On using a multiphase combustion configuration to evaluate detailed kinetic mechanisms of gasoline/biofuel blends

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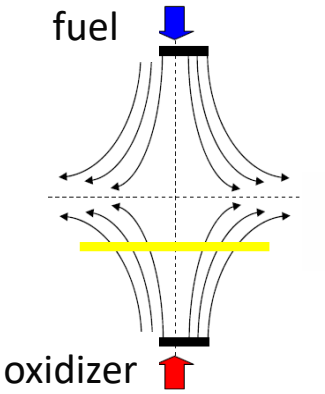
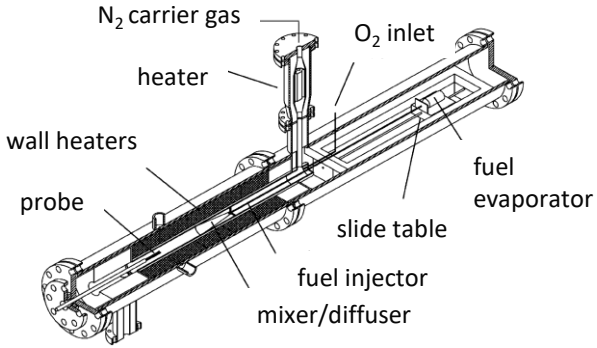
U.S. Department of Energy
EE-0007978
Alicia Lindauer

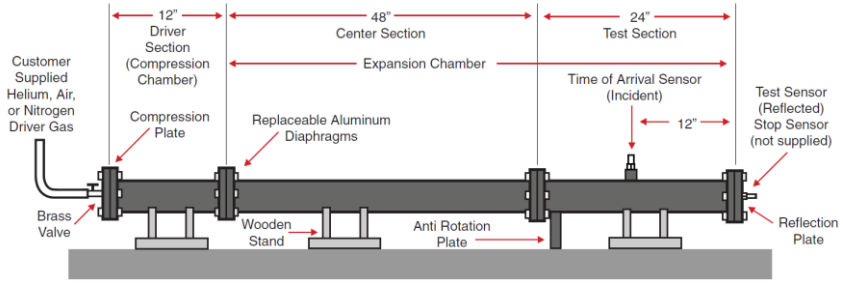
CF Flame



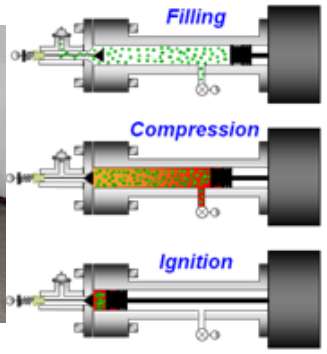
Flow Reactor



Shock Tube



RCM



JSR

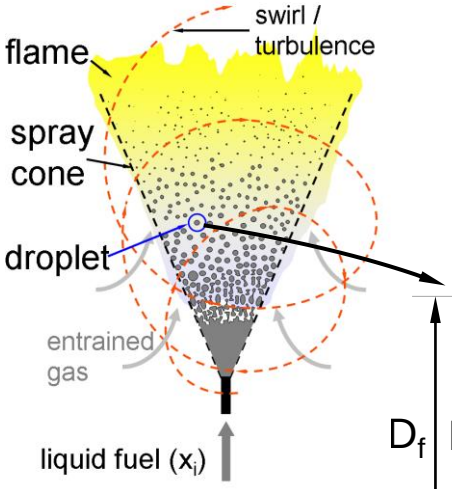
- Common features;
- **-fuel is pre-vaporized**
- **-transport 0D or 1D**
- **-ab-initio models exist**

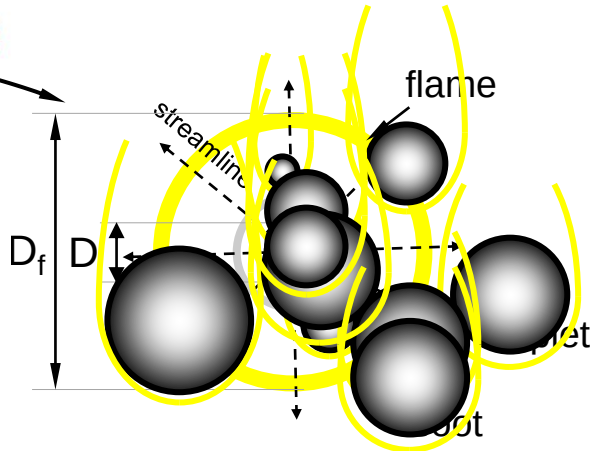
a spray is logical multiphase choice;
"sets initial condition for combustion in engines"…but
sprays can't be ab-initio modeled

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

look to sub-grid element of a spray:

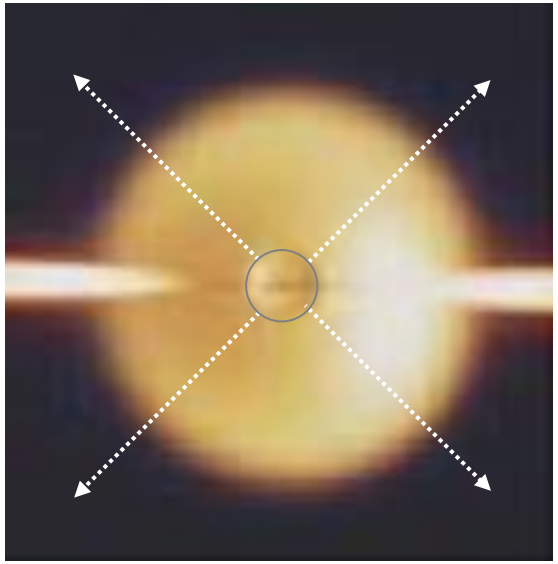
- ***isolated droplet***
  - ***-can model above effects (currently the only configuration)***



