the problem of computing chemically reacting turbulent gas flow using the integral form of the Boltzmann equation. Here we make an attempt to see the feasibility of this approach by considering the simplest case of turbulent flow of binary gas mixture of hot oxygen with dissociation and recombination reactions in a square region bounded by a cool wall with constant temperature. We employ the co-planar model for the molecular kinetics and assume the diffuse reflection at a non-catalytic wall for molecular interaction with the wall. The reaction production term is assumed to be proportional to the local Maxwellian distribution and the reaction rate.

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Wave Dynamic Process in Detonation Reflection from Wedges *Z. Jiang, Z. Hu, J.H.S. Lee; Institute of Mechanics, Chinese Academy of Sciences* The detonation reflection from wedges is investigated aiming at the wave dynamic process occurring in the wave front, including transverse shock motion and detonation cell variations behind the Mach stem. More cases were done on transition on regular to Mach reflection, and the critical angle was found to be 48°, which is smaller than most of the experimental data of 50°-53°, but agrees with that predicted with the CCW theory. The detonation reflection leads to a higher pressure rise behind the Mach stem, and the transition from regular to Mach reflection results in an even higher pressure increase.

Deflagration-to-Detonation Control by Nanosecond Gas Discharge *V.P. Zhukov, A.Yu. Starikovskii; Moscow Institute of Physics and Technology, Dolgoprudny, Russia* We performed an experimental demonstration of an application of high-voltage nanosecond gas discharge for initiation of a detonation. The experiments were carried out in mixtures C3H8+5O2 and C3H8/C4H10+5O2+xN2 (0 $\le x \le 10$), where C3H8/C4H10 is liquified petroleum gas (LPG). The position of the flame front was determined by simultaneous measurements through the side-wall with help of the IR sensors. The discharge chamber consists from a system of distributed electrodes, which provides uniform excitation over length of 80 mm. The electrodes were supplied with a positive pulse with amplitude of 4–70 kV and duration at the half-width of 50 ns At relatively low pressures we observed the deflagration with a weak acceleration. At relatively high pressures we observed the C–J detonation. At intermediate conditions we observed transient detonation.

Detonation Initiation by the Electrical Discharges in the Plane Channel *V.A. Levin, V.V. Markov, T.A. Zhuravskaya, S.F. Osinkin; IACP, Far Eastern Branch of RAS, Vladivostok, Russia* In the present research, the numerical investigation of detonation initiation by the electrical discharges in the plane channel of constant width filled by a stoichiometric hydrogen-air mixture under normal conditions is carried out. It was supposed that the electrical energy is transformed instantaneously into internal energy of the gas mixture. The possibility of a decrease of critical initiation energy by means of using several electrical discharges has been investigated.

Propagation of Detonation Wave in the Encumbered Channels *V.A. Levin, V.V. Markov, T.A. Zhuravskaya, S.F. Osinkin; IACP, Far Eastern Branch of RAS, Vladivostok, Russia* Examination of the initiation and propagation of detonations is one of the fundamental branches of gas dynamics. Detailed information about the features of these processes is very important for solving the problems connected with the prevention of detonation in order to increase blast safety, and for applications of detonation to technological processes. In the present research, the numerical investigation of detonation propagation is carried out for a plane channels without obstacles and filled with a stoichiometric hydrogen-air mixture under normal conditions. Detonation was initiated by the electrical discharge a the narrow layer. It was supposed that the electrical energy is transformed instantaneously into internal energy of the gas mixture.

Application of Direct Monte-Carlo Method for Simulation of Gaseous

Detonation Z.A. Walenta, A. Teodorczyk; Warsaw University of Technology The urgent technological problem is connected with detonation quenching in pipelines. The devices used for this purpose usually consist of matrices of very narrow channels. Cooling the gas by cold walls of such channels may extinguish the flame and stop detonation. The Direct Monte-Carlo Simulation (DMCS) technique has proven to be an excellent tool for simulating flows in various geometrical configurations - particularly in narrow channels. It also offers the possibility of taking into account the relaxation phenomena and chemical reactions. These, unfortunately, increase the complexity of the computer programs and the necessary computing times. However, in the case of detonation, considerable simplifications can be made thanks to the fact that, in a detonation wave, combustion proceeds at high temperature and at very high speed. Therefore, all relaxation processes at the molecular level may be disregarded. The only important factor that remains is the thermal energy produced. We propose a very simple model of a molecular collision, which makes it possible to increase the thermal energy of a gas, which is similar to the processes in the flame. We show then that this model can produce the wave, which has the features characteristic of a detonation wave.

