Combustion of petroleum-based transportation fuels and their blends with biofuels:

a new approach for developing surrogates and understanding the effects of blending

March 7, 2019
Technology Session Area Review

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Goal Statement

-*develop*:

--*kinetic mechanisms matched with thermophysical properties that enable predicting combustion performance of liquid petroleum-fuel /biofuel blends relevant to Co-Optima*

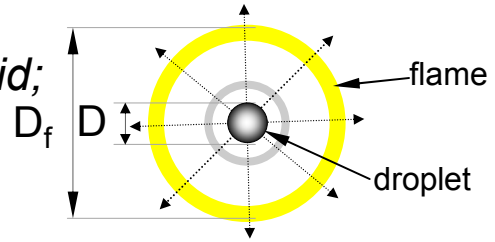
-*approach*:

--*surrogate-based for combustion chemistry: petroleum fuels are highly multicomponent;*

--*validation involves measuring, simulating, comparing*

--*sprays? engines?; current art for measurement prevaporizes liquid;*

--*our approach:conjoin the phases: 1-D droplet flame is bridge*



-*project outcome*

--*capability to enable detailed numerical modeling of combustion of biofuel blends to predict burning properties used for validating surrogates and kinetic mechanisms*

-*broad effort addresses Co-Optima Goals*

--*decreasing transportation-sector particulates and greenhouse gas emissions*

--*aligned with ADO-E barriers and challenges by its focus on a generalized predictive capability for biofuel combustion that can accommodate co-development of fuels and engines.*

Quad Chart Overview

Timeline

Project start date: January 15, 2017
(work began December 15, 2017)
Project end date: December 14, 2020
Percent complete: 36%

	FY 18	Total Planned Funding (FY 19 - Project End Date)
DOE Funded	$259,667	$872,124
Project Cost Share	$14,750	$111,036

•**Partners:**

Cornell (80%):

C. T. Avedisian, P. Pepiot, I. Keresztes

UCSD (20%):

K Seshadri, F.A. Williams

NREL:

R. Grout (national laboratory technical mentor)

Barriers Addressed

...lack of ab-initio models of fuel sprays or engines for validating biofuel kinetic mechanisms. This problem is addressed by using a sub-grid element of a spray – burning droplet – as a platform for developing such a capability. It is aligned with ADO-E barriers and challenges by its focus on a generalized simulation capability that can accommodate co-development of fuels and engines.

Objective

The objective is to develop a predictive capability of biofuel blends relevant to Co-Optima Program using simulated and experimental data for validation from the 1-D droplet flame. This capability will facilitate DOE's objectives to decrease particulate emissions and accelerate deployment of advanced biofuels.

End of Project Goal

Open-source code for direct numerical modeling of petroleum/biofuel combustion that predicts biofuel burn rates and conditions to form soot precursors; and experimental methodology to provide data for validation. Ultimate goal is to identify fuel properties that optimize engine performance, improve fuel economy, and reduce emissions.

1. Project Overview

"sprays set initial condition for combustion in engines"

***modeling is necessary to...**

- ***-predict influence of biofuel concentration***
- ***-facilitate new engine design concepts***
- ***-limit prototype testing***
- ***-reduce time to market***
- ***-lower consumer cost***

***BUT...sprays can't be ab-initio modeled**

- ***-soot/particulates***
- ***-evaporation (moving boundaries)***
- ***-detailed combustion kinetics***
- ***-variable properties, radiation***
- ***-multicomponent phase equilibrium***
- ***-turbulence,swirl,droplet interactions***

***sub-grid element of a spray: isolated droplet**

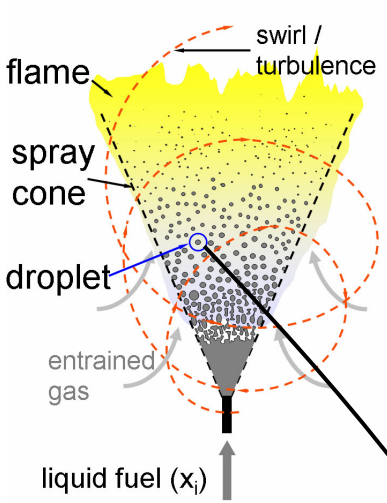
- ***-currently only configuration amenable to detailed modeling***

***team expertise:**

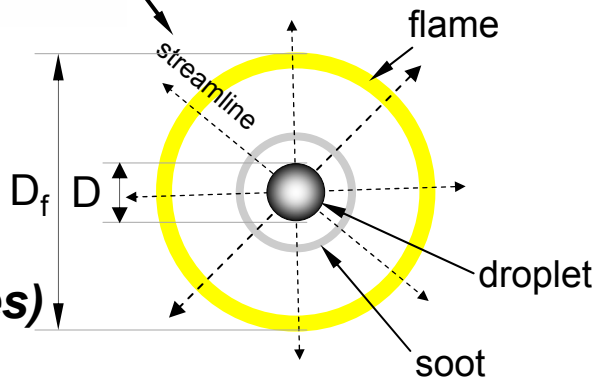
- ***-experimental (CU); modeling (CU, UCSD)***
- ***-surrogate-based approach***

***provide information on blending (burn rates, particulates)**

- ***-fundamental understanding***
- ***-practical guidelines***



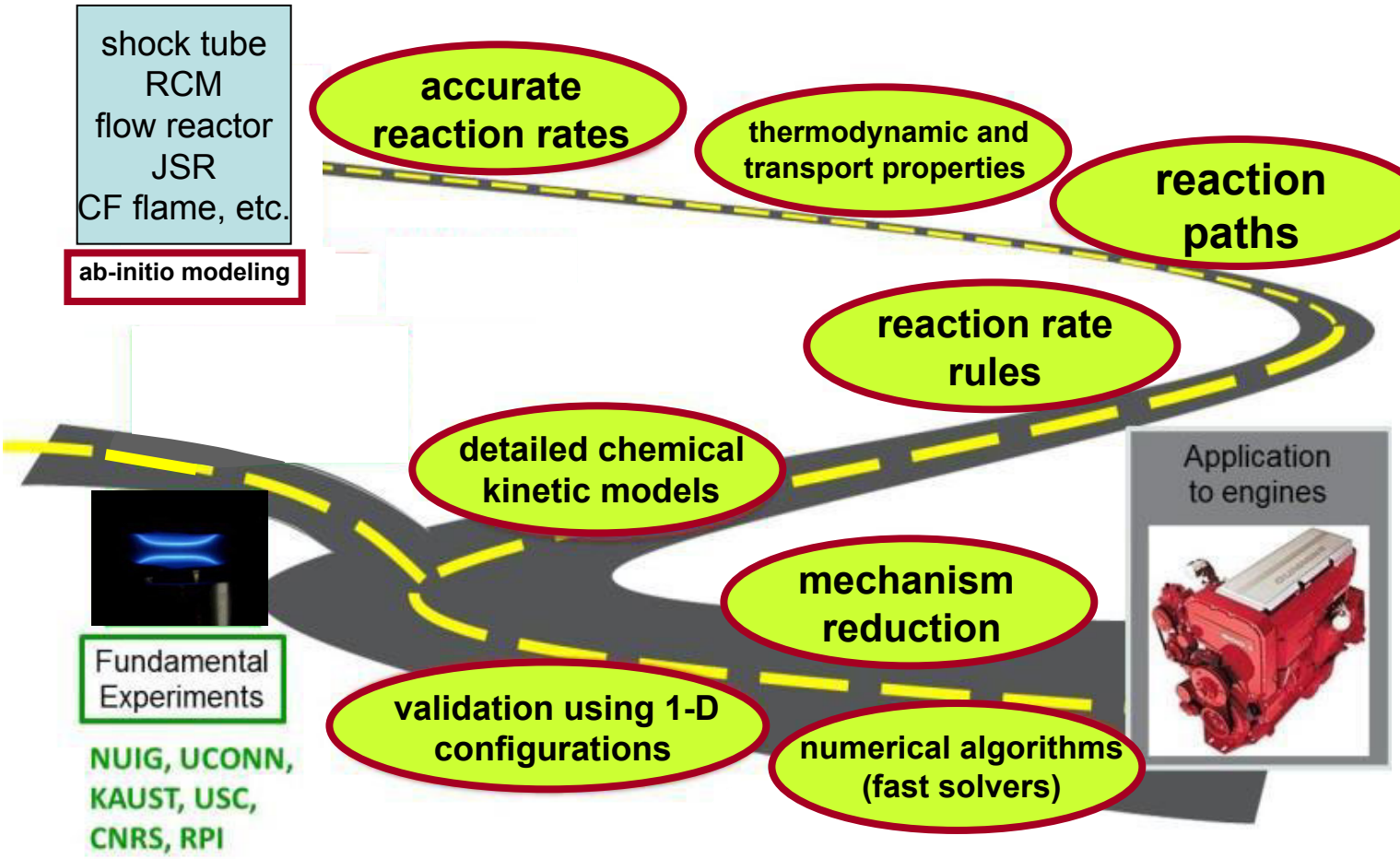
https://www1.eere.energy.gov/vehiclesandfuels/pdfs/presice_rpt.pdf