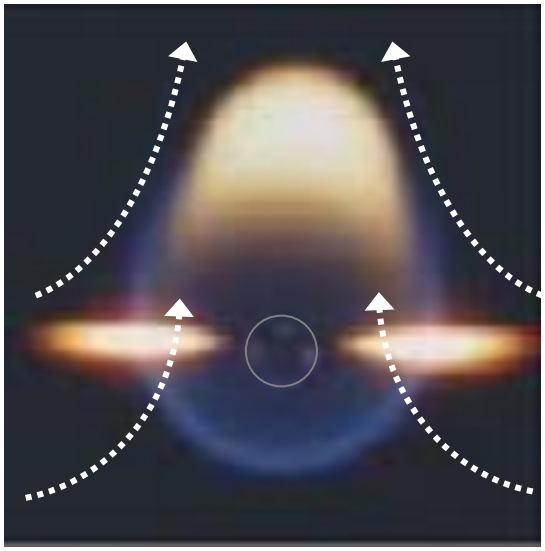


How to create spherical symmetry

creating canonical configuration for liquid fuel combustion



1-D

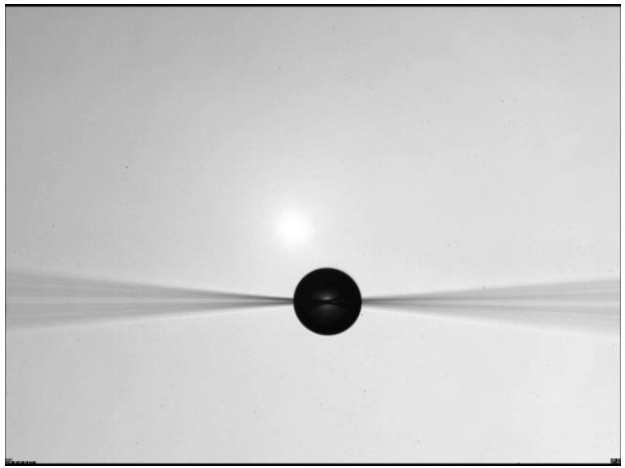


2-D

-perform experiments in buoyuancy-free environment; stagnant ambience (restrict droplet motion)

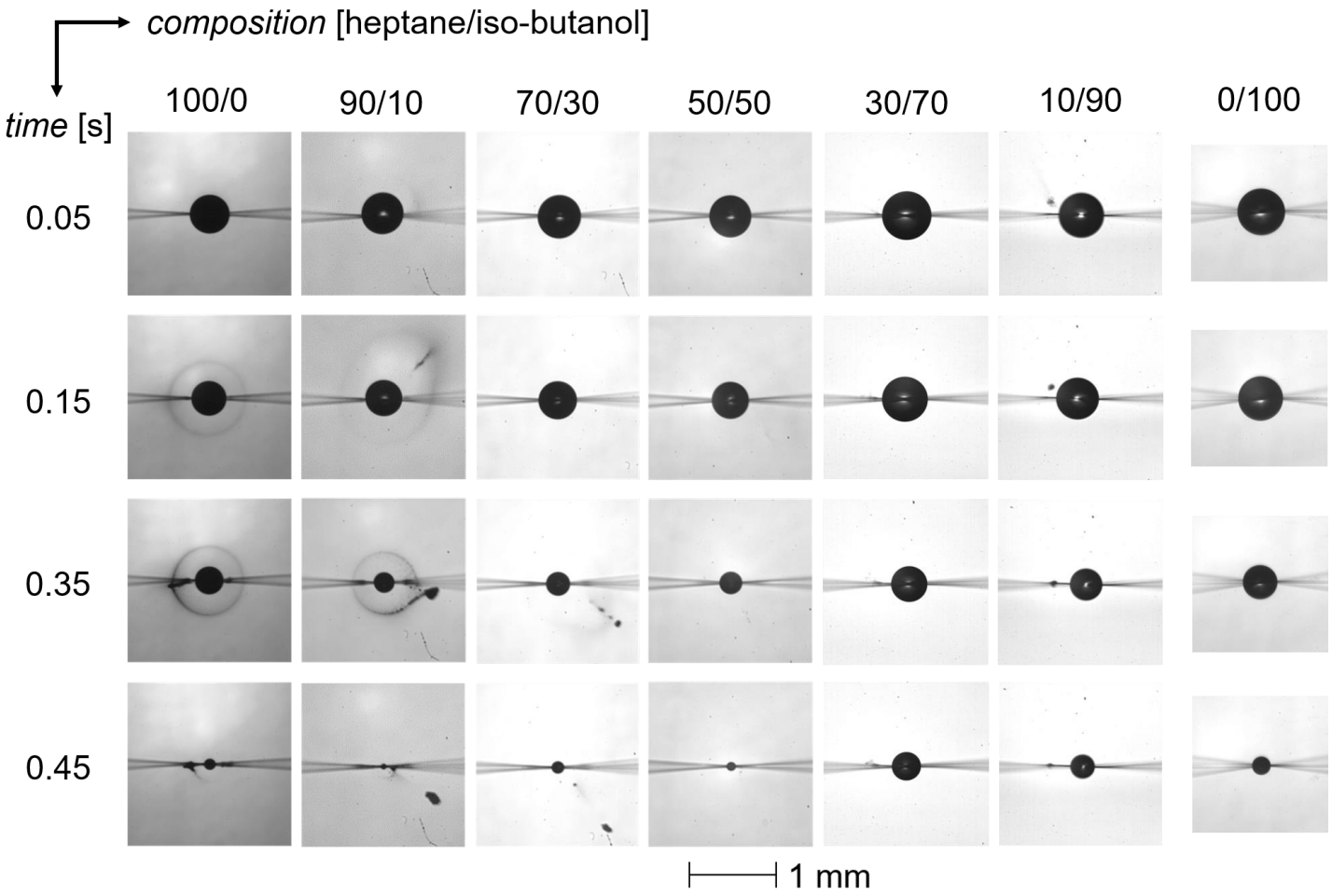
-1-D useful to benchmark biofuel blends and their surrogates;