Chemical Spike in Multiheaded Detonation *A.A. Vasiliev, A.V. Trotsyuk; Lavrentyev Institute of Hydrodynamics* The results of experimental investigation of chemical spikes in multifront detonation waves at DW reflection are presented. 2D numerical simulations of this process in a gaseous mixture were carried out. It was established that the dimensionless ratio of the length of the chemical spike in the multifront DW to detonation cell size increases with the growth of the initial pressure value.

Detonation Properties of Mixed-Fuel-and-Air Gas Mixtures *A. Yoshida, Y. Okuda, T. Yatsufusa, T. Endo, S. Taki, S. Aoki, Y. Umeda; Hiroshima University* We carried out experiments on the detonation properties, mainly on the detonation cell width, of the gas mixtures of mixed fuels and air at the atmospheric conditions of temperature and pressure. The mixed fuels were propane-hydrogen or propane-methane mixtures. In the experiments, the mixture ratios of these mixed fuels were varied keeping their equivalence ratio unity. The dependence of the detonation cell width on the mixture ratios of the mixed fuels was qualitatively understood by considering the number of hydrogen atoms each component of the mixed fuels includes. In the experiments, the detonation waves propagated in the 100-mm-diameter tube in two of the triplicated measurements in the case of the mixed fuel of 80%-methane and 20%-propane with air stoichiometrically. This suggests the possibility that a mixed fuel whose main component is methane could be used in practical pulse detonation engines.

Development of Shock Diffuser for Pulse Detonation Turbine Engines *K. Yoshinaga, T. Ofuka, A. Ochi, T. Yatsufusa, T. Endo, S. Taki, S. Aoki, Y. Umeda; Hiroshima University* For high-efficiency pulse detonation turbine engines, the interface between the combustor and the turbine is one of the critical issues because strong shock waves are disgorged from the combustor and hit the turbine blades which are optimized against a situation of stationary turbine-inlet pressure. As an important element of the combustor-turbine interface, we developed the shock diffuser, which deforms a strong shock wave into a series of weaker shock waves, of white gasoline and air was used. The experimental results clearly showed that the prototype of the shock diffuser was effective. **Re-initiation of Detonation Waves Behind a Perforated Plate** J. Sentanuhady, Y. Tsukada, T. Yoshihashi, T. Obara, S. Ohyagi; Saitama University Propagation of detonation through a perforated plate located inside a tube is of interest for practical uses to suppress accidental detonation bazards in industry. This study focuses on the

uses to suppress accidental detonation hazards in industry. This study focuses on the re-initiation process behind a perforated plate with a single hole or multiple holes. The results show that when the ratio of the diameter of the hole to the cell size is smaller than 10, the detonation wave is re-initiated behind the plate. The re-initiation depends not only on the ratio but also on the thickness and the tube size. The re-initiation processes are visualized from the soot-track records. For a multiple-holed plate with the same thickness, the re-initiation processes are shortened due to rapid ignition.

Equilibrium-Chemistry Model for Multiphase Reactive Premixed and Nonpremixed Flows *B. Khasainov, A. Kuhl, S. Victorov; Laboratoire de Combustion et de Détonique, UPR 9028 CNRS, ENSMA* Our new model is developed to simulate numerically multiphase reactive flows of premixed and nonpremixed mixtures based on an equilibrium chemistry approach for describing the equation of state of a heterogeneous mixture of fresh gas, suspended metal particles, and reaction products. As a result, the same pair of tabulated equations of state can be used for a wide range of metal content in premixed mixtures and even for nonpremixed mixtures, i.e., in the shock dissemination problem of metal particles. Another important advantage of the model is that it provides a detailed description of the evolution of all chemical species present in the conversion process including phase transitions. Reasonable agreement with the experiment is obtained simulating (i) detonation propagation in a premixed hybrid mixture of a gaseous explosive with suspended metal particles and (ii) shock dissemination and after-burning of metal particles in the closed bomb.