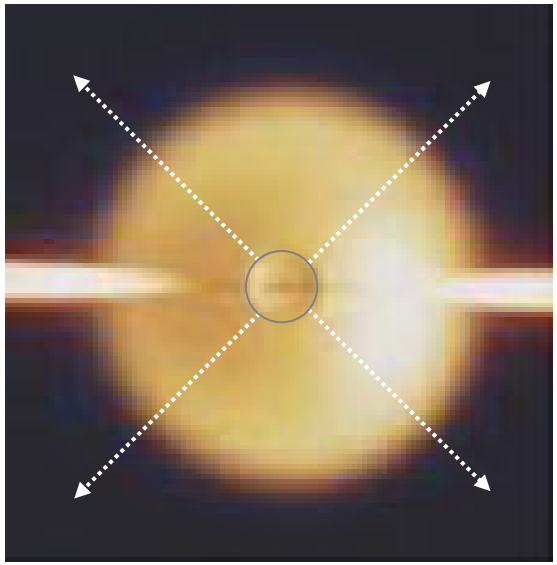
2. Approach

Roadmap for predictive capability of petroleum fuel blended with a biofuel for kinetic mechanism development

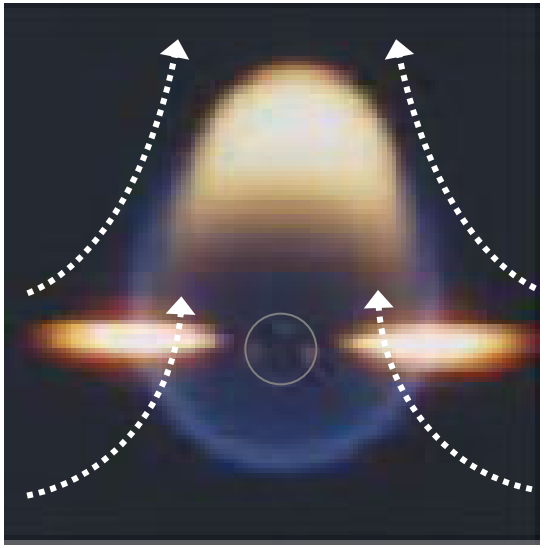
[R.L. McCormick,G. Fioroni, J. Szybist,T. Bays, P. Miles, M. McNenly, W. Pitz, J. Luecke, M. Ratcliff, B.Zigler, S. Goldsborough, PROJECT # FT-038, U.S. DOE, June 9, 2016]



Creating 1-D Droplet Burning Configuration

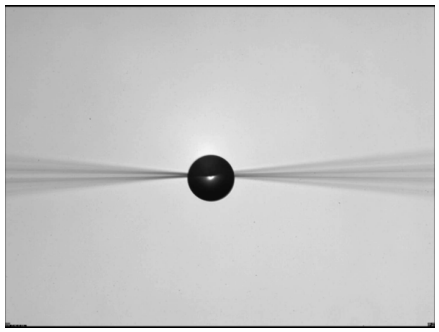


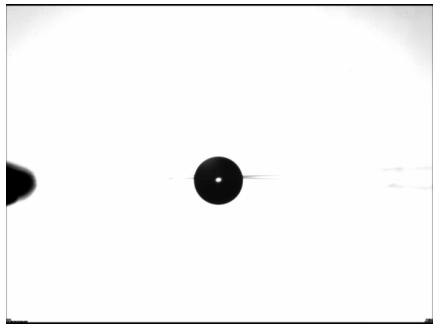
1-D

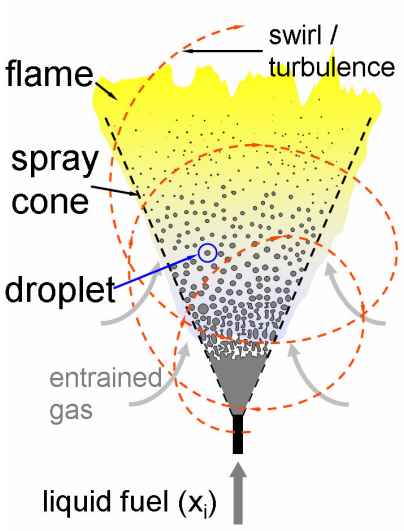


2-D

-perform experiments in buoyuancy-free environment; stagnant ambience (to prevent movement of droplet)
-1-D to provide benchmark data of biofuel blends and their surrogates;
-data important to validate simulation







