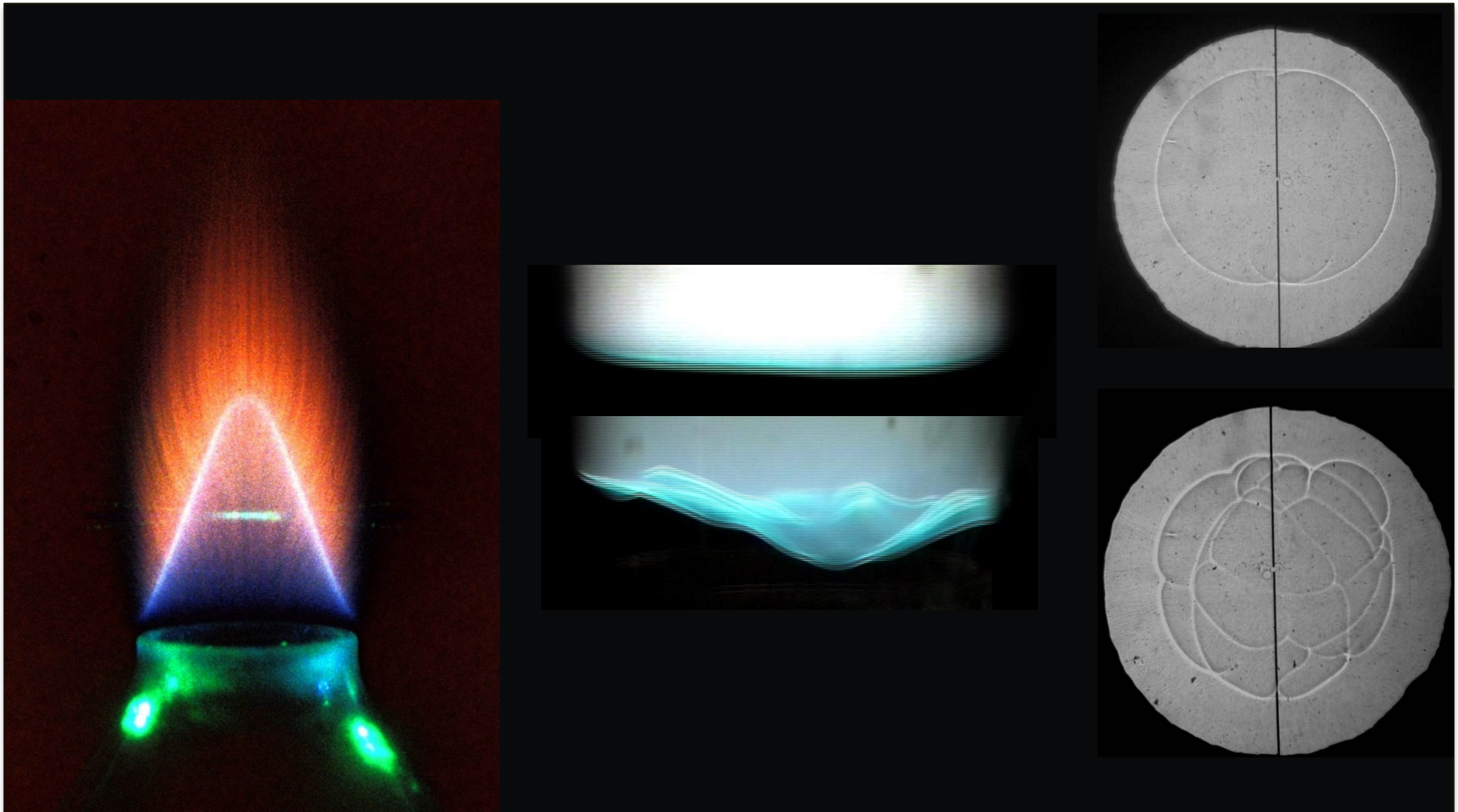
Modeling Tools for Flammability Ranking of Low-GWP Refrigerant Blends

2017 Building Technologies Office Peer Review



U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

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Project Summary

Timeline:

Start date: Oct. 1, 2016 **(New Project)**

Planned end date: Sept. 30, 2019

Key Milestones

1. Burning velocity data/predictive tool for HFCs (9/17) and HFOs (9/18).
2. Generalized burning velocity predictive tool for blends (9/19)
3. Input into codes and standards test method development (9/19).