Detonation in Suspended Aluminum Particles in Tubes *H. Tao, Q. Chengsen, W. Pei; Institute of Applied Physics and Computational Mathematics* Aluminum dust detonation in tubes is analyzed with a two-phase flow model. Development and propagation of aluminum dust detonation is numerically simulated. The velocity of the detonation and ignition distance of particles is obtained. The distribution of pressure, density, velocity, and temperature in the flow field of the detonation wave is also obtained. Development and propagation of aluminum dust detonation with particle diameters of 3.4 mm and 5 mm in a tube with an inside diameter of 15.2 cm is numerically simulated. The detonation velocity and ignition distance of particles from the calculation are in agreement with the experimental results. Also, detonation in aluminum dust with various concentration is numerically simulated. The lower limit of detonation in the aluminum dust is determined from calculation that is equivalence ratio 0.25 in a tube with an inside diameter of 15.2 cm and is 0.16 with infinity inside diameter.

A Thermochemical Code to Model Detonations in Condensed Energetic

Materials Using Genetic Algorithms A. Zayer, U. Riedel, J. Warnatz; IWR, University of Heidelberg We discuss the implementation of genetic algorithms for modeling chemical equilibrium and detonation parameters at the Chapman Jouguet state. Our strategy has the advantage that no initial estimate of the equilibrium product distribution needs to be made. It is also an efficient strategy for finding the global minimum, since for highly non-ideal condensed energetic materials, the calculation of the chemical equilibrium through free energy minimization, using deterministic algorithms, can lead to a local minimum being found instead of a global minimum. This can result in an incorrect prediction of the chemical products distribution. The code was tested for several C-H-N-O energetic materials, namely Cyclotrimethyline- trinitramine (RDX), Nitromethane (NM), 2, 4, 6-Trinitrotoluene (TNT), and Pentaerythritol Tetranitrate (PETN); the results obtained using the genetic algorithm approach are in good agreement with the experimental data available in the literature. Furthermore, a comparison with results of other modeling approaches is presented.

Numerical Simulation of the Combustion of PETN/TNT Products with Air in Closed Chambers J.B. Bell, M. Day, V. Beckner, C. Rendleman, A.L. Kuhl, P. Neuwald; Lawrence Livermore National Laboratory The detonation products resulting from a chemical explosion are typically not completely oxidized and will burn if mixed with oxygen at sufficiently high temperature. In this paper, we present a computational model for the afterburning of these detonation products based on a thermodynamic model developed by Kuhl (2003). This model captures the thermodynamic and chemical behavior of the detonation products as they expand after detonation and provides a thermodynamic model is incorporated into a three-dimensional AMR algorithm and used to study the behavior of a composite TNT/PETN charge in a calorimeter. Numerical results compare favorably with static pressure histories recorded on the calorimeter lid.

The Role of Turbulent Transport for Detonation Initiation at a Turbulent Interface H.D. Ng, J. Chao, J.H.S. Lee; McGill University In this study, the problem of detonation initiation by rapid turbulent mixing at an interface between the combustion product and unreacted combustible mixture is investigated numerically. The role of turbulence mixing is modeled by systematically varying the magnitude of the transport parameters in the mixture. Numerical results demonstrate that the mechanism responsible for the onset of detonation at a turbulent interface is related to that of detonation formation in a free radicals concentration or temperature gradient field via the proper unsteady coupling between the gasdynamic and chemical energy release. In the initiation by turbulent mixing, the mixing process itself creates the gradient field. We illustrate from the numerical results how turbulent transport may play a key role in the initiation event. It is shown that if the turbulent intensity is too low, and thus the diffusion or mixing rate is insufficient, only a flame is formed at the interface which continues to propagate into the unreacted mixture. There is a critical diffusion rate for establishing an adequate gradient field where explosion occurs at the interface, resulting in the transition from flame ignition to detonation initiation.