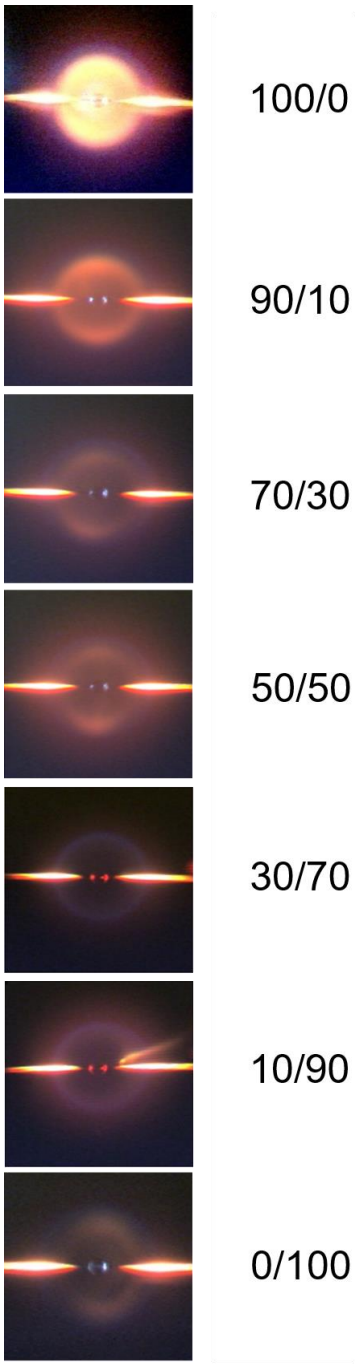
-data important to validate simulation



Collection of photos

Experimental Observations





flame luminosity is measure of sooting propensity
[C.J. Mueller, G.C. Martin, SAE paper no. 2002-01-1631]

Simulation model

detailed numerical modeling (DNM)

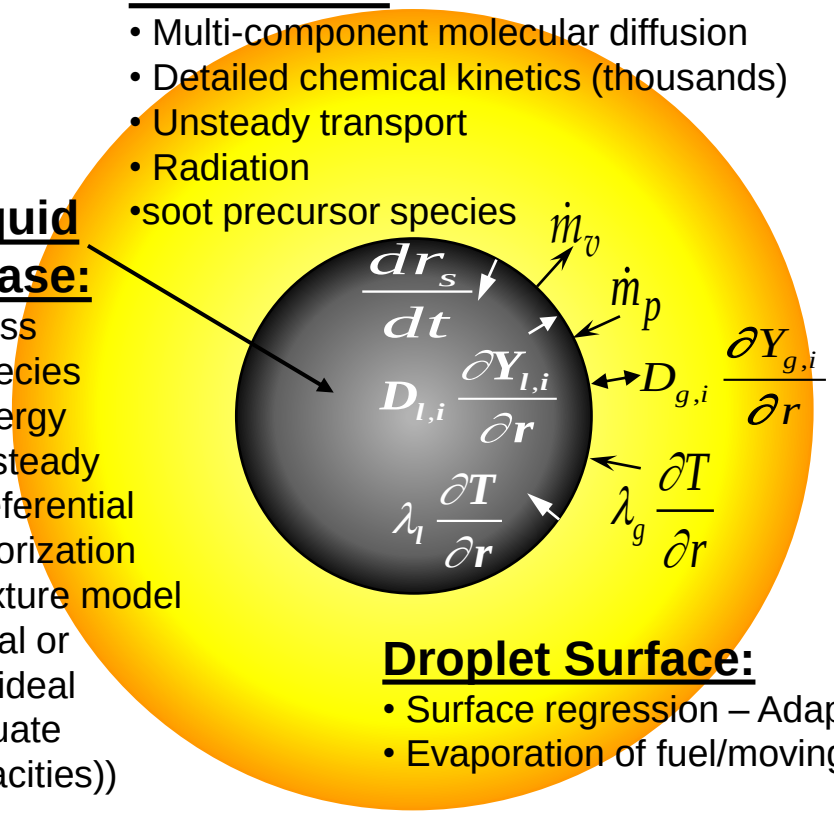
OpenSMOKE++

[1ST principle solver, being modified for miscible mixtures]

Input:
kinetics;
transport
properties

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

Liquid Phase:
- Mass
- Species
- Energy
- unsteady
- preferential vaporization
- mixture model (ideal 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:

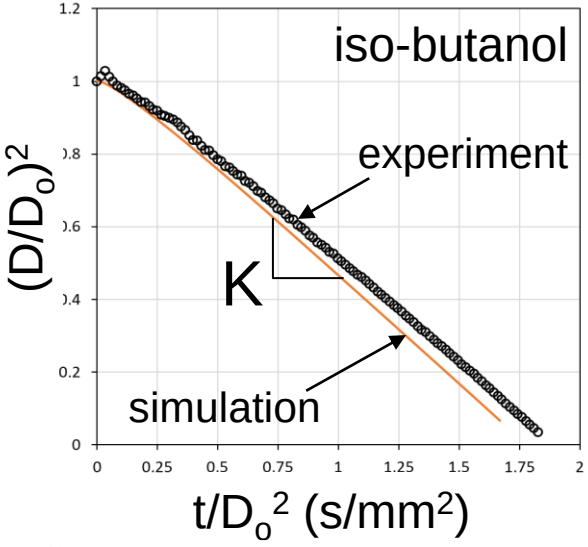
*POLIMI 1800 detailed mechanism of 482 species, 19,072 reactions (for diesel, gasoline, jet fuels, alcohols...)