Key Partners:

AHRI	Japan-AIST
ASHRAE	China - Peking University
ISO	Univ. of So. Cal.
UTRC	NIST Kineticists
Gexcon	

Budget:

Total Project $ to Date:

- DOE: $700k
- Cost Share: $0

Total Project $:

- DOE: $2000k
- Cost Share: $0

Project Outcome:

1. To develop predictive tools for the laminar burning velocity of low-GWP refrigerants, so that blends can be optimized by industry to optimize performance while minimizing flammability.
2. To provide technical input into the codes and standards development process to facilitate the safe implementation of low-GWP, mildly flammable refrigerants.

Purpose and Objectives

Problem Statement: Existing HFC working fluids have high GWP and will be phased out. Low GWP fluids are flammable and there are not yet codes and standards for their safe use. To facilitate the development of effective codes and standards, the present project will provide experimental data, predictive tools, and test method improvement for the burning velocity and flammability test methods being developed and used.

Target Market and Audience: Residential and commercial buildings in the US use about 40 quads of energy, of which most is for heating, cooling, and refrigeration. The focus of the present project is equipment employing vapor compression systems, which are responsible for a large fraction of the total HVAC&R use. The audience is the HVAC&R equipment and refrigerant manufacturers.

Impact of Project: Faster, safer, more effective codes and standards through better fundamental data, measurements, and predictive methods for flammability.

Outputs:

1. Predictive tool for the burning velocity of refrigerants.
2. Technical input into the code-making bodes to facilitate effective and accurate tests and their interpretation.

Approach

Approach: To achieve the performance and GWP goals, industry will use blends (up to five components). To optimize the blends, techniques exist to predict the thermodynamic performance and GWP; however, there are no methods to predict the flammability. The goal of the present project is the develop the ability to predict the burning velocity of arbitrary blends of agents, so that they can be optimized with regard to flammability. To do this, detailed fundamental kinetic combustion models for the pure compounds in the blends will be developed, refined, and tested. Detailed numerical simulations of burning velocity test methods will be used to validate the models and understand the controlling parameters in the test methods.

Key Issues: The blends of most interest are barely flammable, hence the measurements are influenced by usually minor effects such as flame instabilities, buoyancy, radiation, and containment issues. These effects make both the measurements and simulations more challenging.

Why is the Laminar Burning Velocity LBV Useful?

1. A single parameter that combines the effects of energy release, heat and mass transfer, and overall reaction rate.

   $S_L^o = (\alpha\ \omega_i)^{½}$

   S_L^o –burning velocity (1-D, planar, steady, laminar)

   α : thermal diffusivity $= \lambda/\rho C_p$

   ω_i : overall reaction rate = $[f][ox]Ae^{-E_a/RT}$

2. Predictions of turbulent flame speed are based on the laminar flame speed, so over pressure hazard and explosion hazard are both tied to S_L^o.

3. LBV is being adopted in codes and standards by industry.

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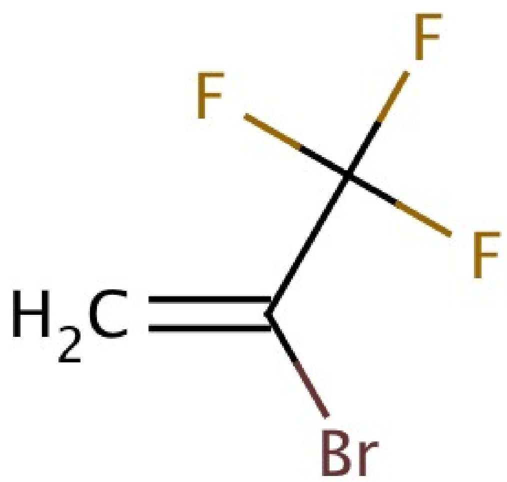
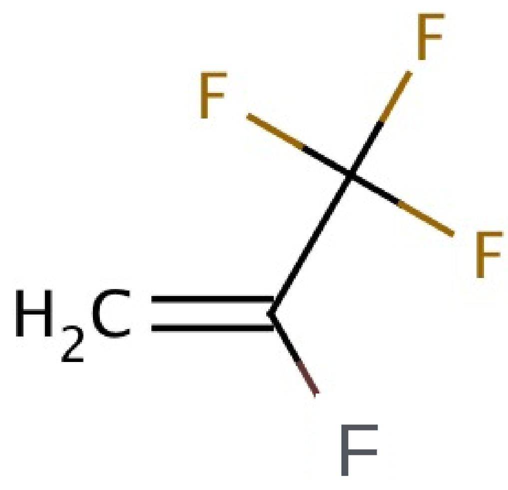
Can we predict LBV? Background: Fire Suppressants