Time-Dependent Dynamics of the Reaction Front Propagation in Detonation

Structure *P.N. Krivosheyev, O.G. Penyazkov, K.L. Sevruk; Heat and Mass Transfer Institute, National Academy of Sciences of Belarus* Time–dependent dynamics of the reaction front propagation along marginal and normal detonation structure in round tubes were investigated. It was shown that before completion of the cell cycle in all studied cases, the flame velocity decays to some critical value, which is very close to the isobaric sound speed of burnt products. The upper velocity level for both marginal and normal detonations at the beginning of the cell cycle is almost two times more than the value of the isobaric sound speed of the mixture.

Applicability Range of Detonation Resonator *S. Taki, T. Fujiwara, Y. Umeda; ATES Corporation* A numerical analysis is given to the resonant detonation phenomenon that occurs in a small cavity containing a fictitious gas mixture constantly supplied from a high-pressure reservoir. The acquired resonant frequency for cyclic and continuous detonation generation is found to be about 4-5 kHz, which is still much higher than conventional PDE operation, but is considerably lower than the value of 25 kHz experimentally observed by Levin et al. [1, 2].

Experimental Study on a Flow Field Behind Backward-Facing Step Using Detonation-Driven Shock Tunnel *T. Obara, T.-H. Kim, S. Ohyagi; Saitama University* In this study, a detonation-driven shock tunnel was built to produce highenthalpy flow, and a model SCRAM jet engine equipped with a backward-facing step was installed in the test section of the facility to visualize flow fields using a color schlieren technique and high-speed video camera. The fuel was injected perpendicular to a Mach 3 flow behind the backward-facing step. The height of the step, the injection distance, and injection pressure were varied to investigate the effects of the step on air/fuel mixing characteristics. The results show that the recirculation region increases as the fuel injection pressure increases. For injection behind the backward-facing step, mixing efficiency is much higher than with a flat plate. Also, the injection position has a significant influence on the size of the recirculation region generated behind the backward-facing step. The schlieren photograph and pressure histories measured on the bottom wall of the SCRAM jet engine model show that the fuel was ignited behind the step.

Numerical Simulation of Detonation inside the Electrochemical Pulse Engine I.V. Semenov, V.V. Markov, S. Wojcicki; Institute for Computer Aided Design, RAS The creation of new types of internal combustion engines based on new principles is important for both theory and practice. A relatively new scheme is an electrochemical pulsejet. In this device the electrical discharge appears in the combustion chamber when the flame front impinges on special electrodes that are attached to a pre-charged energy storage capacitor. Electrodes with the Rogowski profile eliminate electric field enhancement near the electrode edges. A "collar" (ring-type) discharge creates converging shock waves in the combustible mixture. leading to a fast burning process with detonation, high pressure, and an increase in the compression ratio. The energy of combustion of one cycle is thereby much higher than the electrical energy delivered by the electrical discharge. The numerical investigation shows the new gasdynamics problems concerning the engine operation: Initiation of detonation by circular electrical discharge (critical energy); Effective formation of fuel-air mixture in the combustion chamber; Determination of the optimal system parameters; Adaptation to flight conditions.

Mitigation of Strong Deflagrations by Water Mist *M.T. Parra, F. Castro, C. Mendez, J.M. Villafruela; University of Valladolid* The present work focuses on the numerical simulation of the interaction of a premixed flame and a water spray barrier in order to provide its suppression. Propagation occurs in a confined domain of high length and reduced transversal area, which provides the appearance of pressure waves that accelerate the flame front. The water mist is modeled as a uniform cloud of monodispersed droplets. The principal mechanisms of interaction of the water spray against the flame are the break-up, drag, heating, and evaporation of the droplets. They are compared to the propagation of an adiabatic flame and flames interacting with different water mist layouts. The efficiency of water barriers of different diameters is analyzed as a function of the Damköhler number and the propagation velocity of the corresponding perturbed flames.

