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

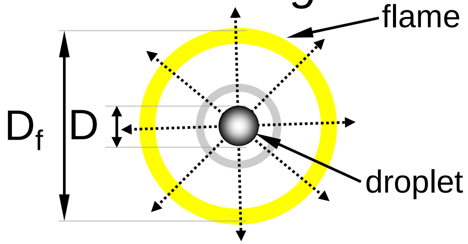
-<u>develop</u>:

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

-<u>approach</u>:

--surrogates, necessary because petroleum fuels are highly multicomponent

--use data for validation from multiphase burning configuration that bridges to sprays and engines which is <u>amenable to detailed numerical modeling</u>: 1-D droplet flame



-<u>project outcome</u>

--simulation capability to enable detailed numerical modeling of combustion of biofuel blends to predict the burning properties relevant to 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.

where we are currently; barriers/objetives how it's done nowb

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)

importance of sprays

Barriers Addressed

The development of petroleum fuel/biofuel blends is facilitated by identifying the operational parameters that influence combustion. The barrier to this end is lack of ab-initio models of fuel sprays which set the initial conditions for combustion in engines. This project addresses this problem by using a detailed numerical model of a sub-grid element of a spray - isolated droplet - as a platform to validate detailed kinetic mechanisms of biofuel blend surrogates that are necessary for simulating engine performance. The project 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 for petroleum fuel/biofuel surrogate blends relevant to Co-Optima Program using 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.

project overview: relevance of 1-D droplet

1. Project Overview

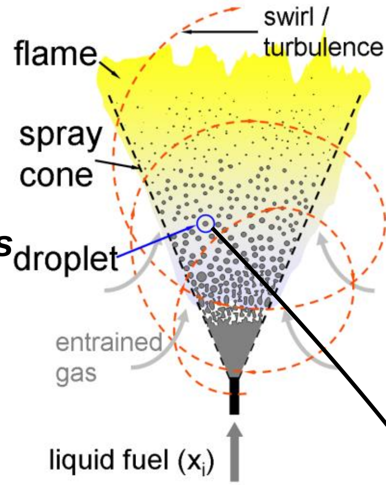
*”sprays set initial condition for combustion in engines”

*blending with biofuels reduces petroleum consumption

*modeling sprays is important to...

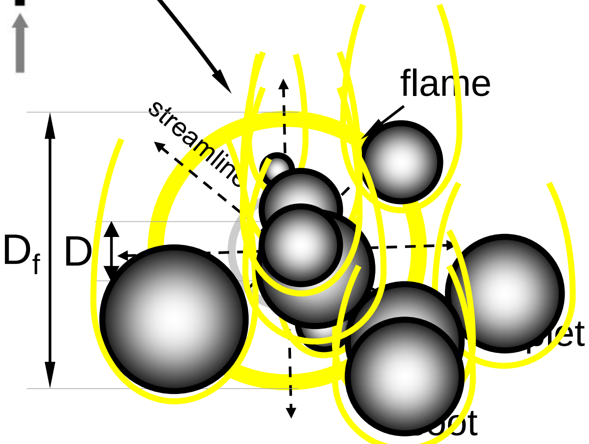
- -predict influence of the biofuel component
- -facilitate new engine design concepts
- -limit prototype testing
- -reduce time to market
- -lower consumer cost
- -validate chemical and property inputs to engine solvers

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



*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

- -can model above effects (currently the only configuration)

*team expertise:

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

*provide information on blending effects (burn rate, particulate)

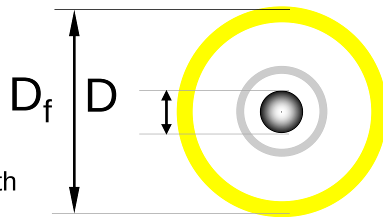
- -fundamental understanding; practical guidelines

Approach: based on roadmap

2. Approach

Roadmap for predictive capability of combustion of a liquid fuel blended with a biofuel

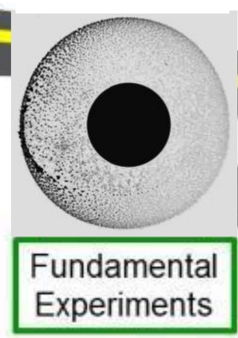
[R.L. McCormick,G. Fioroni, J. Szybist,T. Bays, P. Miles, M. McNenly, W. Pitz, J. Luecke, M. Ratcliff, B.Zigler, S. Goldsborough, PROJECT # FT-038, U.S. DOE, June 9, 2016]



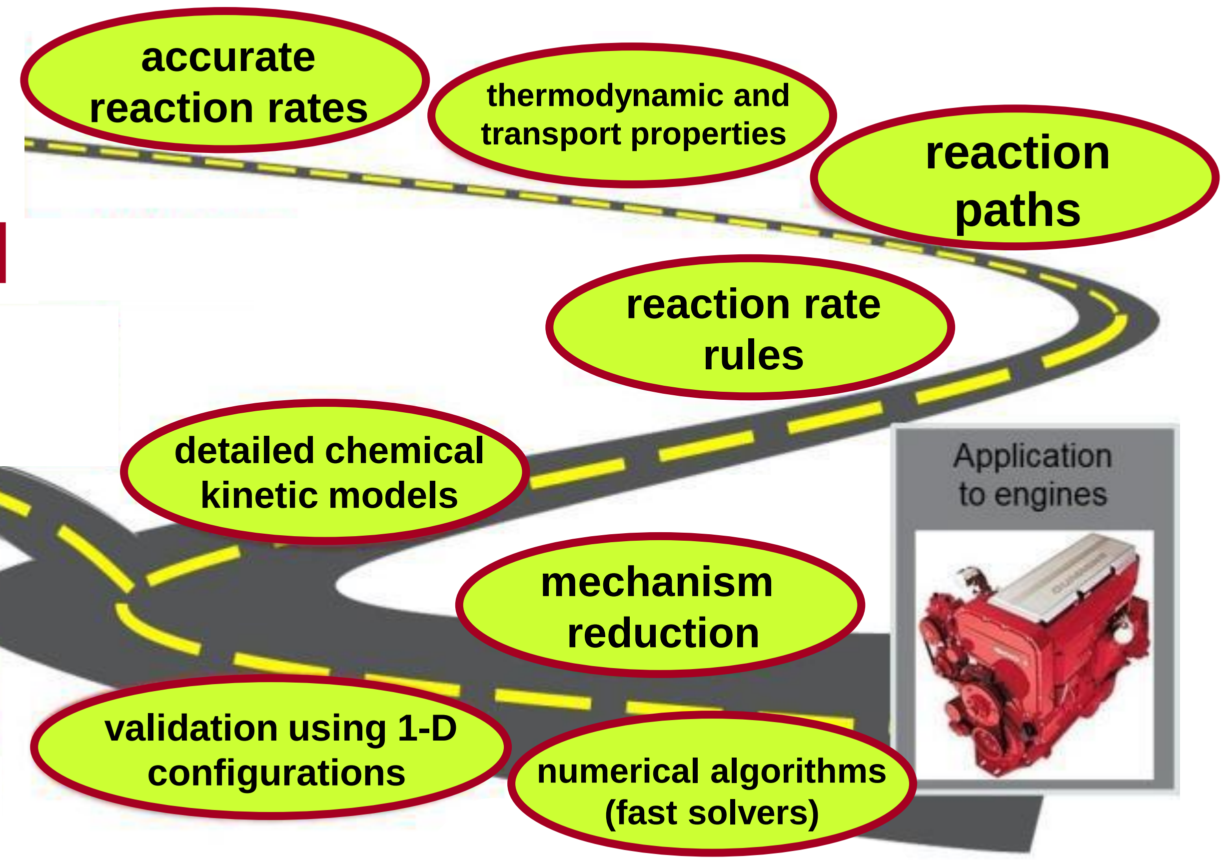
MULTIPHASE with

- unsteady
- variable properties
- moving boundaries (liquid vaporization)
- miscible mixture effects
- radiation
- soot (tractable for 1-D)
- detailed combustion kinetics