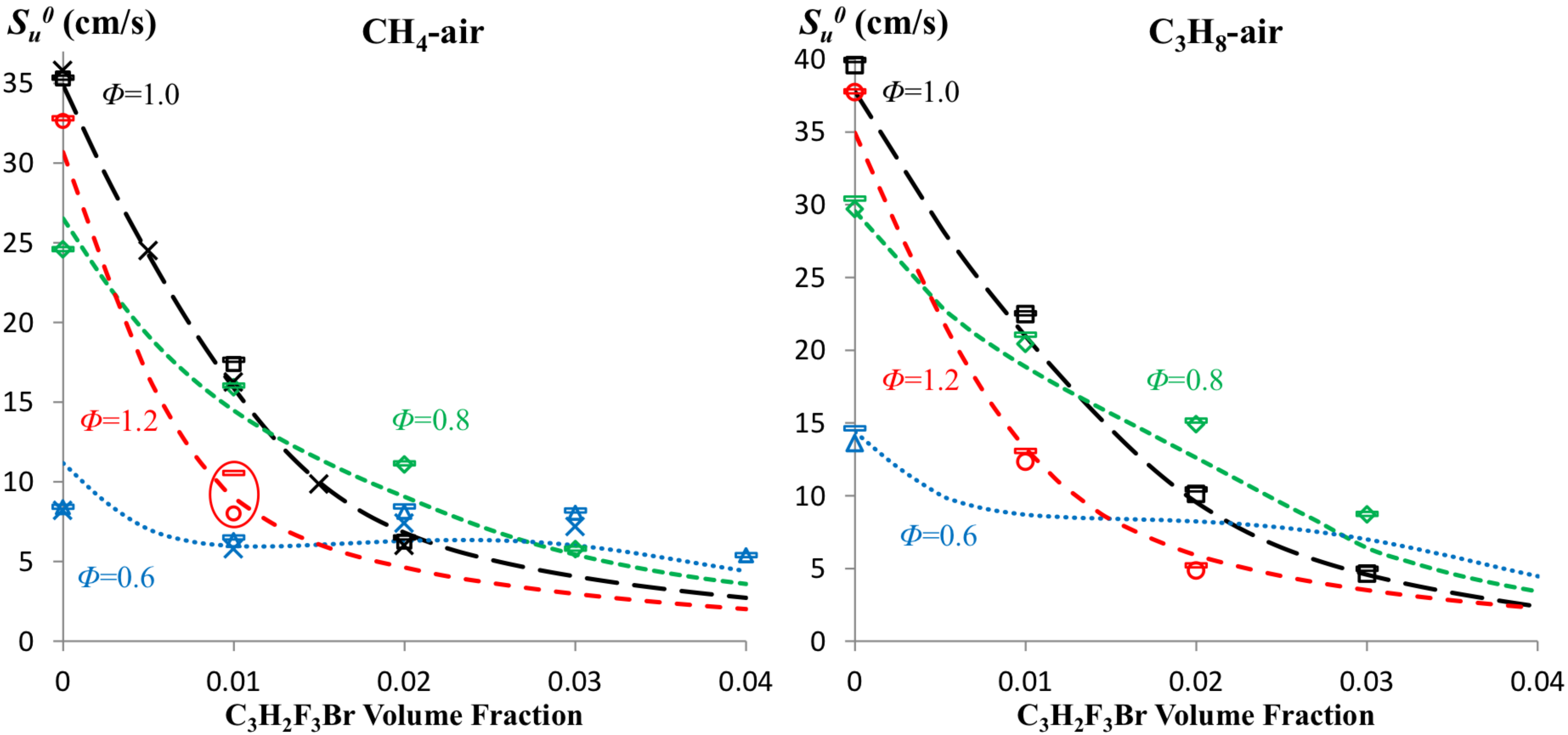




2-BTP

R1234yf

Can we predict LBV? For CH_4- or C_3H_8 with 2-BTP, yes.