Modeling of Turbulent Jet Nonpremixed Flames Using a Scalar Combined PDF/Moment Method S. Noda, K. Yamamuro; Department of Mechanical Engineering, Toyohashi University of Technology Our previous comparative study between the scalar PDF method and the flamelet model method revealed that relative large errors occur in regions where the transport probability of PDF decreases (Noda, 2002). This problem may be resolved with the help of the moment method which is superior in terms of both the numerical resolution and the calculation cost. The PDF method is modeled to reproduce both the mean and the variance obtained by the conventional moment methods. Thus we can now propose a scalar combined PDF/moment method, in which the scalar PDF transport equation and scalar moment equations are simultaneously analyzed to match the low moments. The present scalar combined PDF/moment method does not mean the conventional scalar PDF method which calculates only the flow field by moment methods. In the present paper, we have verified the usefulness of the scalar combined PDF/moment method through a comparison of the scalar PDF, the conventional flamelet model, and the present methods in the configuration of a turbulent jet nonpremixed flame.

Measurement of Local Equivalence Ratio in Partially Premixed Swirling Methane Flame Using Local Chemiluminescence *T.S. Cheng, C.-Y. Wu, Y.-H. Li, Y.-C. Chao; Chung Hua University* Spatially resolved chemiluminescence emissions are measured in laminar methane flames over an equivalence ratio of 0.8-1.4 using two Cassegrain mirrors and two spectrometers coupled with intensified CCD cameras. The measured flame emission spectra indicate that the dependence of the peak intensity of each vibrational band of the chemiluminescence on the equivalence ratio is almost the same as that of the spectrally integrated band emissions of OH*, CH*, and C2*. Experimental results show that the intensity ratios of OH*/CH* and C2*/OH* strongly correlate to the equivalence ratio. The calibration curves between the intensity ratio and the equivalence ratio obtained in laminar methane flames are used to determine the time-averaged local equivalence ratios in a partially premixed swirling methane flame. The measured results indicate that the non-laser based chemiluminescence technique can only be applied to determine the local flame stoichiometry in the reaction zone of partially premixed swirling methane flames.

Deflagrations in Closed and Vented Pipes - An Experimental Study H. Forster, C. Kersten; Physikalisch-Technische Bundesanstalt (PTB) Deflagrations in closed and vented pipes have been investigated experimentally to provide detailed explosion data for practical venting rules and for the validation of possible modelling. The course of explosion pressure and the flame propagation (high-speed video records) are significantly affected by the cooling of the burnt mixture at the pipe walls. The influence of mixture reactivity, pipe length, and pipe diameter is demonstrated for typical examples. A simple semi-empirical relation between transient explosion pressure and flame path shows an acceptable match with the experimatal data and may help to design effective venting systems. By some venting experiments, the significance of the developed criteria is demonstrated.

Thermodynamic Analysis of Closed Explosion of Hexane-Air Mixtures W.A. Trzcinski, P. Wolanski, A. Kuhl; Military University of Technology The thermodynamic theory of combustion in an enclosure was applied to analyse the process of the explosion of hexane vapour or hexane droplets - air mixtures in the chambers of different volumes. The relations between thermodynamic parameters and fuel consumption were determined. These relations and the overpressure histories taken from experiments were used to estimate the combustion rate and the final degree of hexane burned. The modified B. A. Khasainov's law of combustion of particles was applied to describe the process of combustion of hexane droplets in air. The parameters of this equation were estimated.