ab-initio modeling



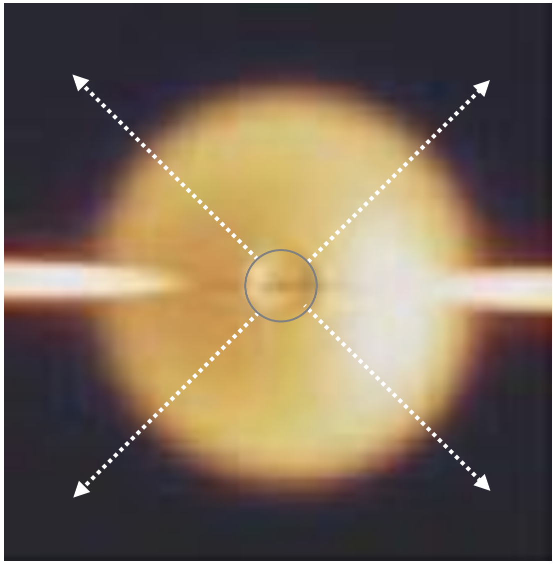
NUIG,UCONN, KAUST,USC, UCSD,CNRS, RPI



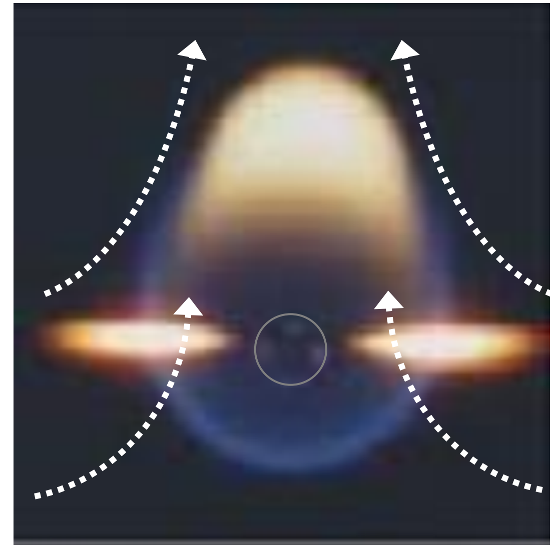
1-D Droplet (multiphase)

experiments (how to create 1-D

Creating canonical configuration for liquid fuel combustion

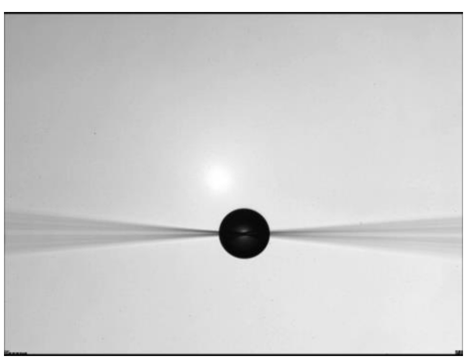


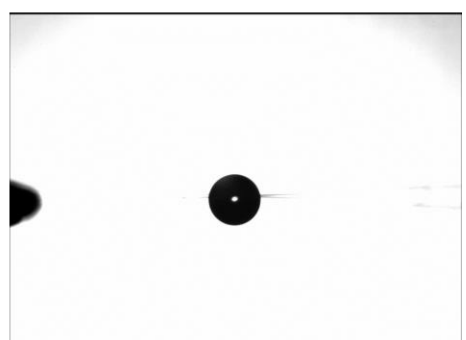
1-D

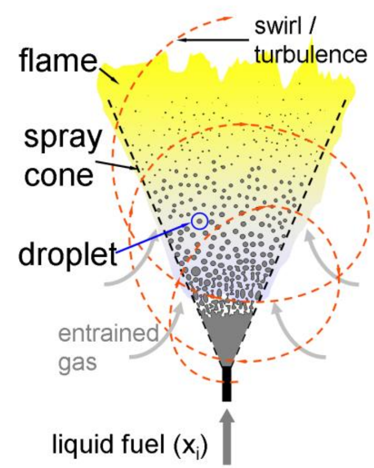


2-D

-perform experiments in buoyancy-free environment; stagnant ambience (restrict droplet motion)
-1-D useful to benchmark biofuel blends and their surrogates;
-data important to validate simulation







project management, timeline, go/nogo;

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:

   --miscible mixtures

   --should be within specified tolerance of experiments

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

   -develop surrogates, kinetic mechanism, transport property database

   -experiments and simulations on fuel system

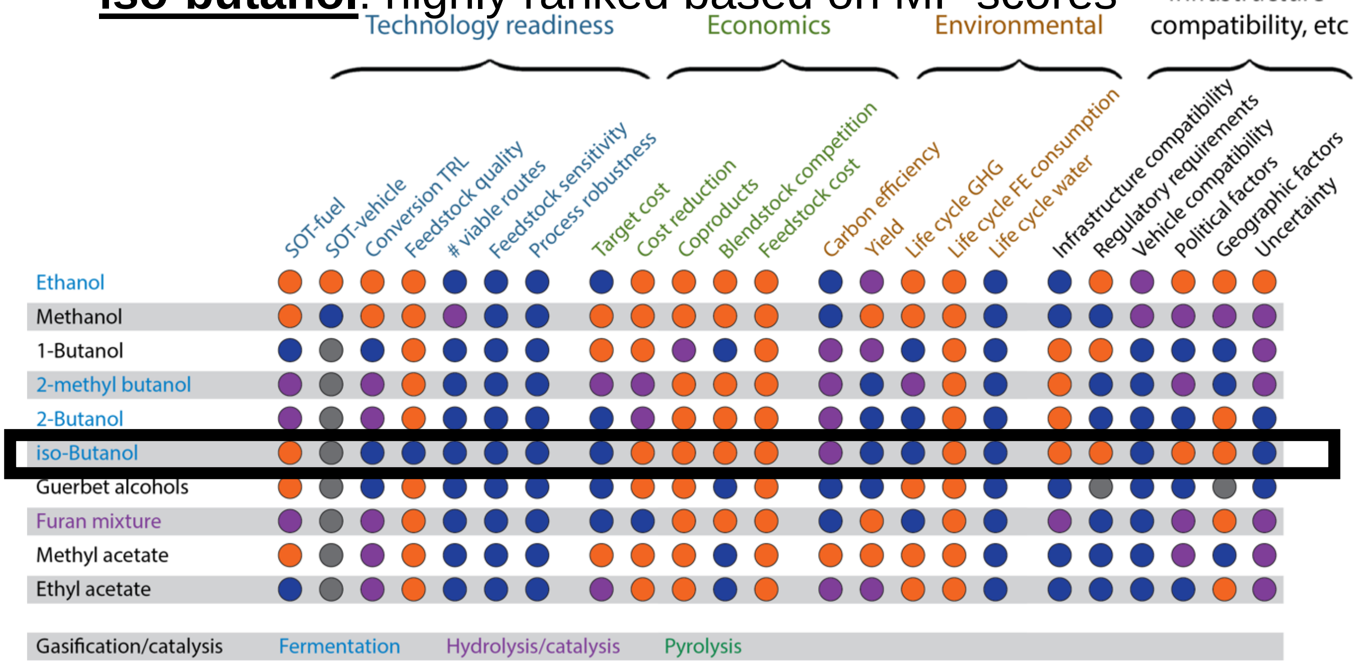
rationale for model fuel system in BP1

2. Approach (contd)

BP1: model fuel system selected is a binary mixture

heptane: simplest diesel surrogate; gasoline "primary reference fuel" component

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

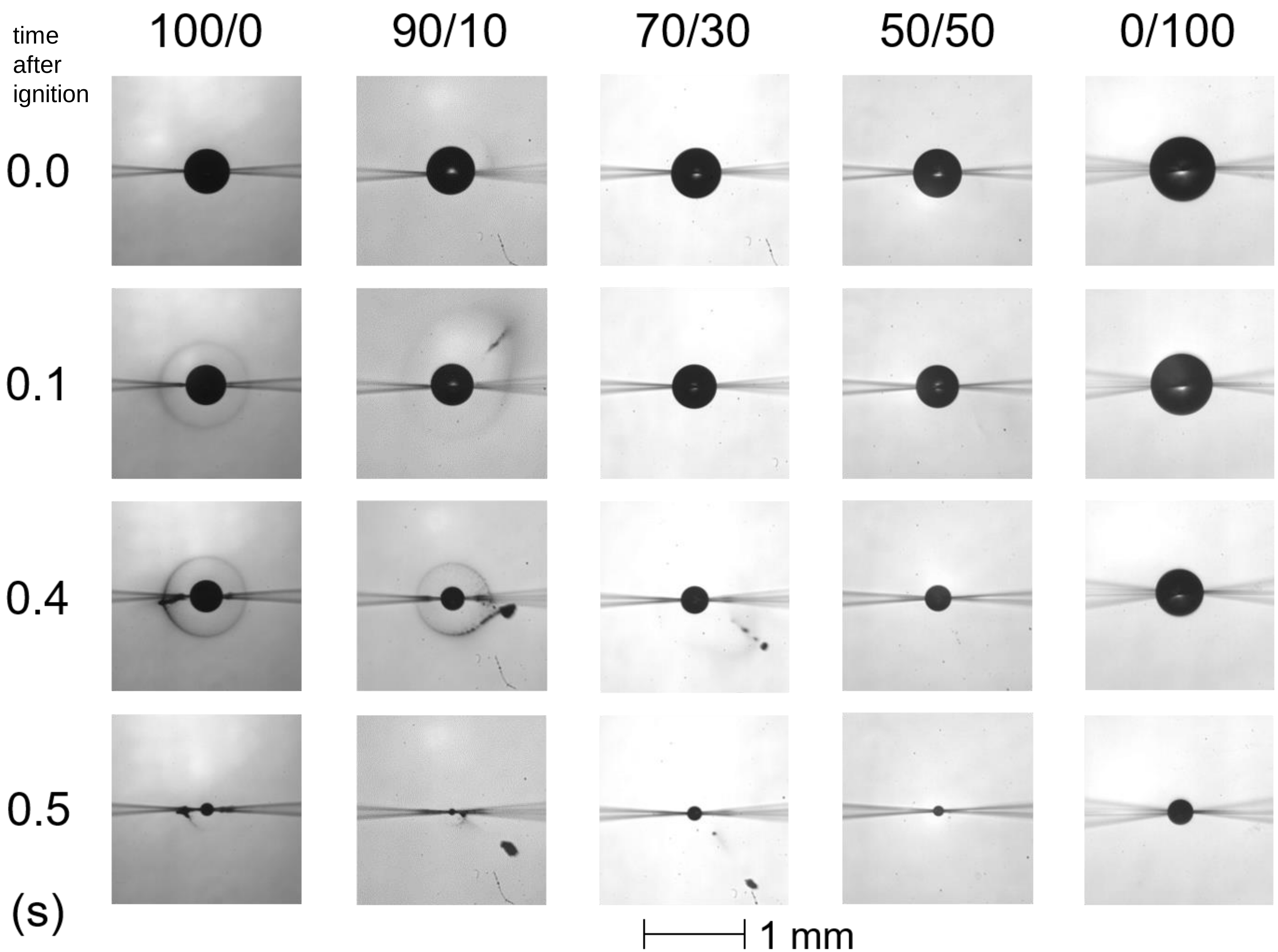
-boiling points are close
-binary simplest mixture (easy sweep through composition space)
-kinetic mechanisms are known
-surrogate not necessary

