Presentation to NETL 2021 Workshop on Multiphase Flow Science

John McQuillen (NASA Glenn Research Center)
Dan Dietrich (NASA Glenn Research Center)
Suman Sinha Ray (Universities Space Research Association)

August 3, 2021
NASA’s Gravity-Dependent Physical Sciences Research

**Combustion Science**
- Spacecraft fire safety
- Droplets
- Gaseous – Premixed and Non-Premixed
- Solid Fuels
- Supercritical reacting fluids

**Fluid Physics**
- Two-phase flow
- Phase separation
- Boiling, Condensation
- Capillary and Interfacial phenomena

**Materials Science**
- Crystal growth
- Metals, alloys
- Electronic materials
- Glasses, Ceramics
- Polymers

**Fundamental Physics**
- Space Optical/Atomic Clocks
- Quantum test of Equivalence Principle
- Cold atom physics
- Critical point phenomena
- Dusty plasmas

**Soft Matter**
- Colloids
- Liquid crystals
- Foams
- Non-Newtonian fluids
- Granular flows
Why Study Combustion in reduced gravity?

To enable space exploration.
- Fire is a catastrophic hazard for manned space flight
- Fire risk mitigation imposes large mass and volume impacts
- Mitigation of the risk requires microgravity testing
- Fire risk changes in low-gravity

To advance science.
- Study classical one-dimensional problems to foster theoretical development
- Create super-lean and super-weak systems to study critical kinetic effects
- Enable study of flame structure and weak forces without gravitational dominance

To enable technologies on earth.
- 85% of our delivered energy comes from combustion
- Combustion generated air pollution is a leading cause of the loss of life
- Greenhouse gas release and climate impact is dominated by combustion processes
- Fire is a major source of the loss of life and property
- Combustion is major source of new materials, nano-tubes, diamond films, ceramics etc.

Macroscopic consequences of gravity on combustion:
- Non-linear buoyant acceleration
- Accelerated mixing and turbulence onset
- Sedimentation (when particles or gases are freely mixed)
- Increased dimensionality

“Progress in combustion studies critically depends on the availability of the CIR facilities on the ISS.”
- NRC Report to NASA, 2003
Why Study Fluids and Soft Matter in Space?

To enable space exploration.
• Two-phase flow systems for heat transfer and life support
• Bubble removal from liquid systems (flowing/static)
• Long term propellant storage, transfer, gauging
• Excavation, material handling and in-situ resource utilization

To advance science.
• Model “atomic” systems at an observable scale (colloids)
• Study self assembly and crystallization – advance knowledge of phase transitions
• Study fluid systems near critical points

To enable technologies on earth.
• Reveal effective rheological properties of non-Newtonian fluids and suspensions
• Stabilization of foams
• Understand the aging of gels and late collapse (P&G) – increasing product shelf life
• Can gain critical insights into strongly non-linear systems (multiphase & interfacial problems) where gravity constitutes a significant perturbation or instability or complicates the interpretation of experimental results

Macroscopic consequences of gravity on fluids include:
• Stratification of different densities
• Hydrostatic pressure gradient
• Sedimentation (when particles are freely suspended)
• Buoyancy-driven convection
• Drainage of liquid films

“When the influence of gravity on fluid behavior is diminished or removed, other forces, otherwise of small significance, can assume paramount roles.”
- NRC Report to NASA, 2003
NASA Glenn Research Center’s ISS Research Program

- **Combustion Science:**
  - Investigating physical combustion phenomena in the absence of gravity.
  - Develop and validate models for future applications.
  - Determine methods for fire prevention, detection, suppression, and selection of proper materials.

- **Fluid Physics:**
  - Study the motions of liquids and gases and the associated transport of mass, momentum and energy in microgravity.
  - Apply knowledge for design of two-phase flow and long-term fluid storage systems for exploration.

- **Soft Matter (Complex Fluids):**
  - Investigation of a large class of soft materials.
  - Bridges the gap between synthetic and living materials with a broad range of industrial, biological, and environmental applications.