Comparison Between Two Liquid Fuels for Pulse Detonation Engines P. Gillard, X. Rocourt, I. Sochet, D. Piton, A. Prigent; laboratoire LEES, université d'Orléans The use of a liquid fuel to supply a PDE is the aim of this study. Although kerosenes are attractive because of their good safety qualities and wide range of storage temperatures, they require large amounts of energy to detonate directly in air. One solution is to carry out a pyrolysis of vapors of such fuels in order to obtain lighter molecules. This work is divided into two complementary parts. In the first one, the thermal degradation of two kerosenes, a kind of JP10 (synthesis fuel) and the decane which is representative of the F34 (obtained from crude oil fuel), is analyzed by means of gas chromatography. A parametric study according to the residence time and the temperature is achieved to seek the pyrolysis conditions which generate the most easy to detonation gaseous mixtures. The second part deals with the detonability of the major gaseous products after pyrolysis of decane and JP10. The limits of deflagration to detonation transition are examined according to significant parameters (nitrogen dilution and equivalence ratio). This comparative study between those fuels leads us to believe that decane, which is representative of classic kerosene of type F34, is more appropriate to supply a PDE than JP-10.

Experimental Study of Pulse Detonation Turbine Engine Toward Power Generator T. Sakurai, T. Obara, S. Ohvagi, M. Muravama: Saitama University Because of high efficiency, research on PDEs has been focused toward air-breathing engines and rockets. Recently, projects have been started to apply the PDE to turbine systems. We have planned to apply the PDE to power generator and the performance of the system has shown to be higher than conventional gas turbine systems by thermodynamic cycle analysis. In this system, problems arise at the turbine interface

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with the detonation wave. Of course, the detonation wave generates an unsteady flow. Unsteady performance of a turbine should be estimated to predict the turbine performance. This paper describes experimental results of Pulse Detonation Turbine Engine (PDTE). An automotive turbocharger was attached to a PDE tube to examine its performance when driven by detonation. Hydrogen was used as the fuel and air was used as the oxidizer and purge gas. The PDE tube was operated at 20Hz for 10 seconds. Estimated thermal efficiency was very low in this test, but it was shown that it is possible to extract power from the PDE by using a turbine system.

Quantitative Analysis of Explosion of an RDF Silo T. Tsuruda; National Research Institute of Fire and Disaster Municipal solid waste is used as an energy source to reduce carbon dioxide emission in large cities. RDF (Refused Derived Fuel) is produced from municipal solid waste in five model areas of medium size cities in Japan. After the death of two firefighters, the National Research Institute of Fire and Disaster investigated the fire and explosion of the RDF silo. The heat accumulation of the RDF pile was studied with small scale and medium scale experiments. The quantitative analysis of the formation of the explosive mixture in the RDF silo was carried out with small scale experiments. In this study, a quantitative analysis of the explosion has been carried out to understand the energy source which blew the roof off the 10 ton RDF silo.

Gas Explosion Simulations with Flux Limiter Centred Method K. Vaagsaether, D. Bjerketvedt; Telemark University College A 2D and 3D numerical code for gas explosion simulations is proposed based on the 2nd order total variation diminishing (TVD) flux limiter centered scheme (FLIC). The equations solved are the Euler equations with an energy source term; these equations are LES filtered. The combustion model used is a reactive Riemann solver for infinitely thin flames. A turbulence model for the turbulent kinetic energy is used to model the subgrid turbulence. The flame propagation is handled by the G-equations for turbulent flames. The FLIC scheme is chosen for its simplicity and its computational speed compared to upwind TVD schemes. To illustrate the performance of the code, results from numerical experiments have been compared with results from physical experiments with hydrogen and air.

Experiments With Flame Propagation in Inhomogeneous Hydrogen-Air Clouds in a Small Vessel O.K. Sommersel, R.L. Shrestha, D. Bierketvedt: Telemark University College Experiments with flame propagation in homogeneous and inhomogeneous hydrogen-air clouds in a small vessel have been carried out. The experimental setup consists of a rectangular steel vessel with dimension L = 445 mm, W = 106 mm and H = 100 mm, with polycarbonate sidewalls and A/V2/3 = 0.075. In the first test series, experiments were performed with pure hydrogen, flow rates ranging from 1.0 l/min to 9.4 l/min, and with ignition after 30, 60, and 120 sec. In the second test series, experiments were performed with pure hydrogen, flow rates ranging from 1.0 l/min to 9.4 l/min, and with the ignition system continuously on. The last test series was performed with homogeneous hydrogen-air clouds. The hydrogen concentration ranged from 16% to 80%. The measured pressures were less than 2kPa. The maximum pressure was slightly higher for the inhomogeneous case than for the homogeneous case. The pressure build-up was controlled by the interaction of the combustion process and the acoustics. Flame propagation in inhomogeneous hydrogen-air clouds in vessels and buildings is very complex and needs to be investigated further, both in small scale and in larger scale.