Can we do it for pure refrigerants in air?

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Why try to predict LBV?

To reach performance goals, industry will use blends

$\Rightarrow$ To optimize a blend, the thermodynamic, heat transfer, toxicity, and GWP performance can be calculated.

Flammability cannot, so the blend cannot be optimized.

$\Rightarrow$ Goal of current project is to develop methods to predict the LBV for arbitrary mixtures so flammability can be included in the optimization.

How do you predict the Laminar Burning Velocity of blends?

$\Rightarrow$ Could measure it, but too many blends (up to five individual compounds at varying composition).

$\Rightarrow$ Empirical methods to predict burning velocity from blends would probably not work (it's too complicated).

=> Calculate it from first principles (a well-established approach for other fuels, e.g., hydrocarbons).

Calculating Burning Velocity:

Use numerical models (1-D, 2-D, steady or non-steady)

- Solve conservation equations for mass, momentum, energy, and species with chemical reaction and radiation.
- Inputs:

1.) a chemical reaction model

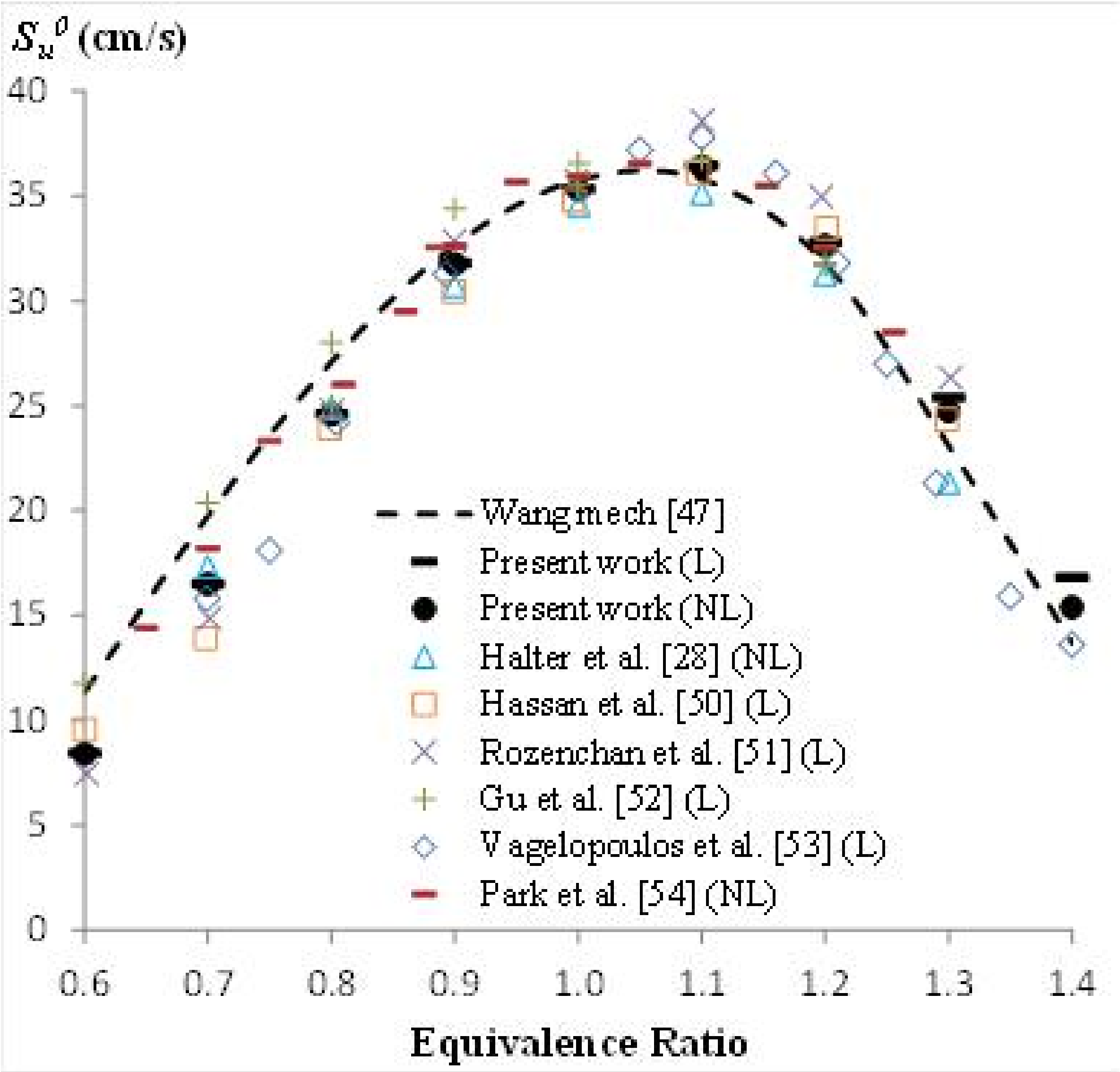
a.) a list of possible species and their thermo data,