2. Approach (contd)

organization/management/key milestones

A. Institutions

-Cornell responsible for experiments, surrogate development, kinetic modeling

-UCSD responsible for simulations of biofuel mixture effects

B. Project organized around two budget periods (BP1,2)

1. BP1 (18 mths): model fuel system (heptane/isobutanol)

GO/NOGO milestone

A. experiments:

--demonstration of ability to ignite heptane/isobutanol mixtures

--extraction of quantitative data from video

B. simulations:

--should be within specified tolerance of experiments

2. BP2: (18 mths): gasoline+biofuel

-develop surrogates

-develop kinetic mechanism and transport property database

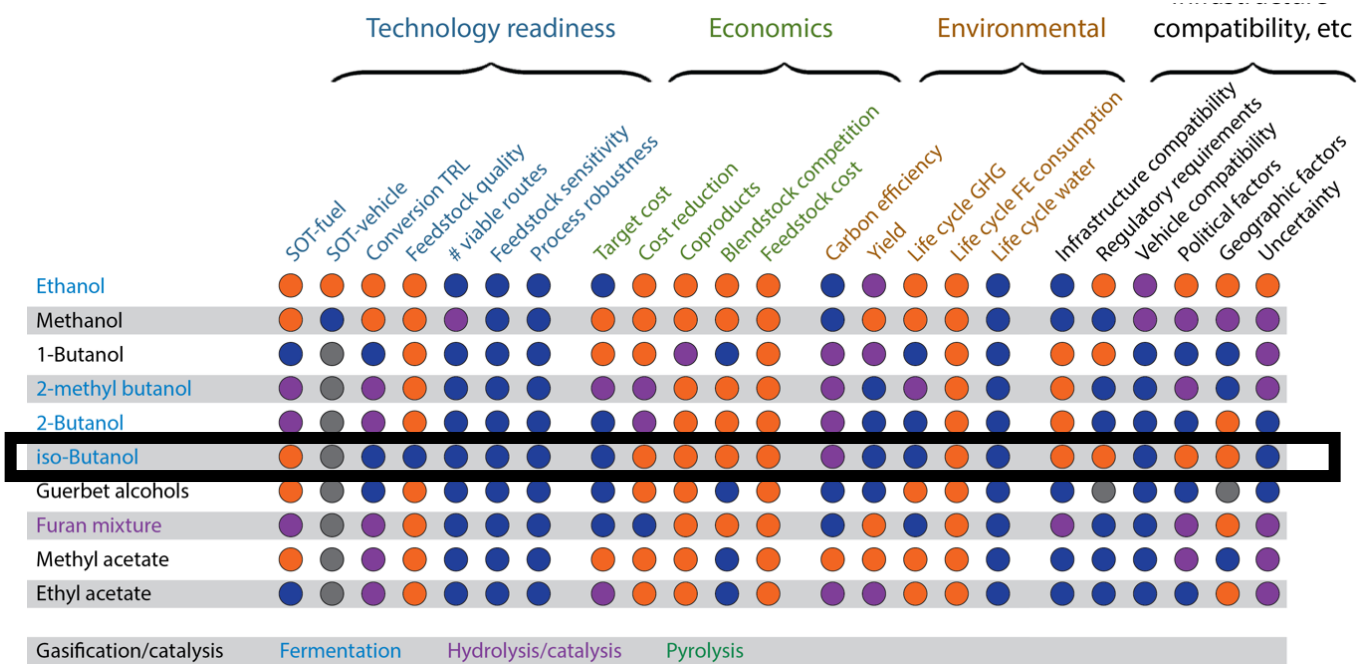
-experiments and simulations on fuel system

2. Approach (contd)

BP1: model fuel system selected is a binary mixture

heptane: gasoline "primary reference fuel" component; diesel kinetic mechanism

iso-butanol: highly ranked based on MF scores



- favorable
- neutral
- unfavorable
- insufficient data

Tier 1: viable feedstock

Tier 2: desired performance (~40)

Tier 3: does it merit focused attention?

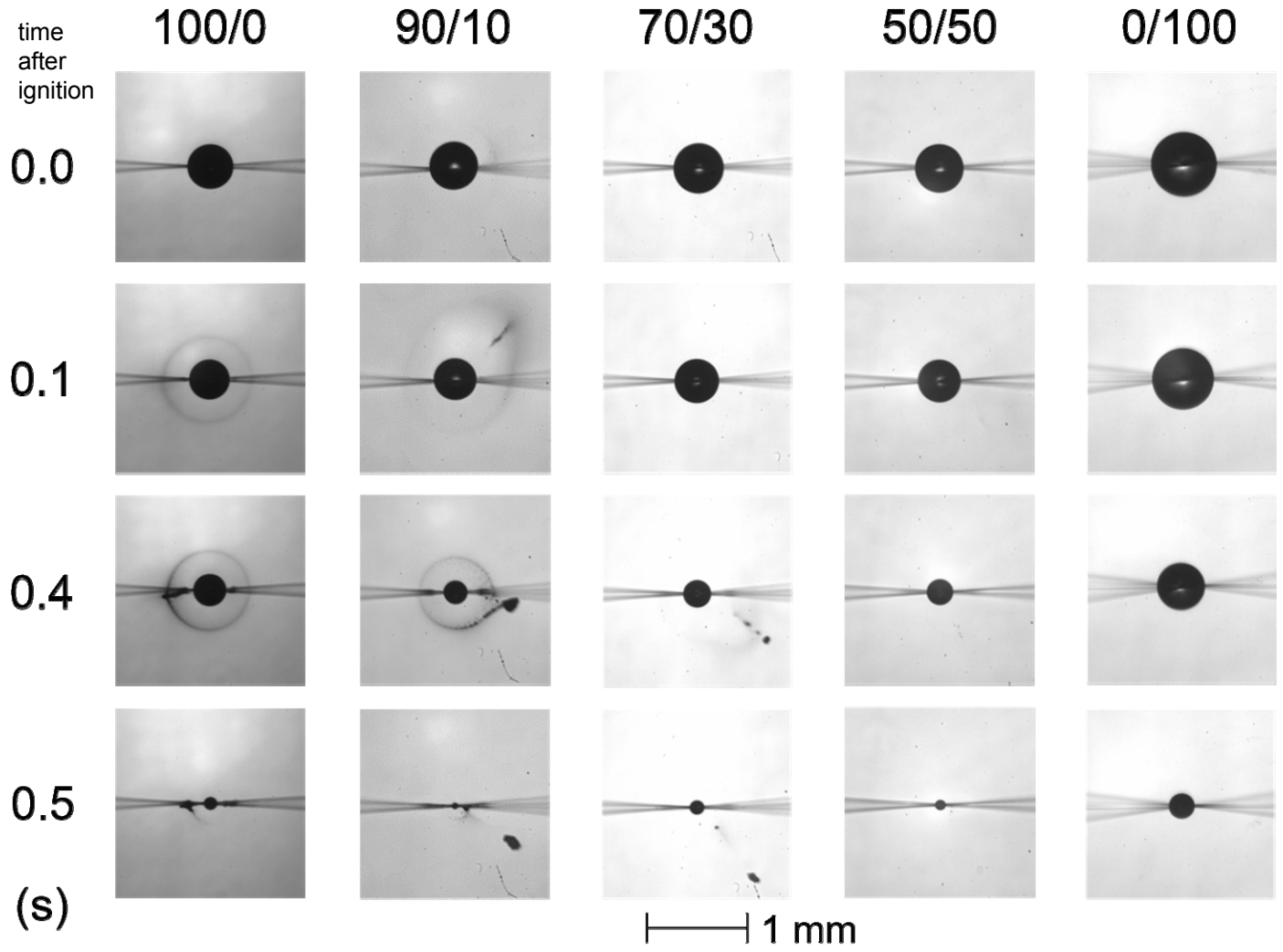
J. Farrell, D. Gaspar, P. Miles, J. Szybist, J. Dunn, M. McNenly, D. Longman, J. Holladay, R. Wagner, C. Moen "Co-Optimization of Fuels&Engines (Co-Optima) Initiative", SAE 13th International Conference on Engines & Vehicles, September 13, 2017, Capri, Italy