Ground-Based and Microgravity Study of Flame Quenching Distance in Metal Dust Suspensions S. Goroshin, J. Mamen, J.H.S. Lee, K. Sacksteder; McGill University A newly constructed apparatus for dust combustion experiments on board parabolic flight aircraft allows investigation of laminar dust flames in a wide range of particle sizes and fuel concentrations. The experiments are based on the observation of a laminar flame propagating through a uniform dust suspension in a semi-opened tube with free expansion and overboard venting of the combustion products. Several sets of the evenly spaced thin steel plates are installed inside a combustion tube to allow observation of the dust flame quenching process within the narrow channels. The apparatus was calibrated and tested in ground-based experiments with micronsize dusts. Flame speeds and quenching distances in air suspensions of fine powders of Al, Ti, Fe, and Cr were measured at close to stoichiometric dust concentrations. Ouenching distances and flame speeds in aluminum and iron dust suspensions of larger particle sizes (Al, d32 » 5.8 mm and 14.7 mm; Fe, d32 » 3.1 and 9.0 mm) were determined in recent microgravity experiments on board the NASA KC-135 parabolic flight aircraft.

Hazard Evaluation of Hydrogen-Air Deflagrations Using Latex Balloons *H. Saitoh, N. Uesaka, T. Ohtsuka, T. Mizutani, Y. Morisaki, H. Matsui, N. Yoshikawa; Nagoya University* In connection with the recent development and test use of hydrogen supply stations for fuel cell automobiles in Japan, the hazards due to deflagrative blast waves were experimentally evaluated in the present work using three different sizes of latex balloons ranging from 5.4 to 1400 liters. It is very important to understand combustion phenomena of hydrogen-air mixtures, especially the relationship between flame propagation in the mixtures and the blast parameters, such as peak over pressure and impulse. In order to examine the influence of the initial condition of the mixture on flame propagation and the blast parameters, the time evolution of flame velocity and pressure were monitored simultaneously using a high-speed camera and pressure transducers. Moreover, we tried normalization of the blast parameters obtained in several kinds of experimental conditions to confirm the blast scaling law. As a result, the blast parameters showed that the validity of the blast scaling law held for hydrogen-air deflagrations.

Simple Analytical Model for Metal Particle Ignition in Condensed Explosive *V. Tanguay, A.J. Higgins; McGill University* A simplified model of the ignition of metal particles contained in a high explosive is developed. The model assumes the detonation products to have a constant ratio of specific heats, and the expansion of the products is planar. Using empirical correlations for the drag and heat transfer coefficients, the trajectory of a single particle and its history of convective heating is solved for. The effects of radiative transport and particle reaction are also considered. The results show that the particle obtains its maximum temperature after the convective heating of the Taylor wave flow of products following the detonation in the high explosive. If a simple ignition criterion (e.g., boiling temperature of metal) is adopted, then this model can be used to predict the size of the charge necessary to obtain particle ignition. The results are compared to experimental results with magnesium particles embedded in nitromethane; the model agrees with the experiment within an order of magnitude and displays the correct trend in relating particle size and critical charge size.