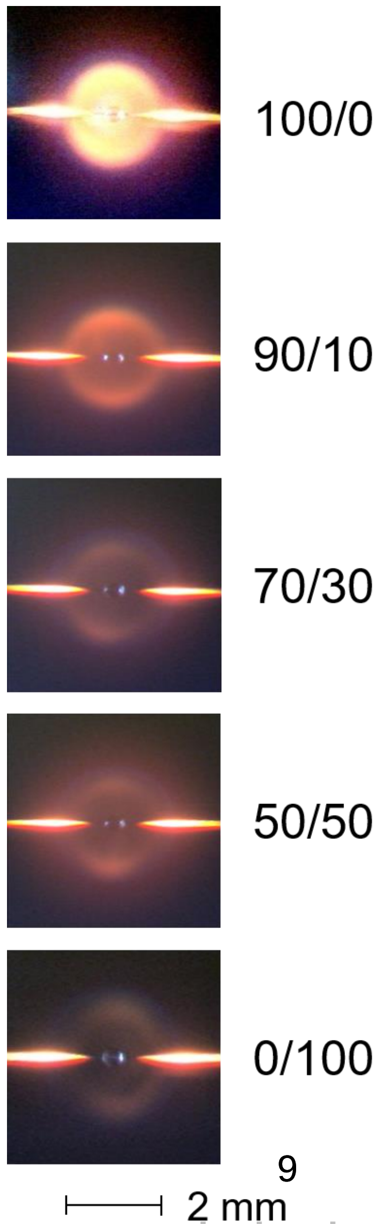
BP2: gasoline/biofuel

now technical accomplishments: experiments first-SWEPT THROUGH compositions

3. Technical Accomplishments

heptane/isobutanol



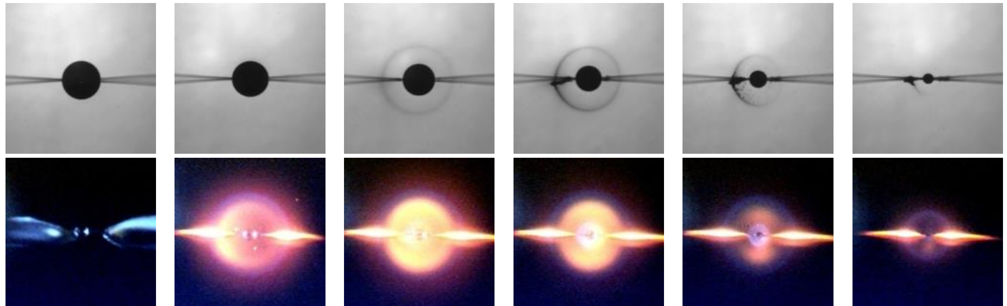


how to get quantitative data

3. Technical Accomplishments (contd)

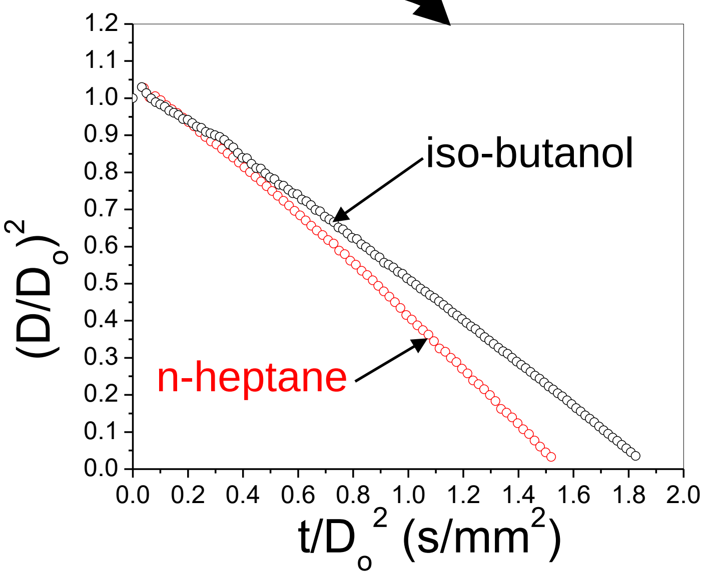
‘raw’ data

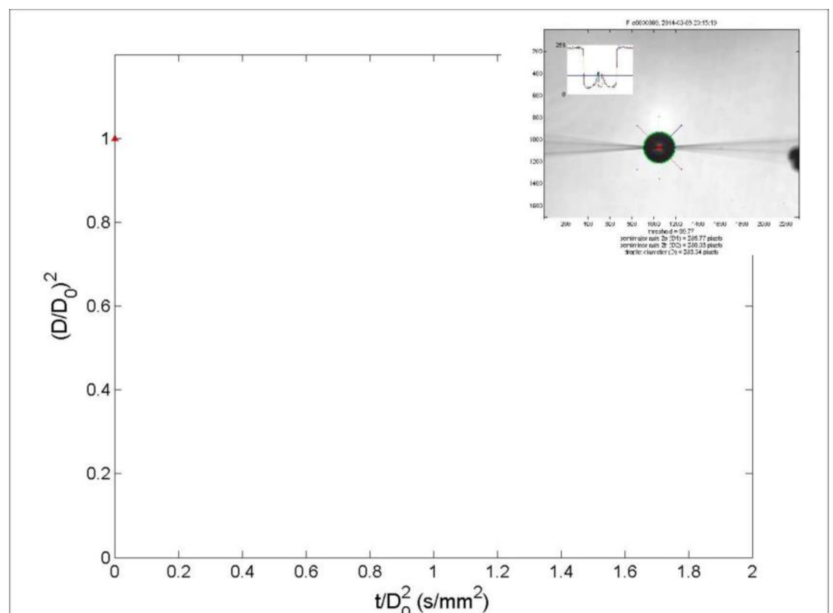
n-heptane



n-butanol

how to get from here to here?





simulations: opensmoke++

3. Technical Accomplishments (contd)

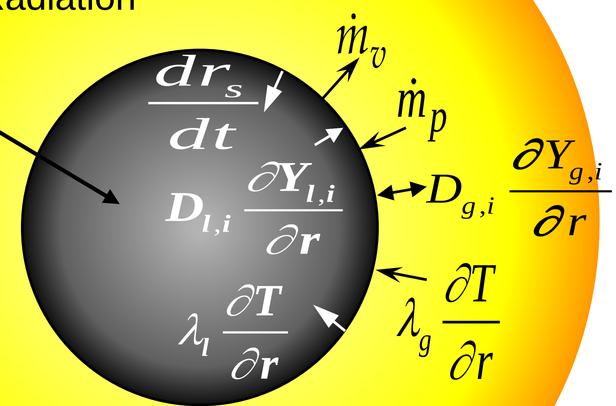
Detailed Numerical Model [OpenSMOKE++]

[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))



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

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

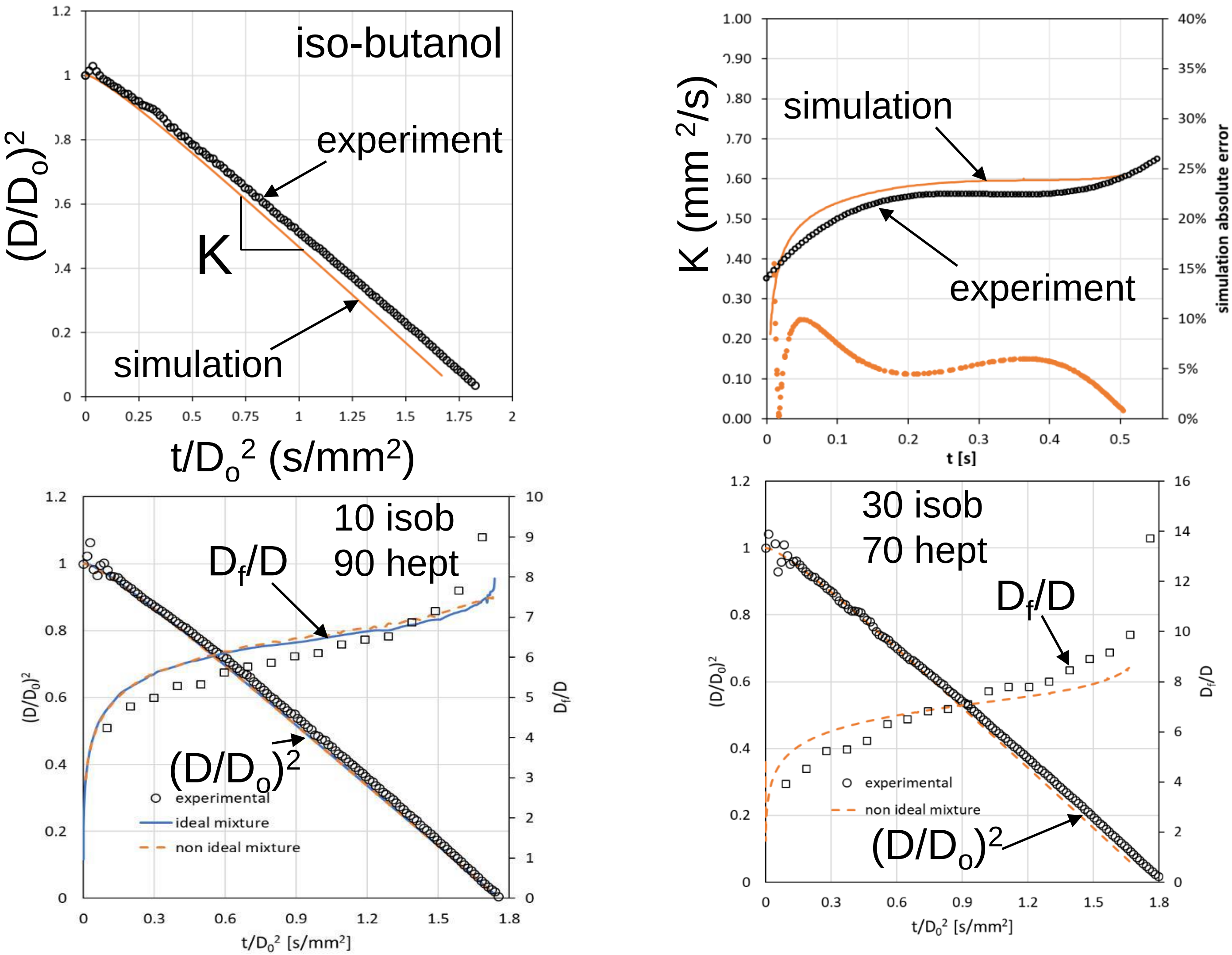
Kinetic Mechanism:

*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...)