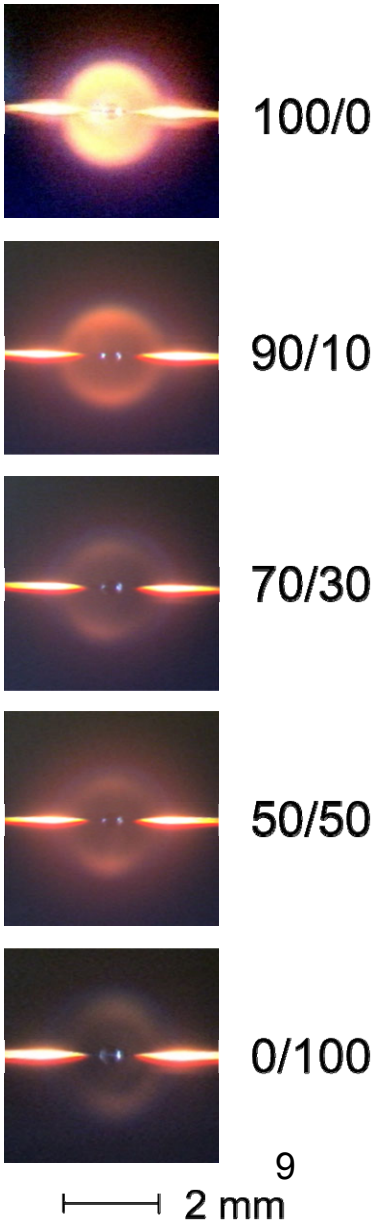
-boiling points are close
-binary simplest mixture (easy sweep through composition space)
-kinetic mechanisms are known
-surrogate not necessary

BP2: gasoline/biofuel

3. Technical Accomplishments

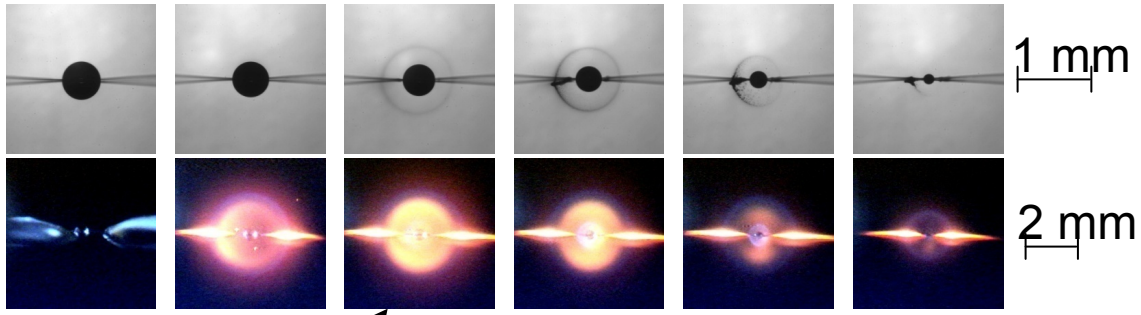
heptane/isobutanol





3. Technical Accomplishments (contd) (data from video images)

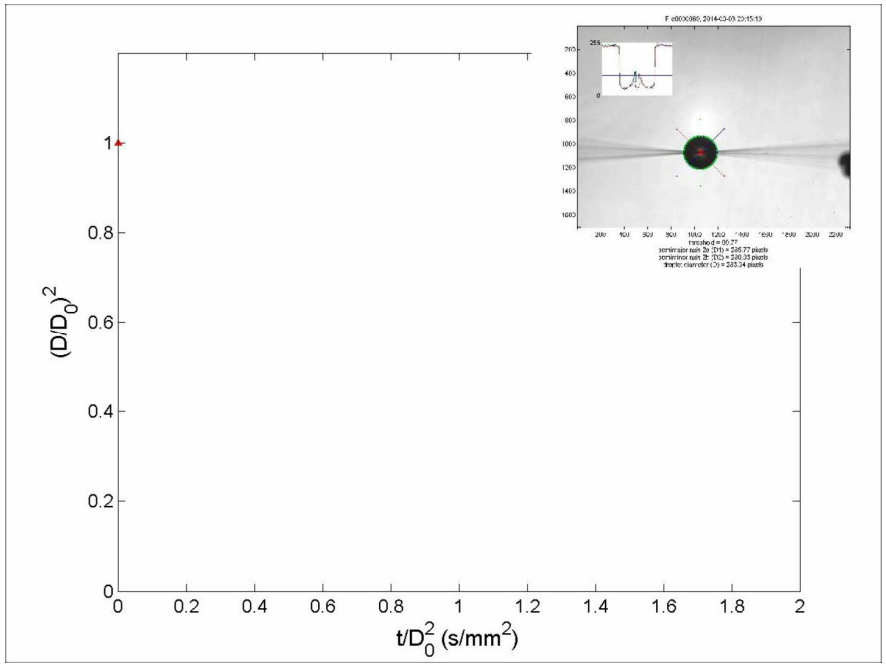
‘raw’ data

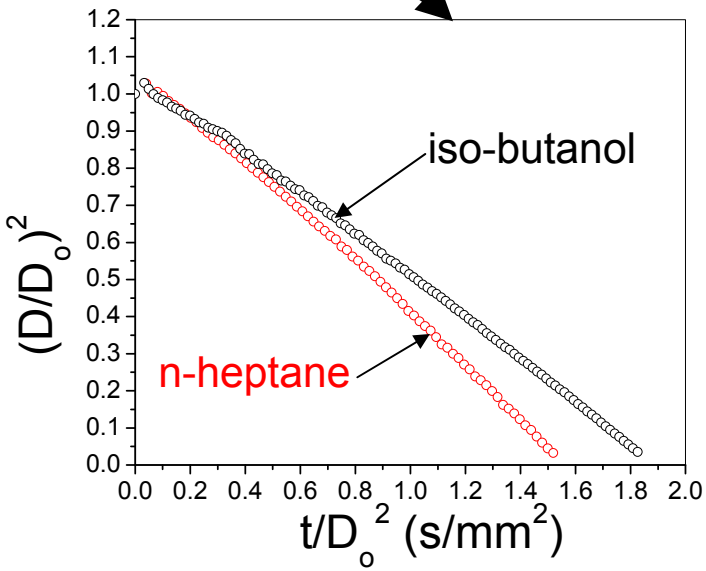


n-heptane

how to get from here to here?

n-butanol





3. Technical Accomplishments (contd)

Detailed Numerical Model [OpenSMOKE++]

[1ST-principle solver, modified for surrogate mixtures]

Input:
kinetics;
transport
properties

Gas Phase:
- Multi-component molecular diffusion
- Detailed chemical kinetics (thousands)
- Unsteady transport
- Radiation

Liquid Phase:
- Mass
- Species
- Energy
- unsteady
- (ideal
- miscible mixtures; or nonideal (equate fugacities))

$$\frac{d r_s}{d t} \quad \dot{m}_v \quad \dot{m}_p \quad D_{l,i} \frac{\partial Y_{l,i}}{\partial r} \quad D_{g,i} \frac{\partial Y_{g,i}}{\partial r} \quad \lambda_l \frac{\partial T}{\partial r} \quad \lambda_g \frac{\partial T}{\partial r}$$

Droplet Surface:
- Surface regression – Adaptive Grid
- Evaporation of fuel/moving boundary

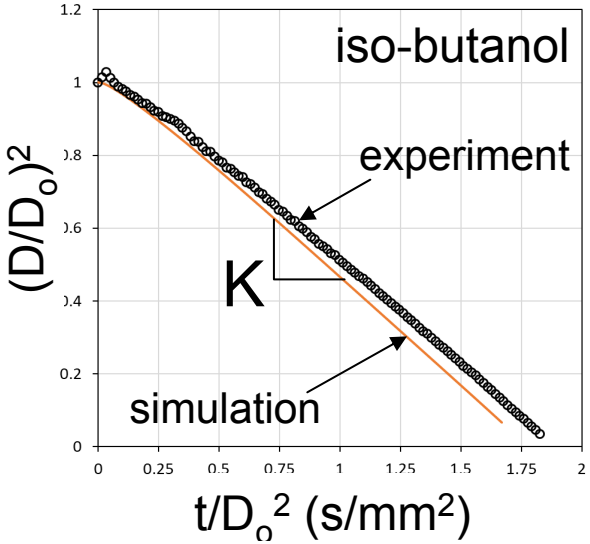
Output:
$D(t)$, $D_f(t)$
D_{fmax}, $K(t)$