Plasma-Wave Initiation of Supersonic Combustion at Low Electric Energy Deposition A. Dovbnya, K. Korytchenko, Yu. Volkolupov, A. Kosoy; National Technical University "KPI" The plasma-wave system has been designed to initiate a detonation in a dense fuel-air environment with frequency not less than 200 Hz at electrical energy deposition on single initiation up to 100 J. The method allows to obtain supersonic combustion due to the achievement of relaxation acceleration and using a designed pulse hydrogen generator. The axial velocities of plasma flow were up to 1000 m/s and radial velocities of expansion of a burning zone were up to 800 m/s by various discharge conditions and electrical energy input in a range from 50 up to 100 J. Due to the changing average intensity of the field, the different methods of ignition of the acetylene-air mixture were observed. The volumetric ignition was observed in a condition of volumetric bombardment of the fuel mixture by a dense flow of electrons or photons. The shock ignition was in case of fast increase in speed of the plasma jet propagation with the formation of an intensive shock wave. The volumetric - shock ignition. The application of PWS will allow to reduce time DDTtransition and to considerably decrease the length of the transitive part of a detonation tube.

Simulating the Influence of Obstacles on Accelerating Dust and Gas Flames *T. Skjold, Y.K. Pu, B.J. Arntzen, O.R. Hansen, I.E. Storvik, O.J. Taraldset, R.K. Eckhoff; GexCon AS and University of Bergen* A new CFD-code called DESC is currently being developed for predicting flow, flame propagation, and pressure buildup during dust explosions in complex geometries. The new code is based on the existing FLACS code for gas explosion modelling, but the combustion model requires empirical input from standardized tests. The main aim of the present work is to test the new code by comparing existing experimental results to results obtained with DESC and FLACS for the same scenarios. The experimental data on the influence of obstacles on flame propagation in cornstarch-air and methane-air mixtures is taken from work by Yi Kang Pu published in 1988. It was possible to reproduce experimental results for lean methane-air mixtures reasonably well with FLACS. However, results obtained with DESC for cornstarch-air mixtures deviated significantly from experimental values.

Formation of SnO2 Nanoparticles from {SnCl4 + H2O} Reactive System at 30 MPa and 415oC Z. Fang, H. Assaaoudi, I.S. Butler, J.A. Kozinski; McGill University Nanocrystalline SnO2 was synthesized in supercritical water at 385-415 oC, 30 MPa and 38-106.2 s in a tubular flow reactor from {SnCl4 + H2O} Reactive System. Conversion rate was 53-81%. It was found that particle size was about 3.7 nm (390 oC and 79.7 s). After calcinated at 450 oC for 2 h, the size changed little (4 nm) and all particles still presented low crystallinity. After calcinated at 600 oC for 10 h, the particle size increased to 9 nm revealing high crystallinity. All SnO2 particles had tetragonal crystalline structure.

Temperature Dependence of the Lower Explosion Limits of Pure Components and Mixtures *E. Brandes, M. Mitu, D. Pawel; Physikalisch-Technische Bundesanstalt (PTB)* The knowledge of the temperature dependence of the Lower

Explosion Limits (LEL) is a very helpful tool in explosion prevention, e.g. for drying processes. Based on experimental results for the LEL of pure flammable liquids at temperatures up to 200 °C, the LEL of mixtures and the temperature dependence of the LEL of the mixtures have been calculated and compared with measured data. The temperature dependence of the mixtures varies from about -9% per 100K to up to -23% per 100K, depending on the respective mixture. Taking a value 20% (rel.) below the calculated temperature dependence gives results safe enough for many technical purposes. If more precise results are required, experimental determination of the LEL at the respective conditions still is necessary. If no data are available, an assumed temperature dependence of -25% per 100K gives safe results under all known conditions without measurements.

Explosions in the Courts: The Intersection of Law and Science *B.A. Davis; CHOATE, HALL & STEWERT LLP, Boston MA* The focus of this presentation will be on the role and effective use of science in the courtroom in cases arising from industrial explosions. Subsidiary topics that will be discussed include: the role of the explosion expert in the litigation process; significant differences in the concepts of scientific proof and legal proof; standard processes for reviewing and ensuring the scientific accuracy of expert testimony; restrictions on opportunities for experimentation and verification often faced in the litigation context; and the divergent presentation approaches necessitated by differences in learned versus lay audiences. These topics will be addressed in the context of three (3) real-world case studies involving actual court actions arising from industrial explosions.