Providing Technology Push and Pull and Pioneering Science
Recent ISS Research Accomplishments

**Cool Flames Discovery**
- Confirmed on the ISS that fuels initially burn very hot, then appear to go out — but they continue burning at a much lower temperature in microgravity, with no visible flames (cool flames).
- Understanding cool flame combustion helps scientists develop new engines and fuels that are more efficient and less harmful to the environment.

**Wickless Heat Pipe**
- Normally when a liquid is heated above its boiling point, it evaporates, turning into a vapor.
- Observed on the ISS that vapor near a heat pipe end condensed into a liquid even when the temperature was 160 K above the substance's normal boiling point.
- Understanding the limitations of heat pipes as cooling devices for spacecraft can guide the design of improved versions.
Zero Boil Off Tank Experiment

- Examine issues associated with the long-term storage of volatile fluids.
- Pressurization as tank is heated.
- Mixing tank as a cooling and depressurization strategy.

Fast Flow Jet Mixing

Slow Flow Jet Mixing

Rapid Cooling
Capillary Phenomena

Capillary Flow Experiment

Microgravity Coffee Cup

Hydroponic Plant Watering
Colloidal Behavior

- Colloidal Rearrangement as a Function of Temperature

**Spontaneous Syneresis**

Gel "fault" caused by temperature stress

**Bijel Reformation**

ACET5_4x_S2201_C1_TRQuench_Stack_26C_to_20C
Evolution of Droplet Combustion
Multi-User Droplet Combustion Apparatus (MDCA)

• Droplet Deployment
• Hot Flame Ignition
• Extinction
• Cool Flame
• Hot Flame Reignition
High Pressure Transcritical Combustion

- Recommended by 2014 Combustionlab Workshop
- Science Definition Team Convened:
  - M. Colket, United Technologies Research Center (ret.)
  - S. Aggarwal, Univ. of Illinois, Chicago (emeritus)
  - H. Wang, Stanford
  - H. Curran, National University of Ireland, Galway
  - S. Goldsborough, Argonne National Lab
  - R. Yetter, Pennsylvania State University
  - M. Ackerman, Air Force Office of Scientific Research
Granular Media

In-Situ Resource Utilization

• Processes
  – Excavating
  – Transporting
  – Processing

• Products
  – Propellants
  – Oxygen
  – Water

Apollo 16 Astronaut John Young driving Lunar Rover Vehicle (note dust kicked behind wheels)

OSIRIS-REx Sampling of Asteroid Bennu

OSIRIS-REx Sampler
Decadal Survey on Biological and Physical Sciences Research in Space 2023-2032

• Seeking input from the scientific community into the next decadal survey.

• The call for 2 to 5 page white papers have the following due dates:
  – “Topical” white papers should be received by October 31, 2021.
  – “Research Campaign” white papers should be received by December 23, 2021.

• Report is framework for the vision, priorities, and strategic plan and budget for NASA’s research efforts in the area of biological and physical sciences in space.

• Prior Decadal Reports
Background Information

Previous Workshops:

• Results Outbrief from the 2014 CombustionLab Workshop

• 2019 NASA Division of Space Life and Physical Sciences Research and Applications Fluid Physics Workshop Report

• Grand Challenges in Soft Matter Science: Prospects for Microgravity Research

Experiments

• Project Information about Experiments

• A Researcher’s Guide to: Combustion Science

• A Researcher’s Guide to: Fluid Physics (Fluid Physics and Soft Matter- was complex fluids).

• Researcher’s Guide to: Physical Sciences Informatics System

• Physical Sciences Informatics Database (Need to register for login)
Questions?
Backup: Research Challenges
We do not have a sufficient fundamental, quantitative understanding of basic combustion phenomena to enable the design of next generation combustion systems.

1. We do not have predictive tools to design the next generation combustion systems for high pressure transcritical environments.

1.1 Measure thermophysical properties in multi-phase systems at trans- and super-critical conditions.

1.2 Characterize the transition from classical two-phase flow dynamics to diffusion-controlled interfacial mixing conditions.

1.3 Examine multi-stage ignition, burning and extinction phenomena at trans- and super-critical conditions.

1A. Benchmark Data
- Thermodynamic/Transport properties
- Mixture properties
- Chemical kinetic data

1B. Predictive Models
- Molecular Dynamic Simulations
- Analytical
- Mixing models
- CFD

Design guides and reference databases.
We do not have a sufficient fundamental, quantitative understanding of basic combustion phenomena to enable the design of next generation combustion systems.