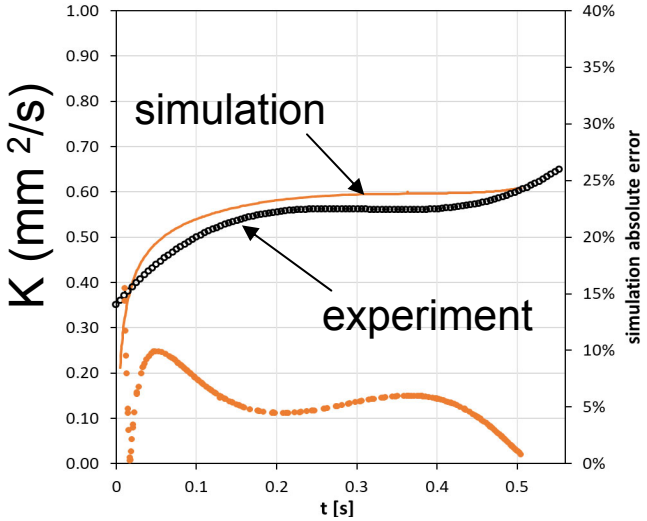
Kinetic Mechanism:

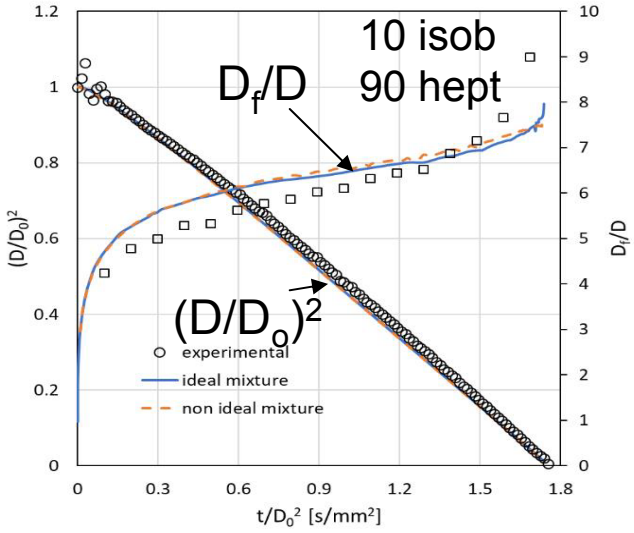
*POLIMI PRF 1412 mechanism 225 species, 7645 reactions (reduced from the POLIMI 1800 mechanism of 482 species, 19,072 mechanism (for diesel, gasoline, jet fuels, alcohols...))

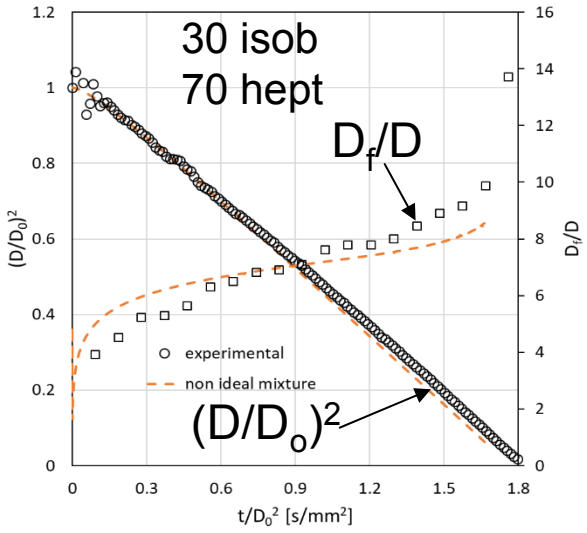
3. Technical Accomplishments (contd)

Comparing simulated and measured mixture burning properties







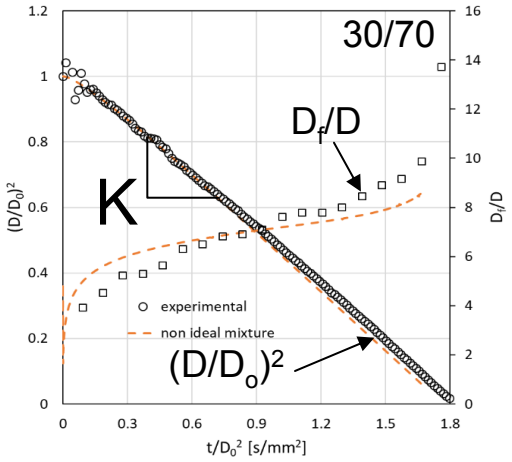


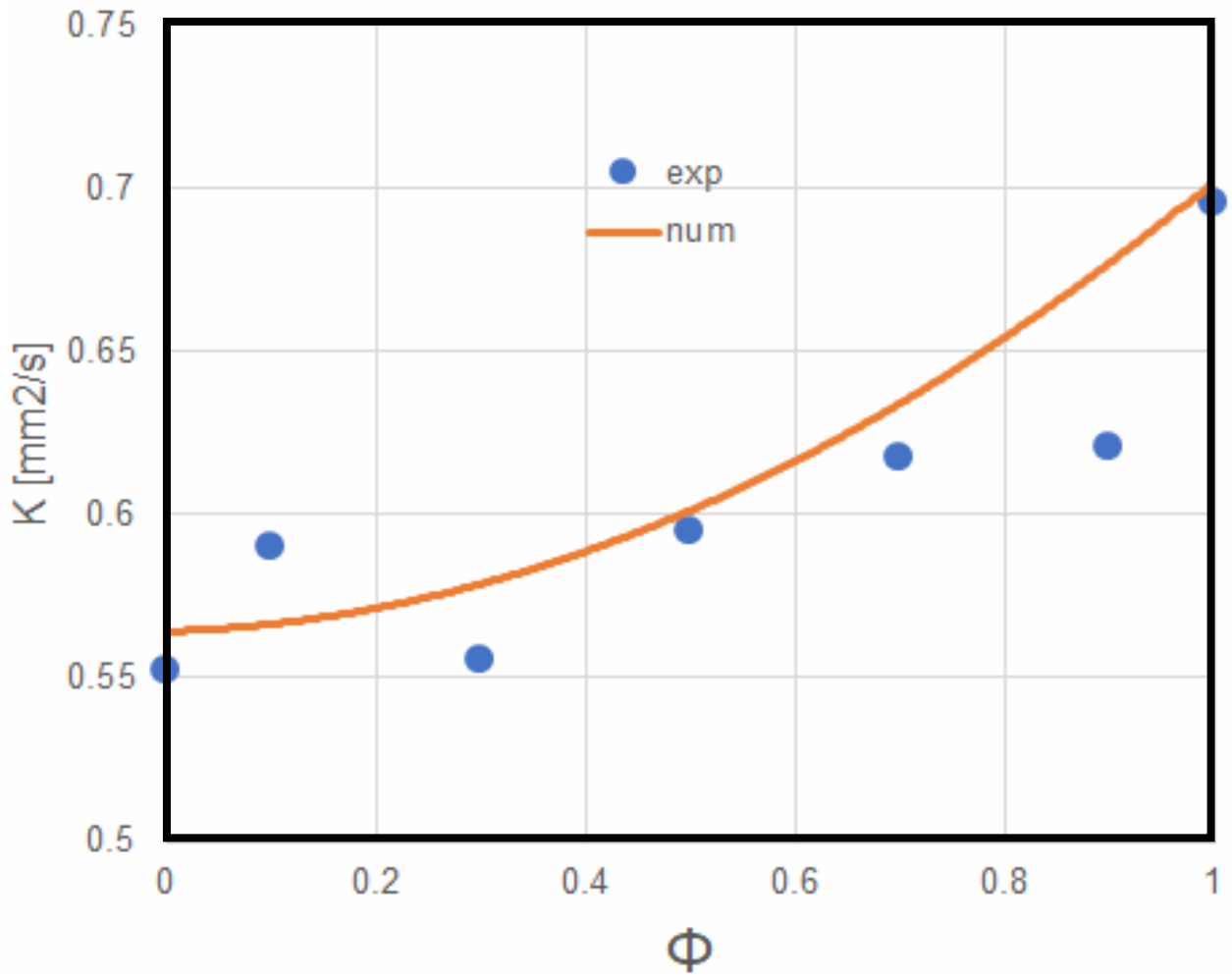
--excellent agreement; compositional space investigated: **0/100, 10/90, 30/70, 50/50, 70/30, 100/0**