results to date: D2 and Df vs time

3. Technical Accomplishments (contd)

Comparing simulated and measured mixture burning properties



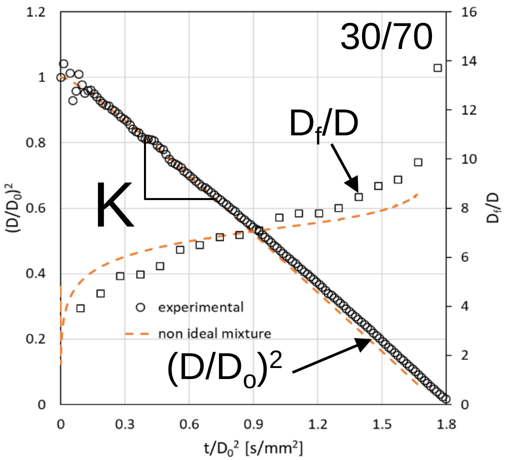
--excellent agreement; compositions investigated: **0/100, 10/90, 30/70, 50/50, 70/30, 90/10, 100/0**

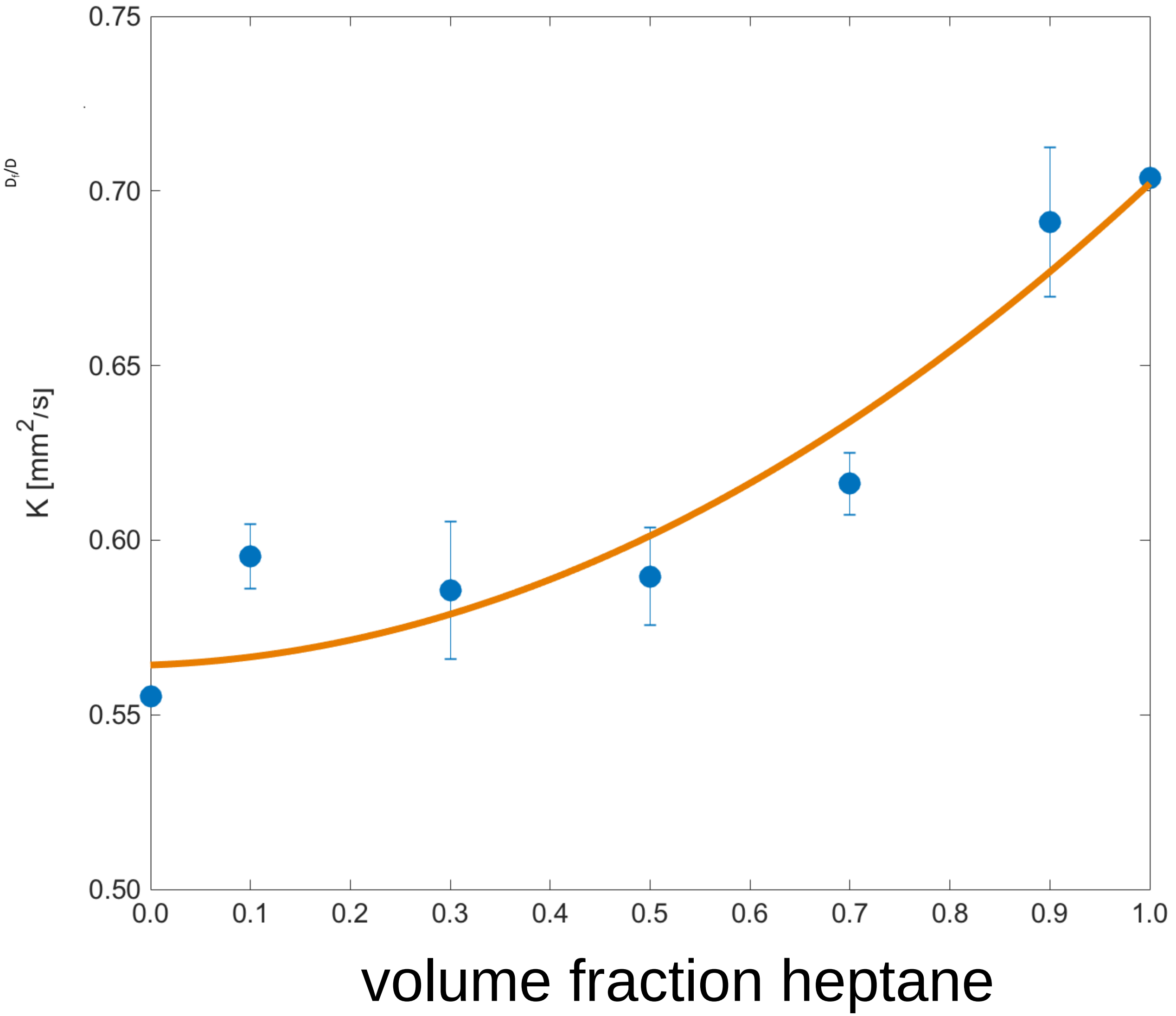
--heptane/isobutanol behaves as a nearly ideal liquid mixture: Raoult's law

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

simulated K vs composition

3. Technical Accomplishments (contd)



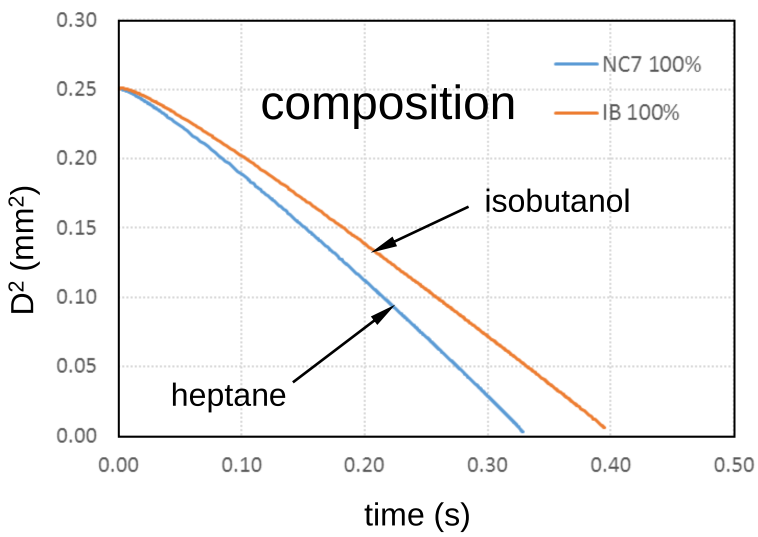


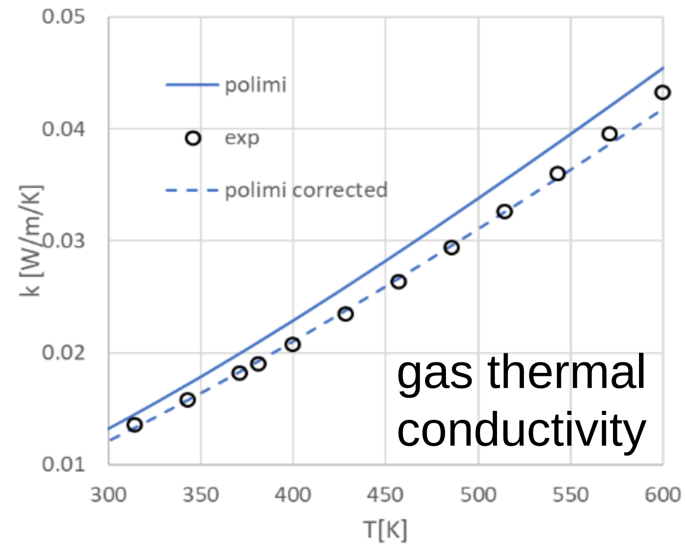
differences are within 20% GO/NOGO decision point