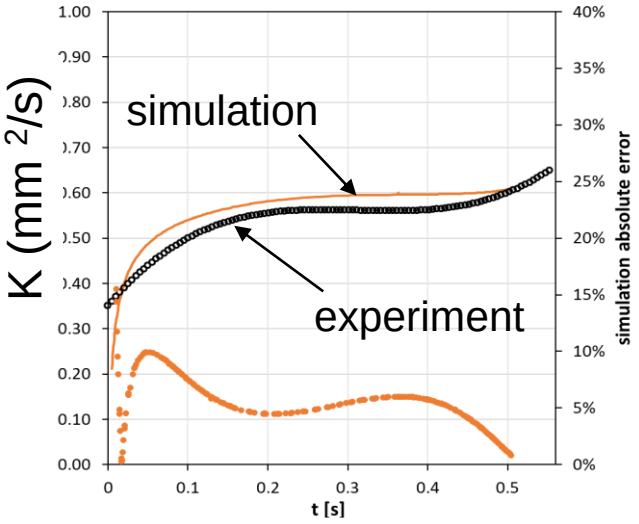
*POLIMI 1421 skeletal mechanism 225 species, 7645 reactions (reduced from POLIMI 1800)

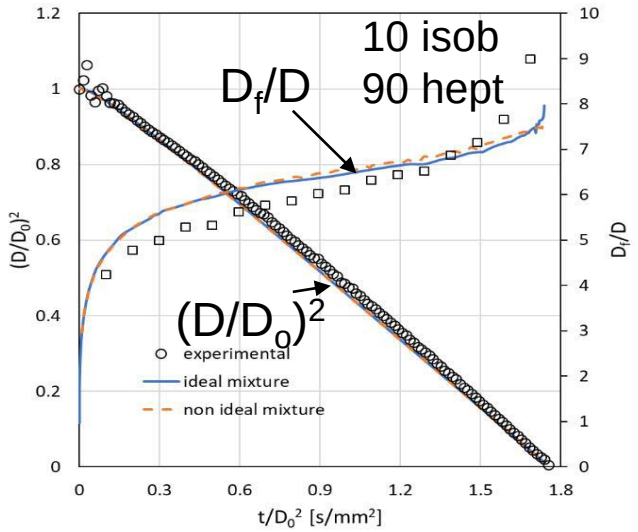
results to date: D2 and Df vs time

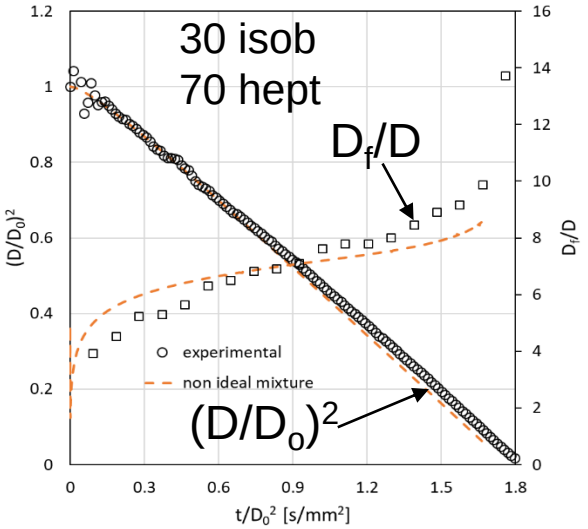
representative results

Compare simulated and measured mixture burning properties









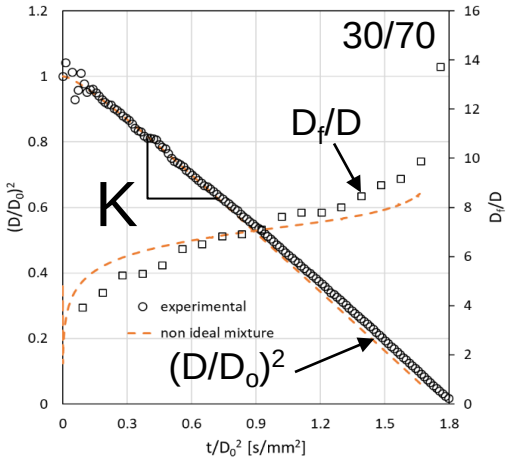
--excellent agreement; compositions investigated: **0/100, 10/90, 30/70, 50/50, 70/30, 90/10, 100/0**

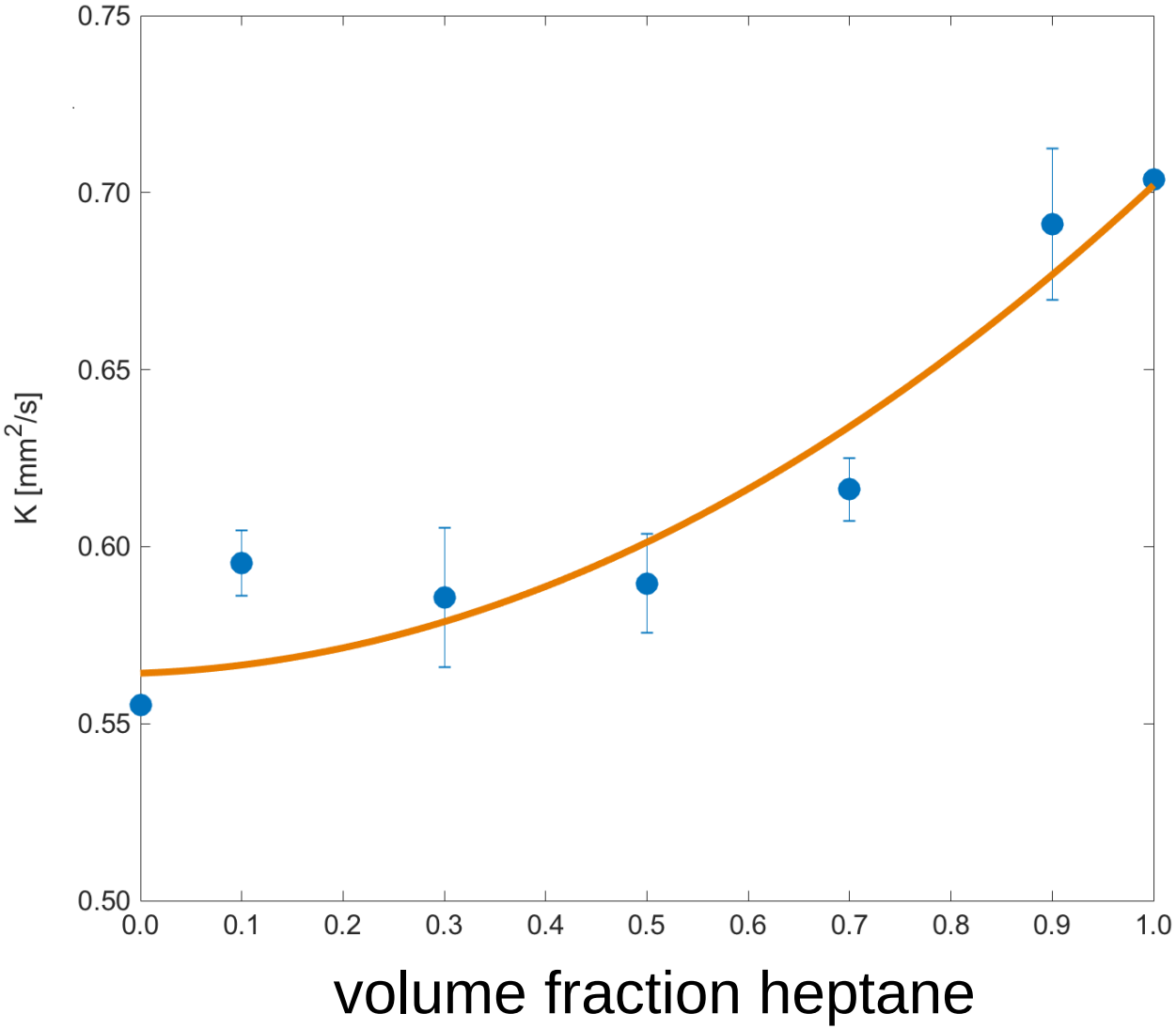
--heptane/isobutanol behaves as a nearly ideal liquid mixture: Raoult's law