--heptane/isobutanol behaves as a nearly ideal liquid mixture: Raoult's law

--nonideal: $f_{iL} = f_{iv}$ (Peng-Robinson EOS (1976) used)

3. Technical Accomplishments (contd)



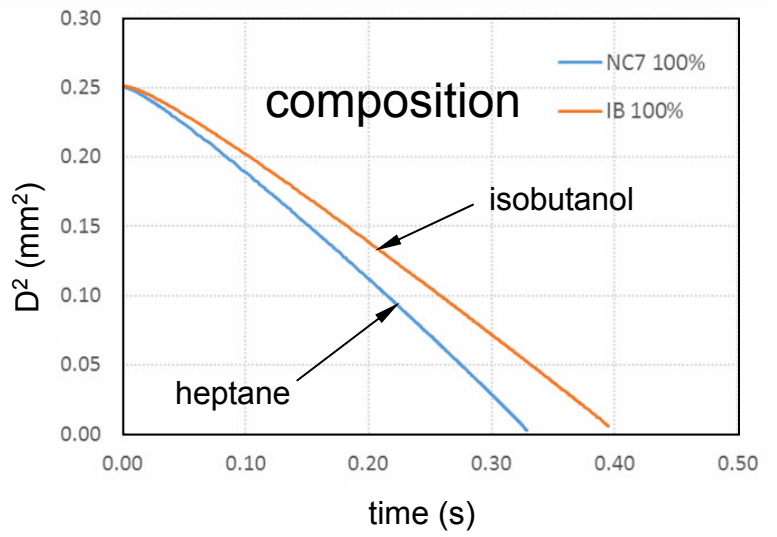


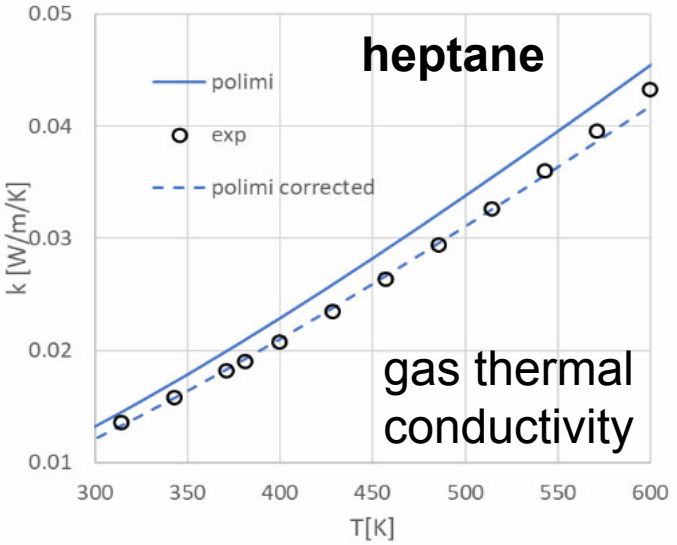
volume fraction heptane

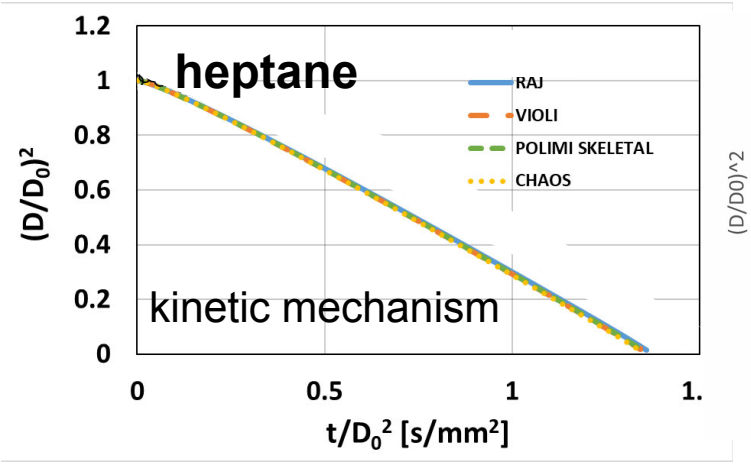
differences are within 20% GO/NOGO decision point

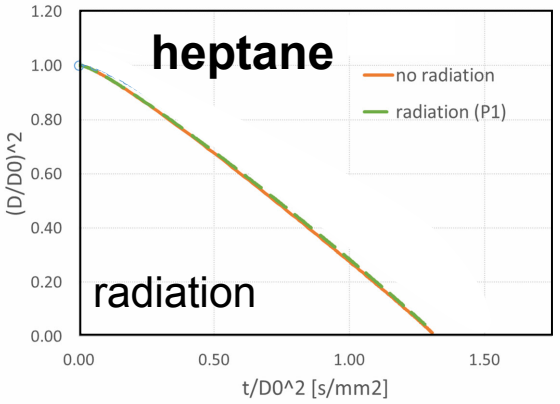
3. Technical Accomplishments (contd)

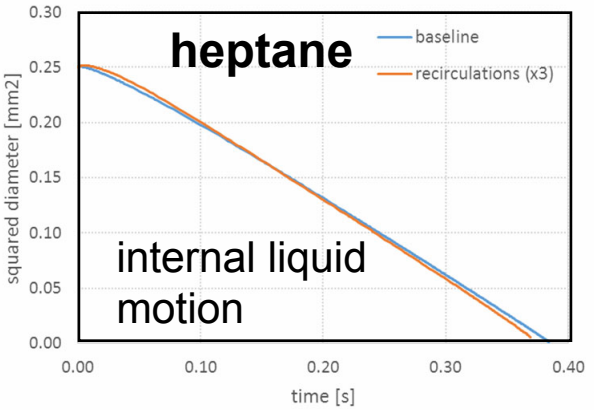
What most influences burning?