b.) a list of possible reactions and their rates (Arrhenius parameters, A, E_a, etc.),

2.) transport model and parameters (diffusion coeff.)

3.) radiation model and parameters (extinction coefficient)

Predicted Laminar Burning Velocity for Methane-air Mixtures



Approach in Project:

1. Assemble team (experimental, modeling, kinetics).
2. Get experimental LBV data for select pure compounds, over range of fuel/air mixtures.
3. Build kinetic models (shock-tube studies, quantum mechanical calculations).
4. Get flame modeling tools. (1-D, 2-D, time-dependent, spherical, with radiation).
5. Understand what's modelled and what's measured.
6. Compare experiments with model.
7. Validate model.
8. Develop predictive tool. f(humidity, T_{init}, P_{init})
   First for pure compounds.
   Then mixtures.
   Then add humidity.
9. Goal: Usable tool.

=> Understand what controls LBV, and if this approach is possible for refrigerant-air flames.

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Approach

Distinctive Characteristics:

1. Results based on fundamental, detailed kinetics
2. Numerical simulations of the flame structure: various levels of sophistication, depending upon the experiment.
3. The goal is a <u>usable design tool</u> that can predict the fundamental laminar burning velocity of refrigerant blends.

Progress and Accomplishments

Accomplishments: New Project.

1. Software installations and updates (NIST Senkplot, Cantera)
2. Updates to the NIST one- and two-carbon HFC combustion model (in work).
3. Burning velocity measurements for R32-air mixtures.
4. Burning velocity simulations for R32-air mixtures.
5. Assessment of influence of flame curvature on the measurements.
6. Observation of the effect of HFO species heat of formation on the calculated burning velocity of R32.
7. Simulations of burning velocity for R143, R143a, R152, R152a, 134, C2H5F,and CH3F.
8. Modifications to the NIST shock tube for kinetic studies.
9. Assembly of research team.

Market Impact: New Project.

Impact will be achieved through close interactions with industry groups via AHRI, ASHRAE, and ISO committees, publications, collaborations, presentations.

Awards/Recognition: New project. N.A.

Lessons Learned: New project. N.A.