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

simulated K vs composition

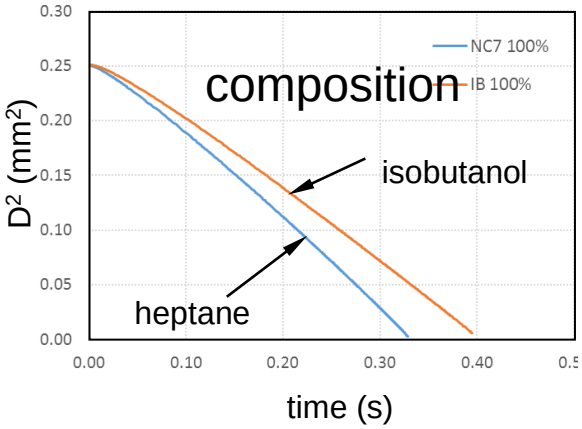
burn rate is important metric for comparison

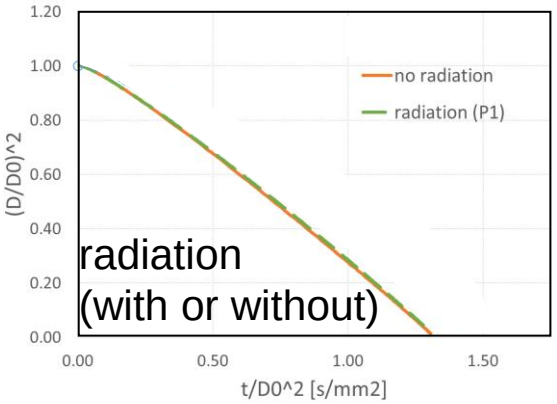


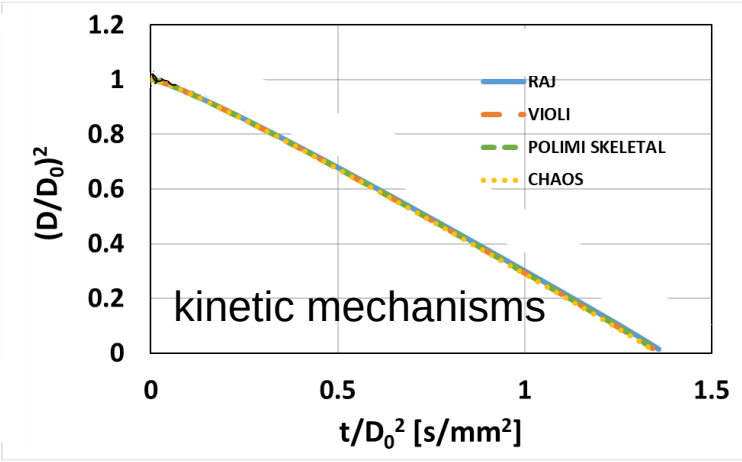


final thought, use simulation as test

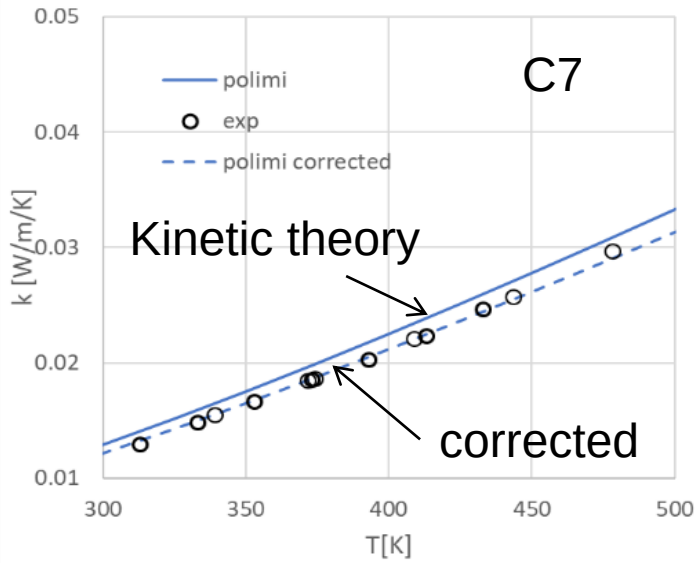
sensitivity

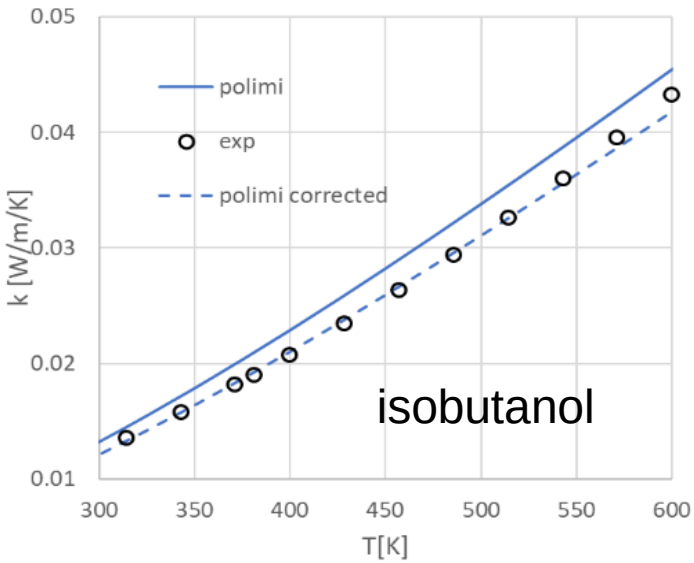






gas thermal conductivity



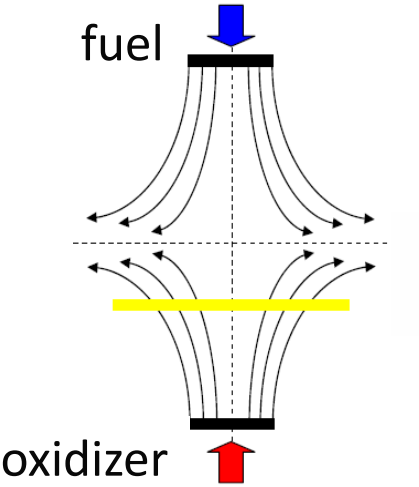


Thank you

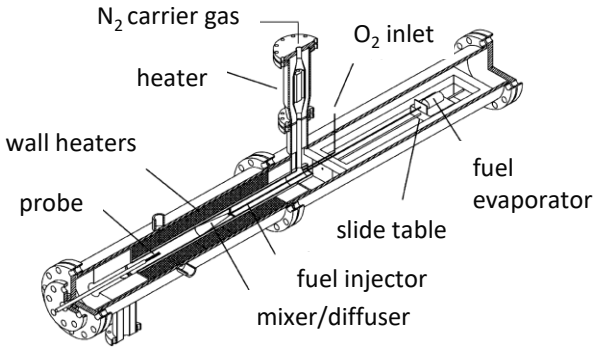
Questions?

important configurations for generating combustion properties for validation

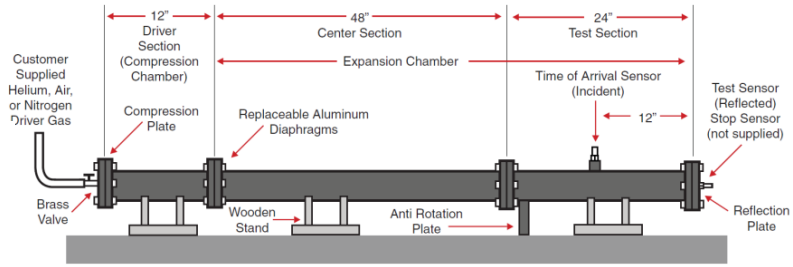
CF Flame



Flow Reactor

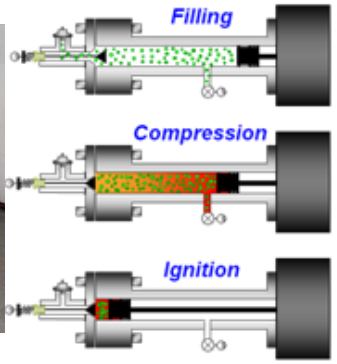


Shock Tube



JSR

RCM



Common features;

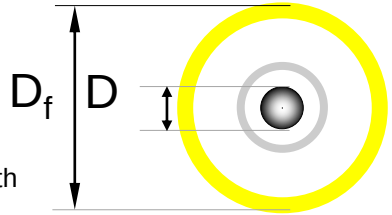
-**fuel is pre-vaporized**

-transport is 0D or 1D

-ab-initio models exist

the process

[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