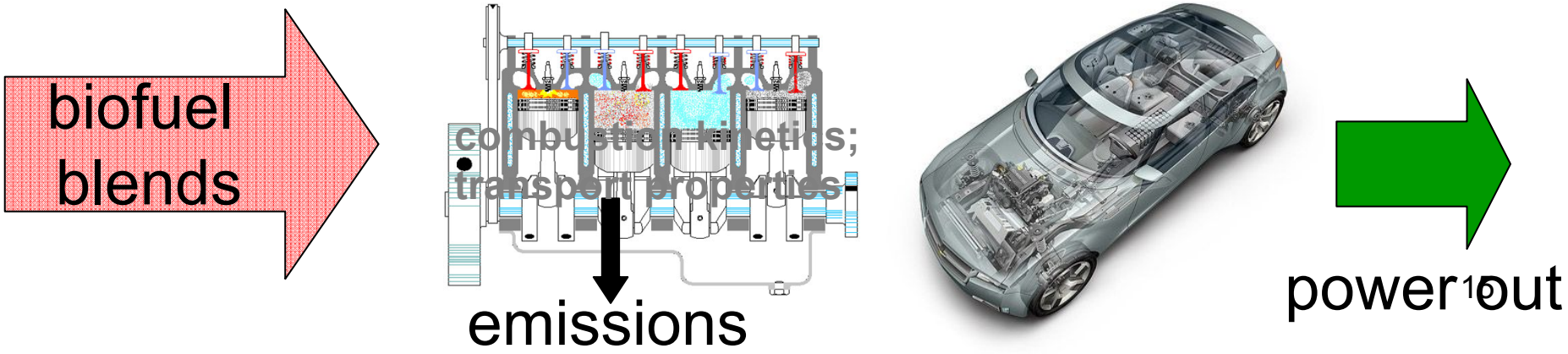


4. Relevance

-liquid fuel burning is complex (sprays, unsteady, phase equilibrium, moving boundaries, radiation, emissions, etc.); 1-D multiphase (droplet) simplifies while allowing consideration of other effects that are challenging (currently) to model for a spray

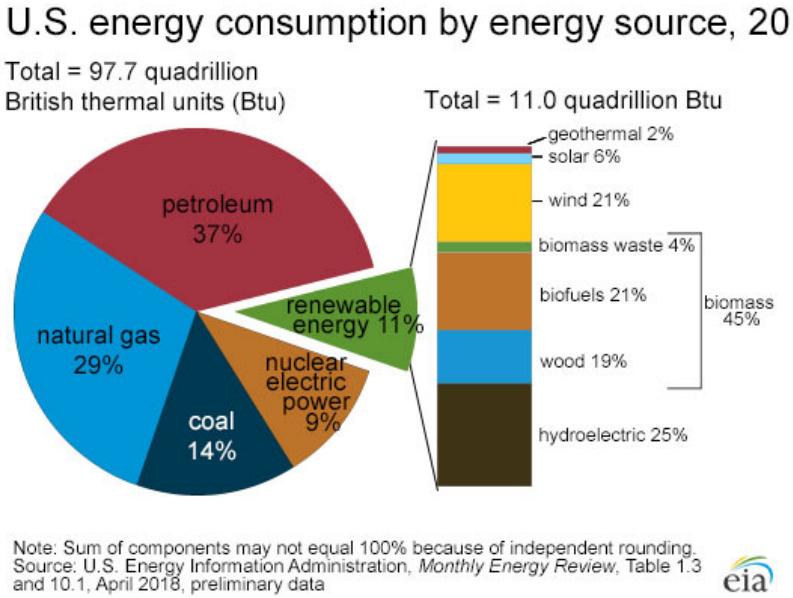
-opensource simulation capabilities enhance development

Liquid fuels and combustion engines will be dominant



4. Relevance (contd)

"The needs of power and transportation systems...will very likely require *liquid hydrocarbon fuels for years to come*..."



blending is simple strategy; current understanding of performance (on fundamental level) is lacking; liquids complicate the understanding; project provides sound basis for predicting blend performance

"...*combustion will remain a dominant energy* and power *source* for world society *for another century*"

https://epdf.tips/transforming-combustion-research-through-cyberinfrastructure.html

https://www1.eere.energy.gov/vehiclesandfuels/pdfs/presice_rpt.pdf

5. Future Work

BP1: (December 15, 2017- June 15, 2019)

**complete heptane/isobutanol model system experiments and simulations (achieve go/nogo decision point for experiments (ignition/data, simulations of soot precursor distribution))*

BP2: (June 16, 2019 - October 15, 2020)

**select biofuels for BP2 (probably isobutanol and a furan mixture)*
**develop gasoline/biofuel surrogates using one or more droplet properties as targets (constrained optimization process*
**experiments (gasoline; biofuel; gasoline/biofuel mixtures)*
**develop combustion kinetic mechanism of surrogates and reduced mechanisms*
**simulations: data to validate kinetic mechanism and surrogate formulation with droplet burning properties*
**availability of open-source code for simulation*

Risk factors:

fuel ignitability (sparks and alternatives); code convergence (mesh; simulating initial condition; alter mixture model; mixing rules)

Summary

1.Overview

-Project concerns combustion of liquid transportation fuels (gasoline) blended with biofuels and developing their surrogates and combustion kinetic mechanisms

-Kinetic mechanisms will be validated against 1-D droplet flame properties; open source code will be provided to predict mixture effects on fuel burning.

2. Approach

-Sub-grid element of spray (droplet) is configuration for addressing spray complexities (unsteadiness, mixture effects, variable properties, radiation, etc.)

3. Technical Accomplishments

-Simulations show good agreement with experiments for heptane/isobutanol

-Results sensitive to fuel composition and transport properties

4. Relevance

-Sprays set initial condition for combustion in engines but too difficult to model

-1-D droplet flames link to spray flames and can be modeled in detail; building block for spray/engine simulations

5. Future work

-Project on track to move to gasoline/biofuel mixtures in BP2

--surrogate will be needed;

--develop using one or more targets from droplet burning (K, peak droplet flame diameter are possibilities)

-Develop detailed and reduced surrogate kinetic mechanisms; use 1-D droplet flame data for validation

publications

C. T. Avedisian, K. Skyllingstad, R.C. Cavicchi,C. Lippe, M.J. Carrier. "On the initiation of flash boiling of multicomponent miscible mixtures with application to transportation fuels and their surrogates," Energy & Fuels, 32, 9971-9981 (2018).

presentation

A. Dalili, J.D. Brunson, P. Dou, S. Guo, M. C. Hicks, A. P. Reeves, C.T. Avedisian, "Spherical flame characteristics of heptane/iso-butanol mixture droplets," poster ID# 312, 34th Annual Meeting, American Society of Gravitational and Space Research, Bethesda, MD October 28 November 3, (2018).

A. Dalili, J. Brunson, C.T. Avedisian, "A simple biofuel surrogate blend for diesel fuel: heptane/iso butanol mixtures and their droplet burning characteristics," paper no. P55, Spring Technical Meeting, Canadian Section, Combustion Institute, Toronto, Ontario, Canada, May 14-17 (2018).

A. Dalili, J.D. Brunson, C.T. Avedisian, "Combustion Characteristics of Heptane/iso-butanol Mixture Droplets," poster #1, American Society of Engineering Education, St. Lawrence Section, 2018 Conference, Ithaca, New York, April 20-21 (2018).

P. Sharma, H. Goyal, P. Pepiot, An Analytical Jacobian Generator for Reduced Chemical Kinetic Models Involving Quasi-Steady-State Assumptions, Eastern States Section, Combustion Institute, Spring Technical Meeting, Pennsylvania State University, PA. (2018).

Thank you

Questions?