Progress and Accomplishments

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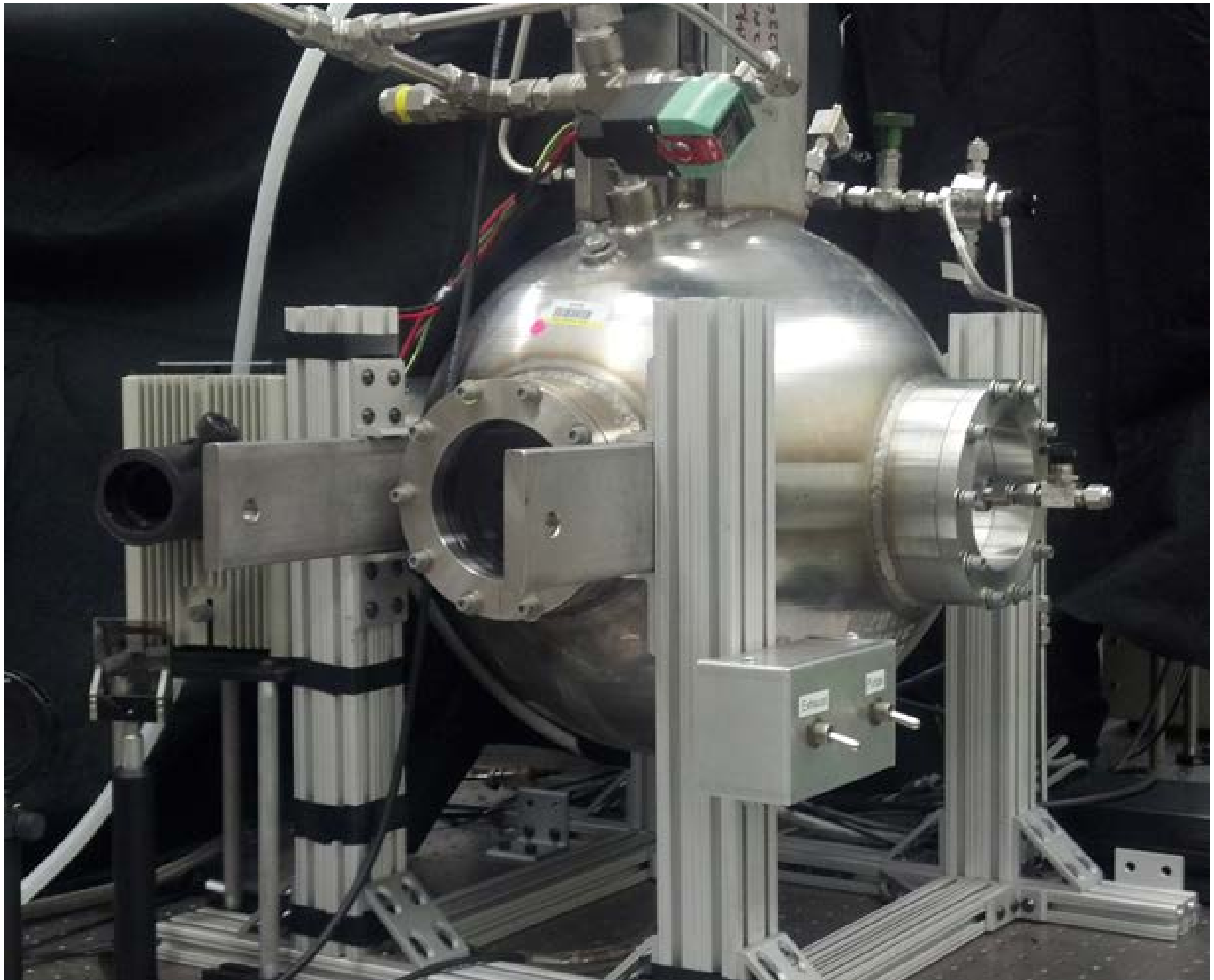
Lessons Learned:

New project. N.A.

Progress and Accomplishments

Constant Pressure Method, 30 L chamber:



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Project Integration and Collaboration

Project Integration:

Dr. Linteris is a member of committees addressing refrigerant flammability in AHRI, ASHRAE, and ISO. He actively collaborates with other refrigerant flammability researchers at Univ. of Maryland, UTRC, AIST (Japan), and Gexcon.

Partners, Subcontractors, and Collaborators:

Valeri Babushok (Kineticist, contractor),
Jeff Manion, Don Burgess (NIST Chemical Kinetics),
Piotr Domaniski, NIST HVAC Performance Group,
Mark McLinden, NIST Applied Chemicals and Materials Division
Prof. Zhang Chen, Peking Univ.,
Roe Burrell, Univ. So. Cal., NRC Post doc.

Communications:

Participation and presentations at AHRI, ASHRAE, ISO, and Combustion Institute meetings.

Next Steps and Future Plans

1. Work with researchers in MML to develop kinetic mechanisms and transport data for new low-GWP refrigerants.

2. Perform LBV experiments for low-GWP refrigerant-air mixtures.

3. Predict the LBV for 1-D, steady, planar and 1-D, unsteady, spherical flames using available codes.

4. Collaborate with external researchers to model 2-D time-dependent flames in the experiments.

5. Quantify uncertainties in measurements and predictive methods.

6. Develop tools for predicting the LBV of arbitrary refrigerant blends.

7. In the process, provide insight into:
   - the best test methods for characterizing the refrigerant flammability
   - the flammability properties of the refrigerants.

Project Budget

Project Budget: $2000k over three years.
Variances: None, **new project.**
Cost to Date: $100k
Additional Funding: NRC (Post-doc).

Budget History					
(past)		FY 2017 (current)		FY 2018 – FY2010 (planned)	
DOE	Cost-share	DOE	Cost-share	DOE	Cost-share
		$700k		$1300k	

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Project Plan and Schedule