accurate reaction rates

thermodynamic and transport properties

reaction paths

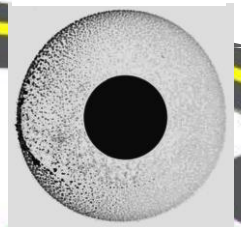
reaction rate rules

detailed chemical kinetic models

mechanism reduction

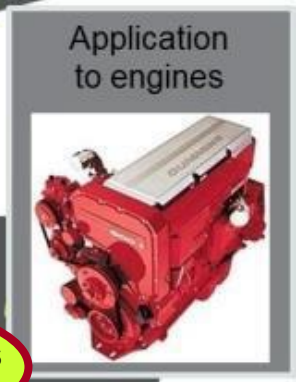
validation using 1-D configurations

numerical algorithms (fast solvers)



Fundamental Experiments

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



1-D Droplet (multiphase)

experiments (how to create 1-D

Summary

Continuing work:

gasoline/biofuel mixtures

- **-biofuel = isobutanol; possibly a furan mixture**

surrogate is needed

- **-include a droplet target (e.g., burn rate, maximum flame diameter)**

experiments to develop surrogate droplet burning data

- **-compare surrogate combustion with gasoline/biofuel combustion**

kinetic mechanism is needed

- **-start with POLIMI skeletal mechanism**

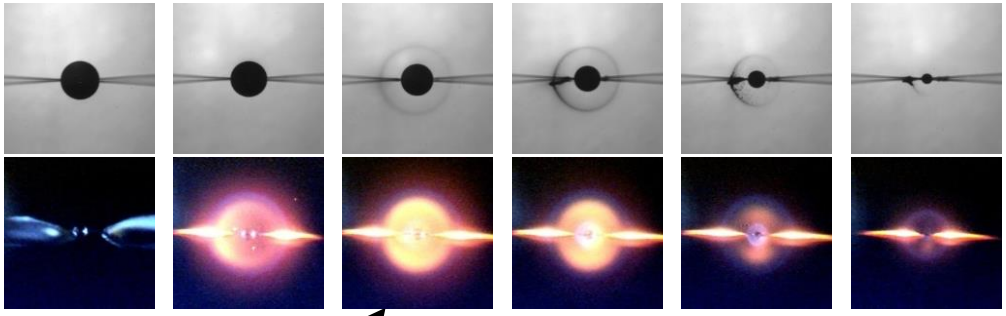
deliverables:

- **-open source code for detailed modeling to simulate burning properties**
- **-experimental methodology to develop combustion properties**
- **-kinetic mechanism that can be used in engine simulation of gasoline/biofuel mixtures**

data extraction from video

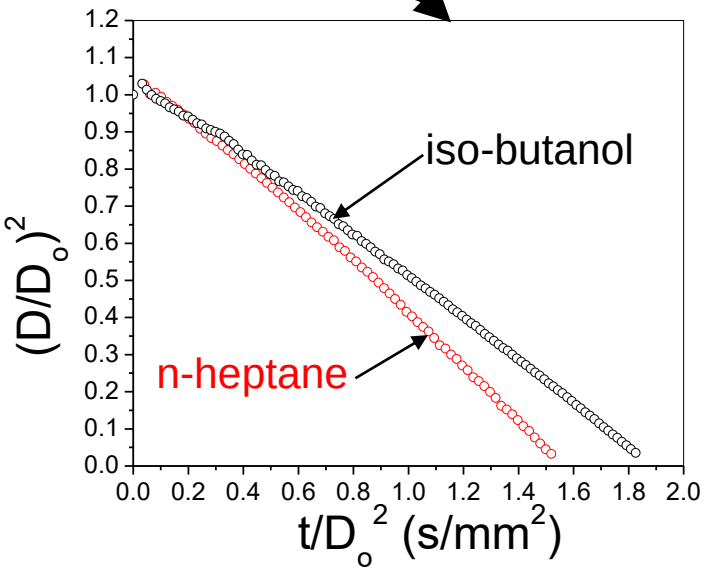
‘raw’ data

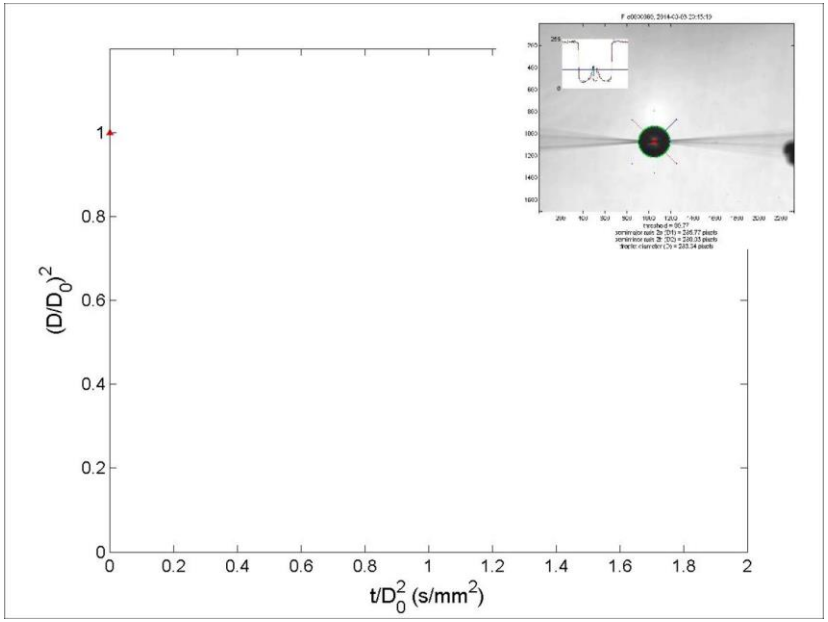
n-heptane



n-butanol

how to get from here to here?



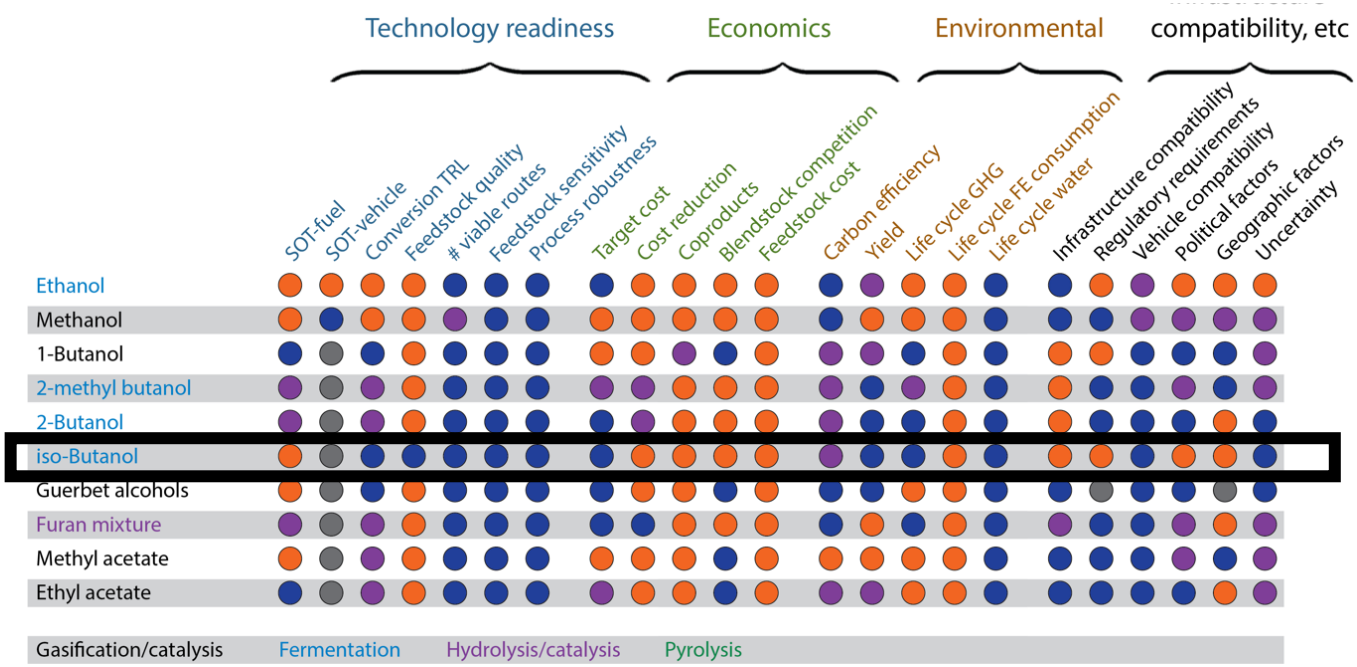


simulations: opensmoke++

why heptane and isobutanol?