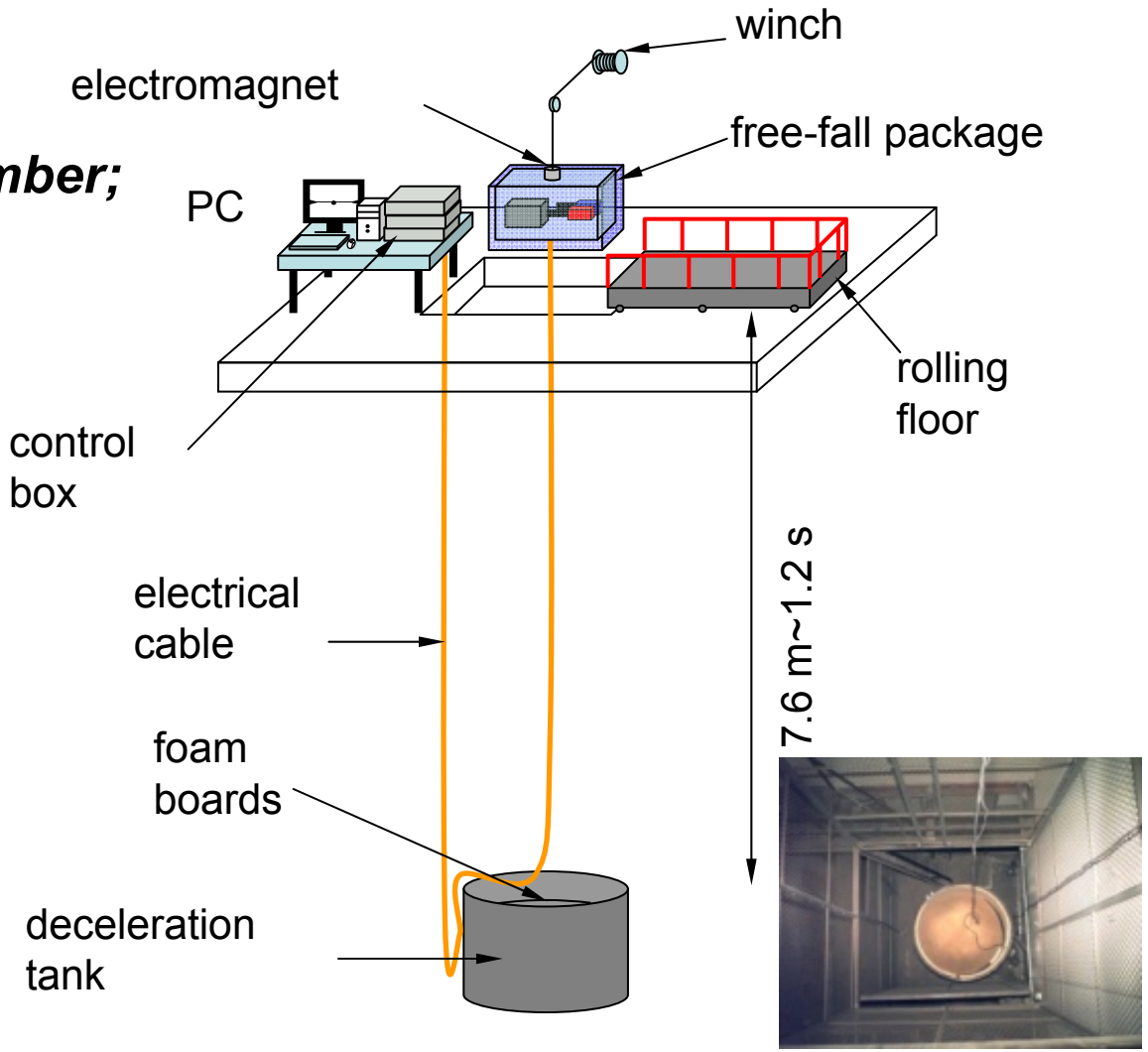
Backup Slides

Experimental Hardware

experiments performed in free-fall

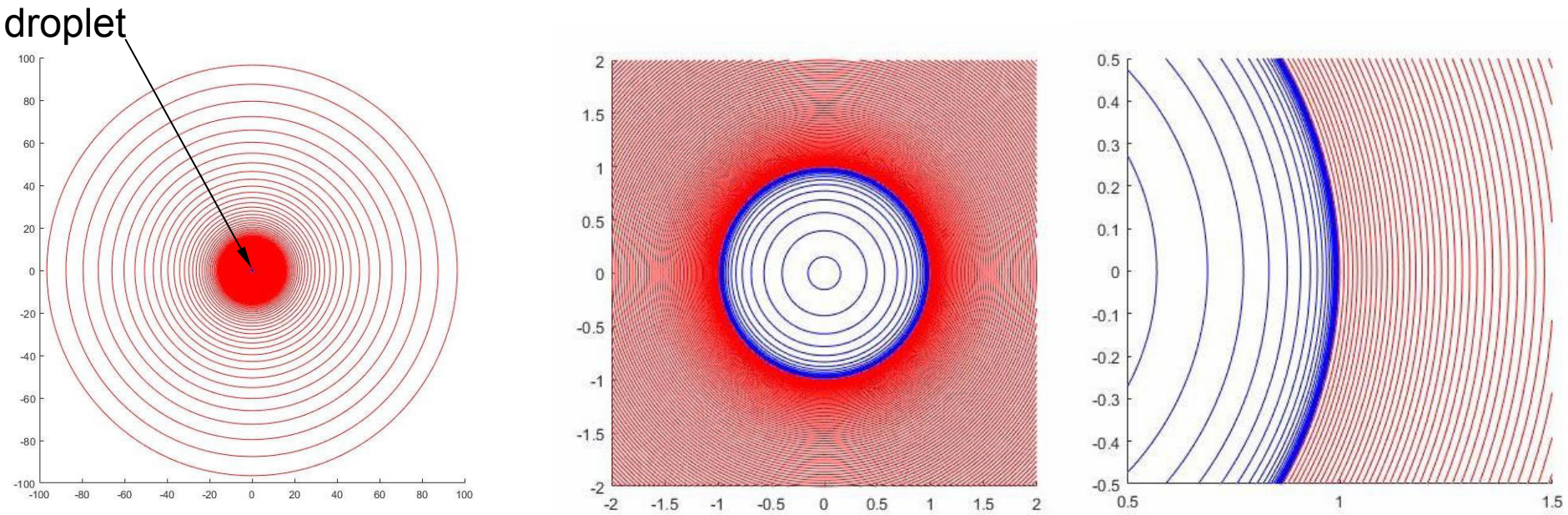
<u>minimize bouyancy</u>
experiments in free-fall chamber;

<u>minimize forced convection</u>:
stagnant ambience;
prevent droplet from moving
stagnant ambience;
(restrain droplet)



Computational Grid

-computational grid of solution domain developed;
(blue, liquid; red, gas)
-50 points for liquid phase; 300 points for gas (grid-independence)
(grid is finer across interface)



Surrogate development process

***Constrained Optimization Approach**

[Narayanaswamy, K., Pepiot, P, Pitsch, H., "A component library framework for deriving kinetic mechanisms for multi-component fuel surrogates: application for jet fuel surrogates," Comb. Flame 165, 288–309 (2016).]

***other surrogate Generators**

Pitz, W. et al. "Chemical kinetic models for advanced engine combustion," Project ID # ACE013, Annual Merit Review, Department of Energy, June 7, 2016 Washington, DC.

C.J. Mueller, W.J. Cannella, T.J. Bruno, B. Bunting, Heather D. Dettman, J.A. Franz, M.L. Huber, M.Natarajan, W.J. Pitz, M.A. Ratcliff, K.Wright, Methodology for formulating diesel surrogate fuels with accurate compositional, ignition quality and volatility characteristics, Energy&Fuels, 26, 3284-3303 (2012)

burning histories of heptane/isobutanol droplets