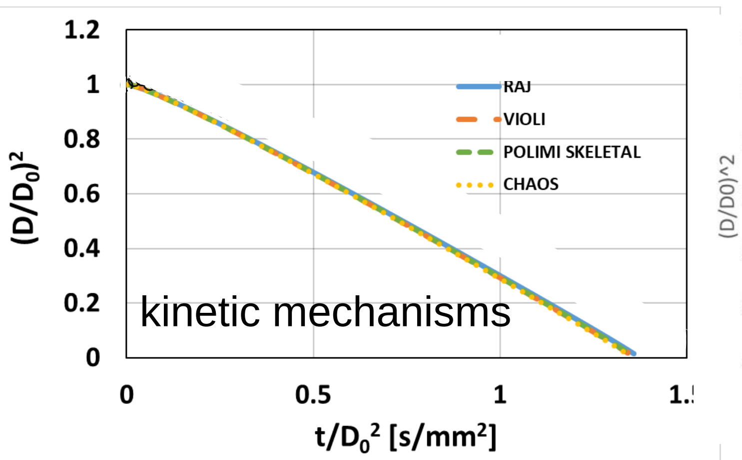
use model to predict what influences burning most

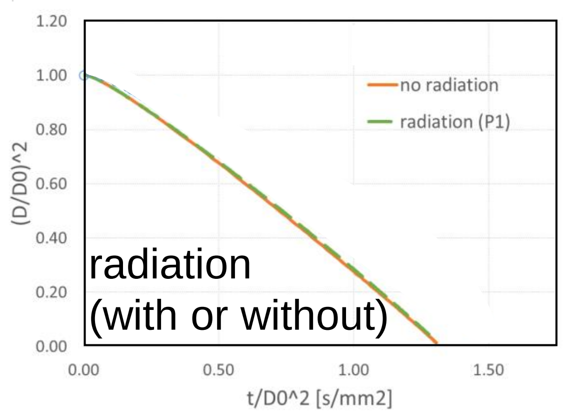
3. Technical Accomplishments (contd)

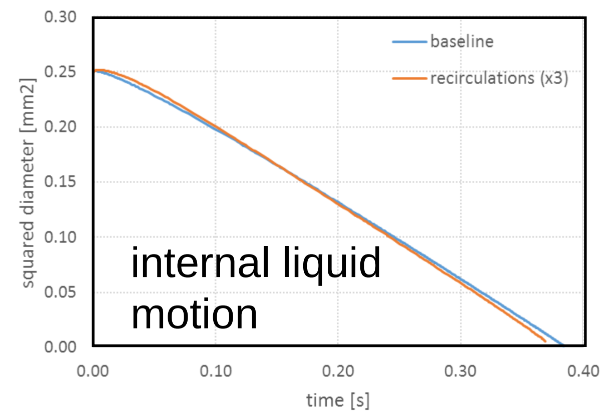
What most influences fuel burning (heptane as an example)?











broad relevance of these results: why liquid fuels

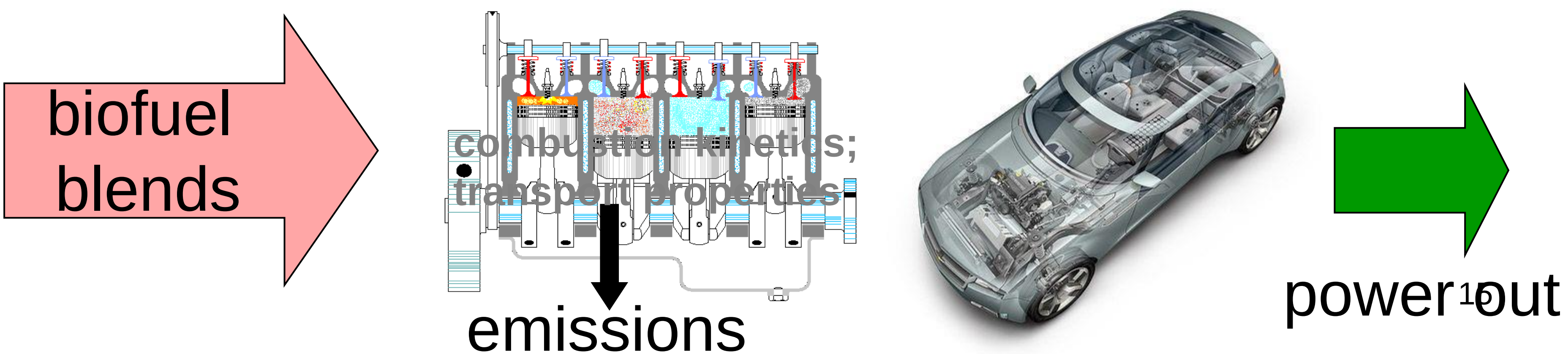
4. Relevance

-opensource simulation capabilities enhance development

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

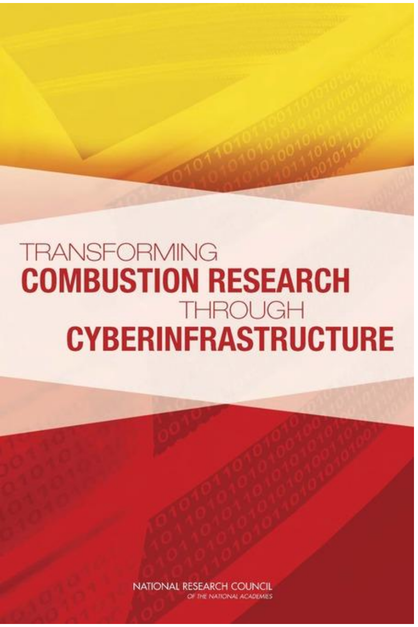
How is combustion of gasoline/biofuel blends influenced by mixture fraction? This project provides answers from a fundamental perspective.

Liquid fuels and combustion engines will be dominant

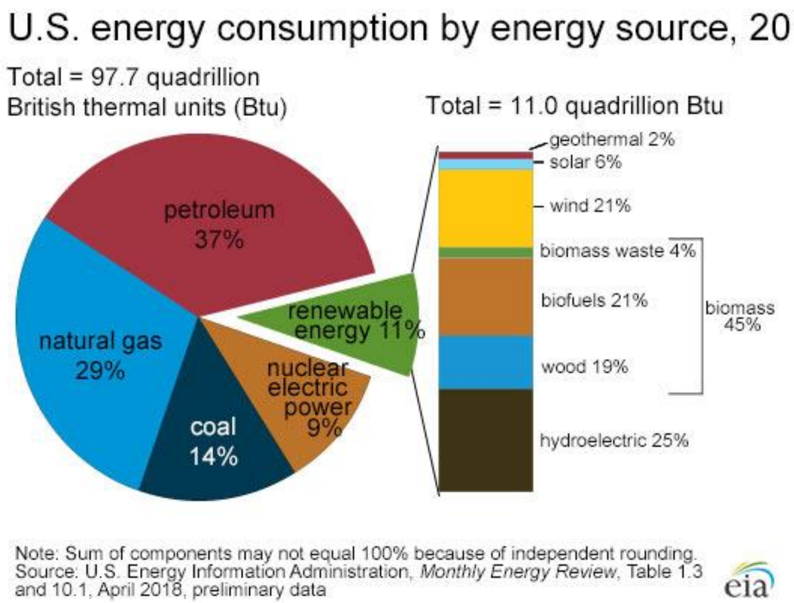


report that notes importance of liquid fuels

4. Relevance (contd)



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



blending simple strategy; current understanding of TFB 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

future/continuing work

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) and simulations

**submit journal article for review.*

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 mixture)*

**develop combustion kinetic mechanism of surrogates and reduced mechanisms*

**simulations*

-validate kinetic mechanism and surrogate formulation with droplet burning properties

**provide access to 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

presentations/publications so far in BP1 publication

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).

conference presentations

A. Dalili, M. Turello, F. Pizzetti, J.D. Brunson, C.T. Avedisian, K. Seshadri, S. Guo, A. Cuoci, P. Dou, F.A. Williams, A. Frassoldati, M.C. Hicks, “Experiments and Analysis of n-Heptane/Iso-butanol Mixture Droplet Combustion,” 11th U. S. National Combustion Meeting, Western States Section, Combustion Institute, March 24–27, 2019, Pasadena, California (2019)

A.Dalili, J.D. Brunson, P. Dou, S. Guo, M. C. Hicks, A. P. Reeves, K.Seshadri, 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?