2. We do not have a predictive understanding of weak, low-stretch, near-limit and cool flames

2.1 Measure flammability limits and stability regimes for low temperature flames

2.2 Examine stability regimes and flammability limits for weak, near-limit hot flames

2.3 Examine flame structure (spatial and temporal species data) for near-limit hot and cool flames

2.4 Measure soot formation and destruction and sooting limits in near-limit flames

2A. Benchmark Data
• Ignition/extinction data
• Flame structure
• Chemical kinetic data

2B. Predictive Models
• Improved chemical kinetic models
• Analytical, reduced kinetic models
• CFD

Design guides and reference databases
We do not have a sufficient fundamental and predictive understanding of basic combustion phenomena to enable the design of next generation combustion systems.

3. We do not have predictive tools validated in the regimes where future engines will operate

3.1 Examine high pressure, turbulent flames

3.2 Examine chemical kinetic effects such as ignition and extinction, flame structure in turbulent flames

3.3 Examine soot formation/destruction in turbulent flames

3B. Predictive Models
- Improved chemical kinetic models
- Analytical, reduced kinetic models
- DNS, CFD
- Kinetic submodels for turbulent models

3A. Benchmark Data
- Ignition/extinction data
- Flame structure
- Chemical kinetic data

Design guides and reference databases
How do we ensure crew safety with respect to accidental fires in human-crewed spacecraft?

1.1 How do we improve our understanding of material flammability through a better predictive understanding of the underlying fundamental physics??

1.1.1 How does sample size and orientation affect material flammability

1.1.2 How do spacecraft cabin environments (P, T, Flow) affect material flammability

1.1.3 How does partial gravity affect material flammability

1.1.4 Are NASA standard flammability tests a conservative measure of material flammability

1.1B Predictive Models
- Empirical
- Analytical
- CFD
- Risk Assessment

1.1A Fire Safety Database
- BPS and AES data
- Flight and ground-based
- Links to NASA partners

Fire Safety Certification
- Design guide
- Certification process
- Risk Assessment
C. Reliably and predictably to control fluids (gasses & liquids) in space like we do on earth?

RQ1. How is the shape of the gas-liquid interface affected by flow and a reduction in gravity?

RQ2. How does the gravity vector affect the transport phenomena along and through the gas-liquid interface?

RQ3. What are characteristics that result in preferential accumulation of a single phase and how does the accumulation and shedding events impact system stability?
C. Reliably and predictably to control fluids (gasses & liquids) in space like we do on earth?

RQ1. How is the shape of the gas-liquid interface affected by flow and reduction in gravity?

T1 Examine capillary effects on interface position and stability
T2 Study influence of flow conduit geometry
T3 Examine interfacial effects associated with bubble and droplet formation and coalescence
T4 Examine dynamics associated with residual accelerations
T5 Establish, verify and validate Design Guidance

P1 Flow Regime Database
P2 Predictive Models
P3 Design Guide
C. Reliably and predictably to control fluids (gasses & liquids) in space like we do on earth?

RQ2. How does the gravity vector affect the heat and mass transfer along and through the gas-liquid interface?

T6 Examine heat transfer into a pool of non-flowing fluid and effect on pressurization of volatile fluid.

T7 Investigate forced convection heating of volatile fluid.

T8 Explore cooling phenomena at and near the Leidenfrost temperatures.

T9 Study influence of gravity on condensation.

T5 Establish, verify and validate Design Guidance.

P4 Heat Transfer Coefficients Database

P2 Predictive Models

P3 Design Guide
C. Reliably and predictably to control fluids (gasses & liquids) in space like we do on earth?

RQ3. What are characteristics that result in preferential accumulation and shedding events of a single phase and impact instability phenomena?

- T10: Examine contact angle and geometry effects capturing flowing phases.
- T11: Explore effects of sudden massive vapor Generation
- T12: Examine effect of compressible volumes
- T13: Data mining Activity
- T5: Establish, verify and validate Design Guidance

P5 Stability Envelope

P2 Predictive Models

P3 Design Guide
**Roadmap Overview**

**Challenge:** Understand, control, and use complex soft matter dynamical systems to improve the understanding of nonequilibrium phenomena from nano- to large-scale systems.

- **RQ1.** How dynamics and cooperativity influence smart reactive materials and systems?
- **RQ2.** How to develop a nonliving self-reliant sustainable/circular ecosystem via better understanding of fundamental dynamical organizational principles of its constituents?
- **RQ3.** How to tailor the microstructure to develop active materials and metamaterials?
RQ1. How dynamics and co-operativity influence smart reactive materials and systems?

**T1. Develop and test robust experimental facilities both on ground and in space**

- **P1. Ground-based Experimental Rigs**
- **P2. Space flight hardware**

**T2. Study force-induced (e.g. potential, chemical activity, flow, external stimuli etc.) dynamics of non-equilibrium self-assembly**

- **P3. Systems capable of moving, morphing, transforming energy**
- **P4. Predictive models/theories**
- **P5. Bio-inspired and bio-machine interfaced soft matter**

**T3. Develop mechanisms of nonlinear co-operativity between neighboring elements**

- **P6. Fundamental principles inter- and intra-connected systems**
- **P7. Optimized protocol for studying impact of stimuli on inter- and intra-connected systems**

**T4. Integrate intelligent processing of data from experiments, simulations and databases (e.g.-PSI) to get better insight**

- **P8. Machine-learning (ML) based hybridized model**
- **P9. Systems integrated with AI/ML/Edge computing-based proactive system**
**Challenge:** Understand, control, and use complex soft matter dynamical systems to improve the understanding of nonequilibrium phenomena from nano- to large-scale systems

**RQ2. How to develop a nonliving self-reliant sustainable/circular ecosystem via better understanding of fundamental dynamical organizational principles of its constituents?**

- **T1.** Develop and test robust experimental facilities both on ground and in space
- **P1.** Ground-based Experimental Rigs
- **P2.** Space flight hardware
- **T5.** Develop an understanding of nonequilibrium organizational principles of systems that recycle their own building material across scales from cellular to planetary via functionalization of elementary building blocks
- **P10.** Non-equilibrium organizational principles
- **P11.** Hierarchical additive manufacturing
- **T6.** For these systems, study the impact of rheology, hydrodynamic interactions, gravity, friction, charging, hysteretic and other effects
- **P12.** Pharmaceuticals & biomedical applications
- **T4.** Integrate intelligent processing of data from experiments, simulations and databases (e.g.- PSI) to get better insight
- **P8.** Machine-learning (ML) based hybridized model
- **P9.** Systems integrated with AI/ML/Edge computing-based proactive system
- **T3.** Develop an understanding of non-equilibrium organizational principles of systems that recycle their own building material across scales from cellular to planetary via functionalization of elementary building blocks
- **P13.** Handling and Processing Granular Media

---

27
**Challenge:** Understand, control, and use complex soft matter dynamical systems to improve the understanding of nonequilibrium phenomena from nano- to large-scale systems

**RQ3:** How to tailor the microstructure to develop active materials & metamaterials to achieve novel capabilities?

- **T1.** Develop and test robust experimental facilities both on ground and in space
- **P1.** Ground-based Experimental Rigs
- **P2.** Space flight hardware

- **T7.** Develop active materials & metamaterials outside the realm of continuum theories constructed from energy minimization.
- **P15.** Metamaterials with multiple functions on deployment

- **T8.** Develop methodologies to encode multiple functions (e.g. controlling propagation of electromagnetic radiation, sound and elastic wave in the same metamaterial).
- **P16.** Active & self-sensing bio-soft metamaterials

- **T9.** Understand the scalability of active materials & metamaterials and how that affects multiple functionality.
- **P17.** Predictive models/theories for metamaterials

- **T4.** Integrate intelligent processing of data from experiments, simulations and databases (e.g. PSI) to get better insight
- **P8.** Machine-learning (ML) based hybridized model
- **P9.** Systems integrated with AI/ML/Edge computing-based pro-active system