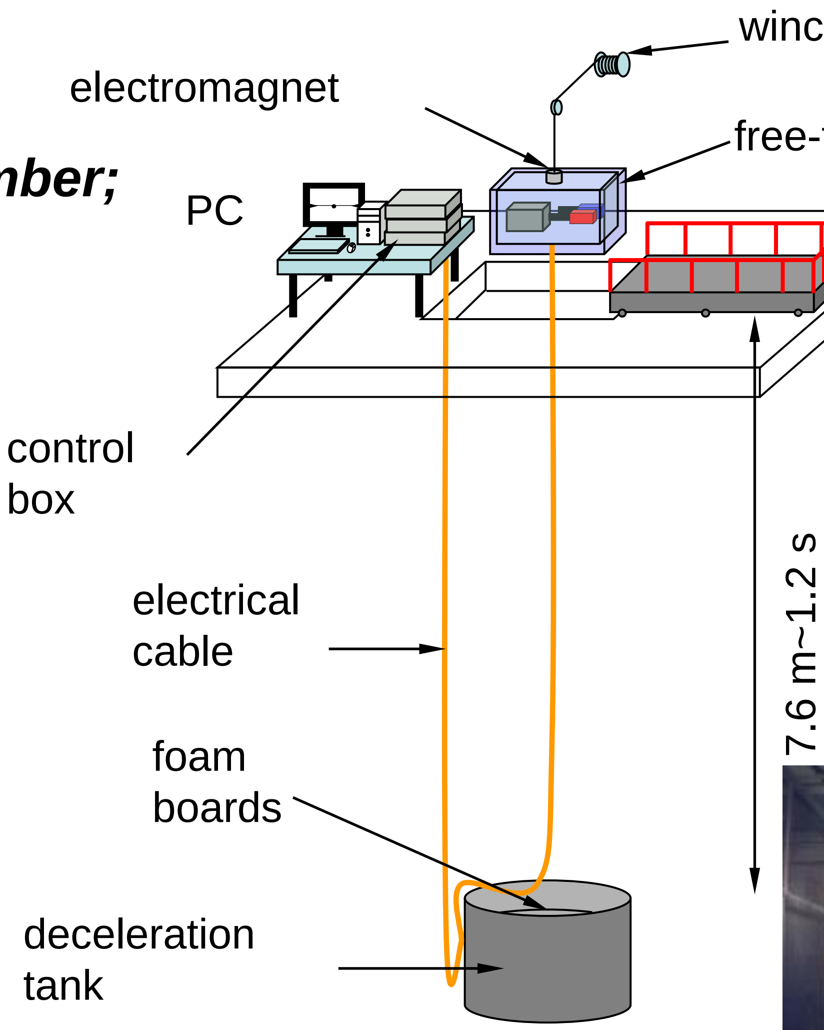
Backup Slides

Experimental Hardware

experiments performed in free-fall

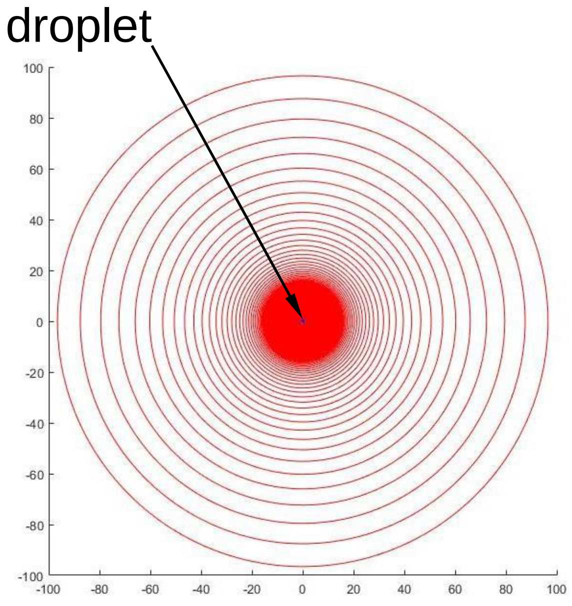
minimize bouyancy
experiments in free-fall chamber;

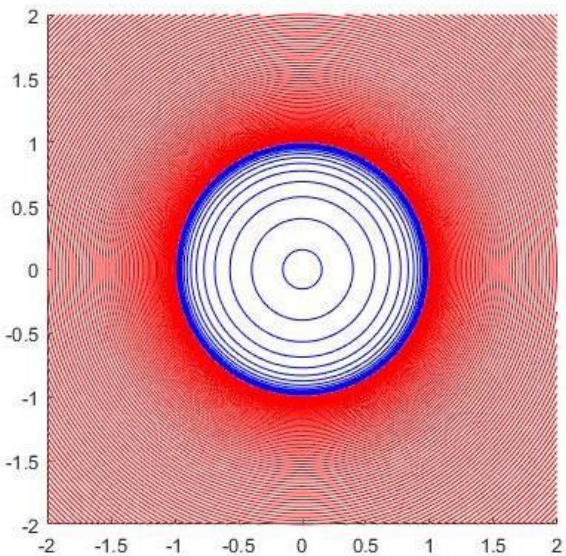
minimize forced convection:
stagnant ambience;
prevent droplet from moving
stagnant ambience;
(restrain droplet)

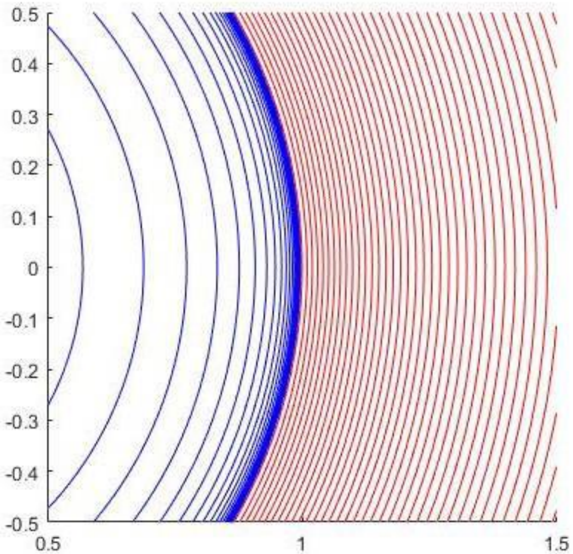


Computational Grid

-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)







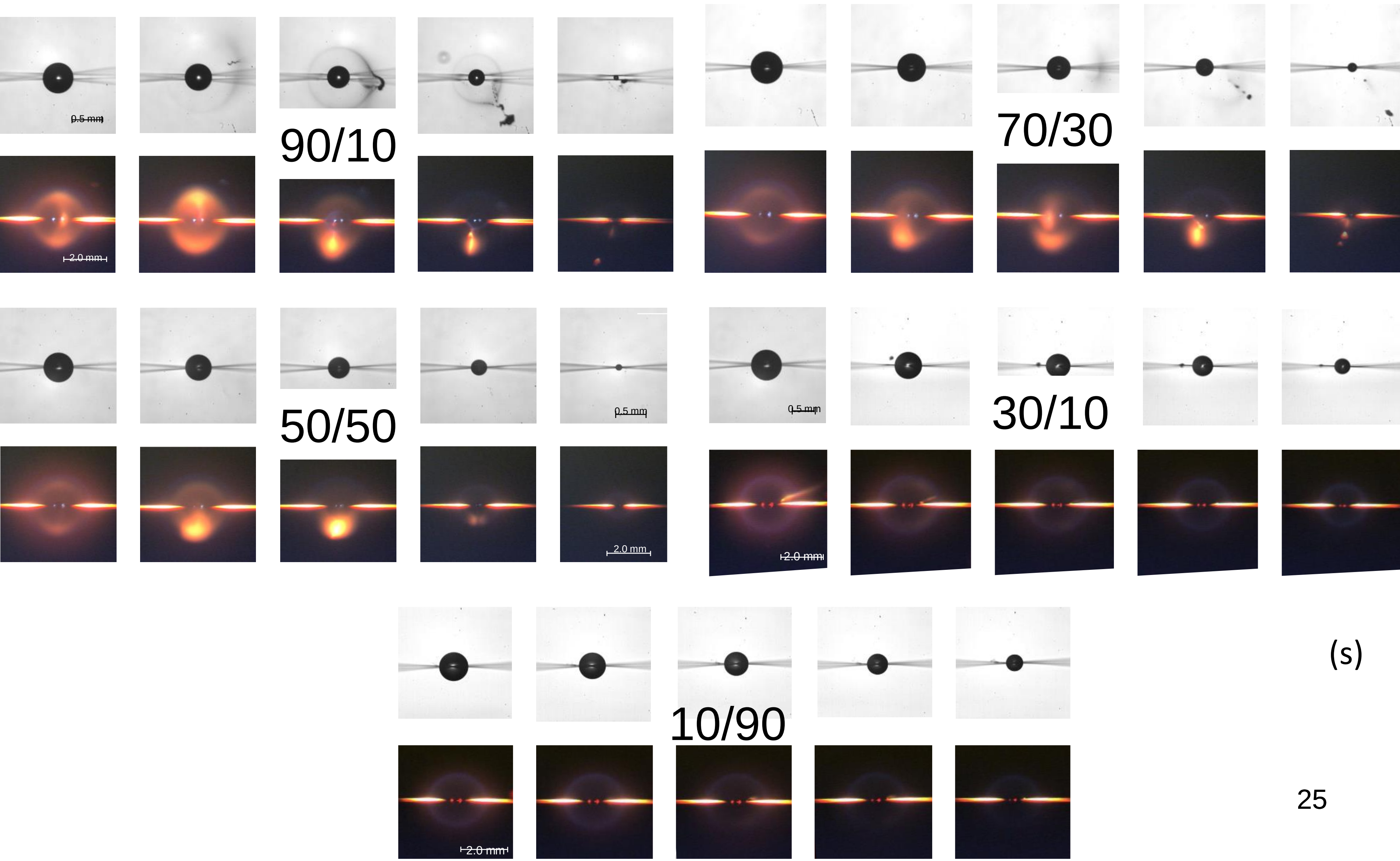
Surrogate development process

***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)

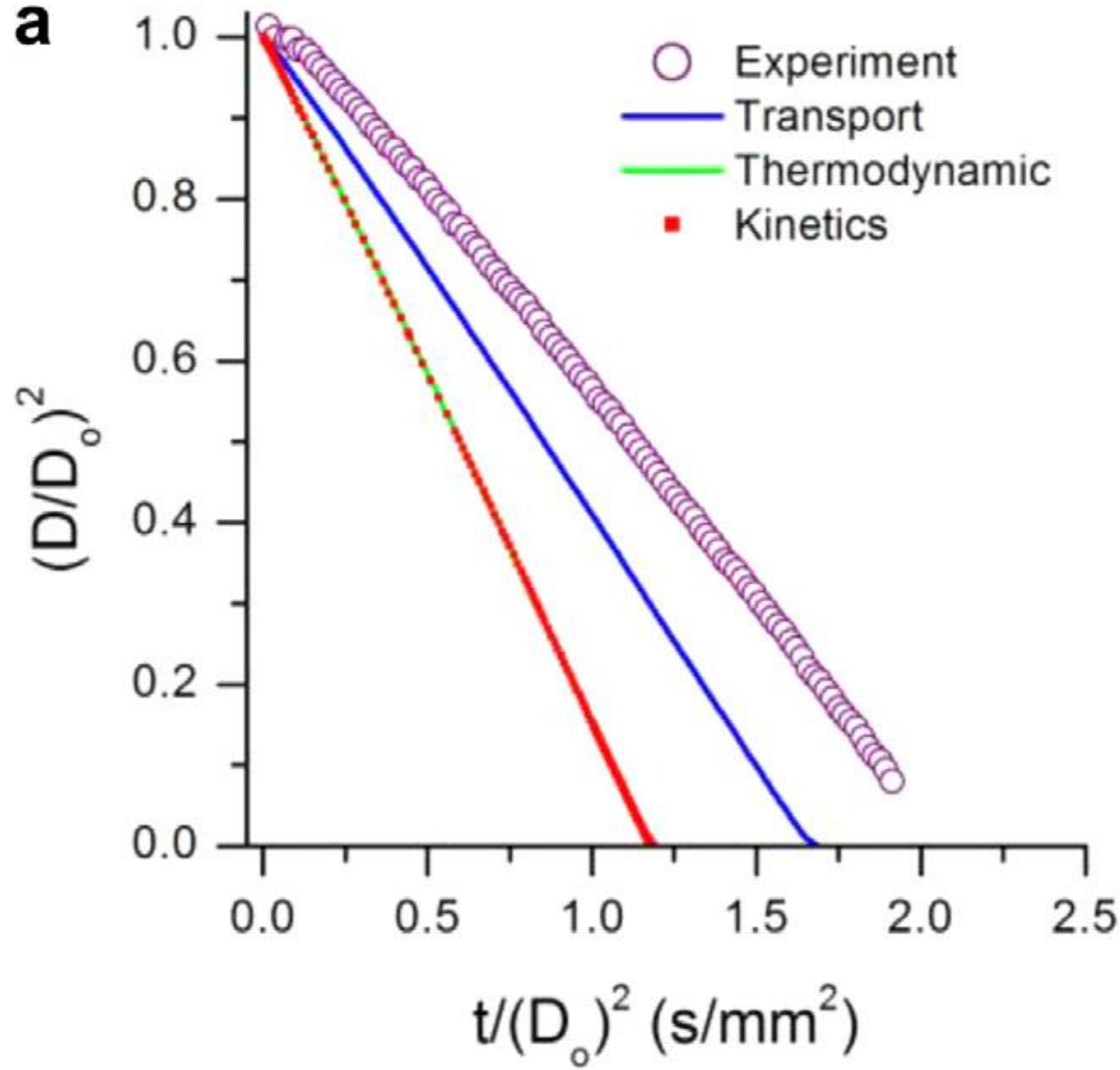
burning histories of heptane/isobutanol droplets



(s)

OEMs (2012): E10 has 3.5 vol% O_2; for same 3.5 vol% O_2, an EPA waiver on O_2 content would allow up to **16.1 vol% isobutanol in gasoline**

Kolodziej; Scheib, R**.**, **“**Bio-isobutanol: the next-generation biofuel,” J. Hydrocarbon Processing, 79-85 (2012)



a
1.0
0.8
0.6
0.4
0.2
0.0
$(D/D_o)^2$
0.0
0.5
1.0
1.5
2.0
2.5
$t/(D_o)^2$ (s/mm^2)
Experiment
Transport
Thermodynamic
Kinetics