model fuel system selected is a binary mixture

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

-we don't need a surrogate (initially; later for gasoline/isobutanol we do)
-boiling points are close
-binary simplest mixture (easy sweep through composition space)
-kinetic mechanisms are known

now technical accomplishments: experiments first-SWEPT THROUGH compositions

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

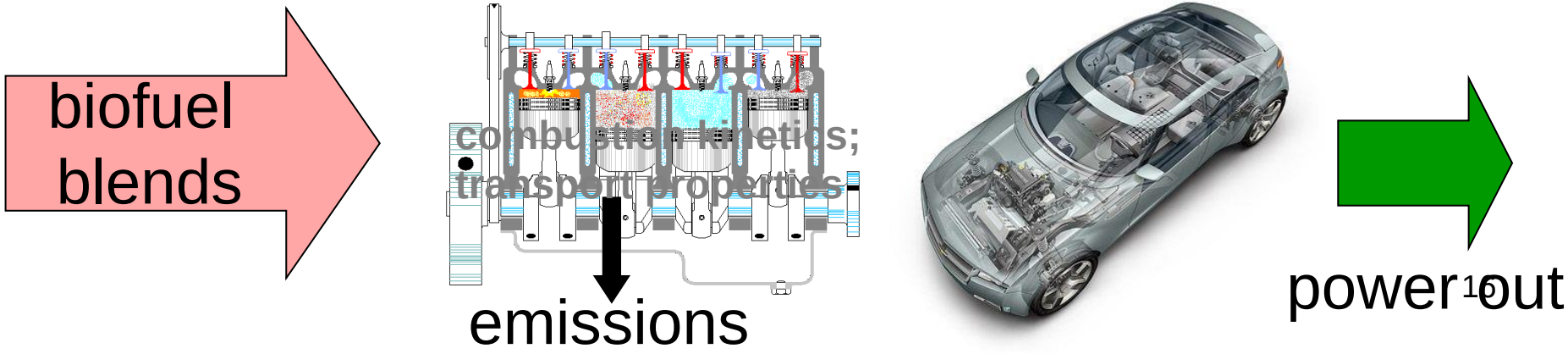
4. Relevance

-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

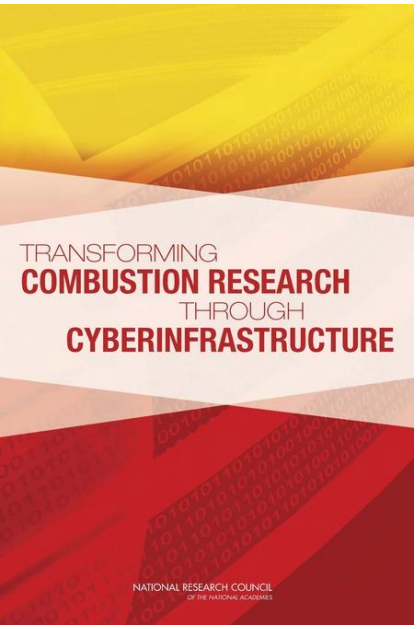
How is combustion of gasoline/biofuel blends influenced by mixture fraction?
This project provides answers from a fundamental perspective.

Liquid fuels and combustion engines will be dominant

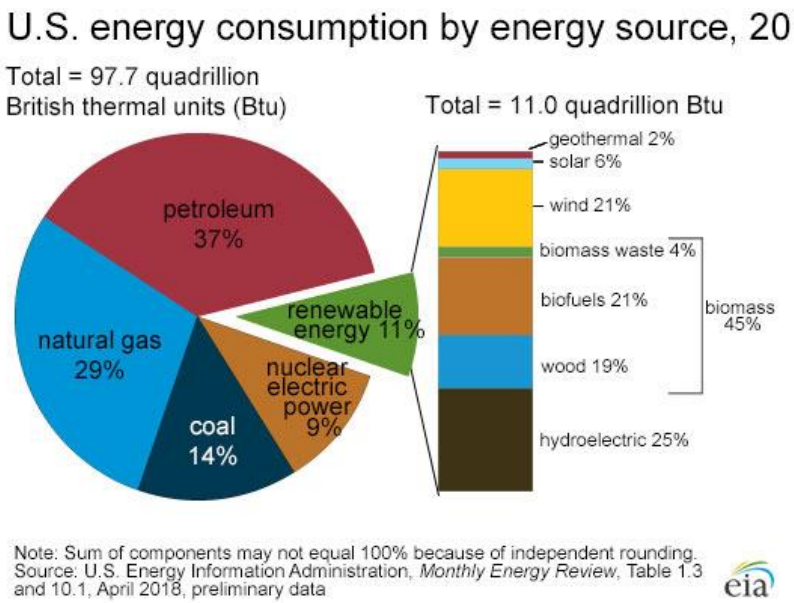


report that notes importance of liquid fuels

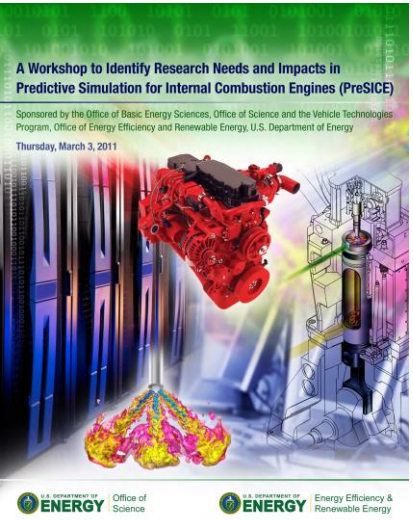
4. Relevance (contd)



"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)

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).

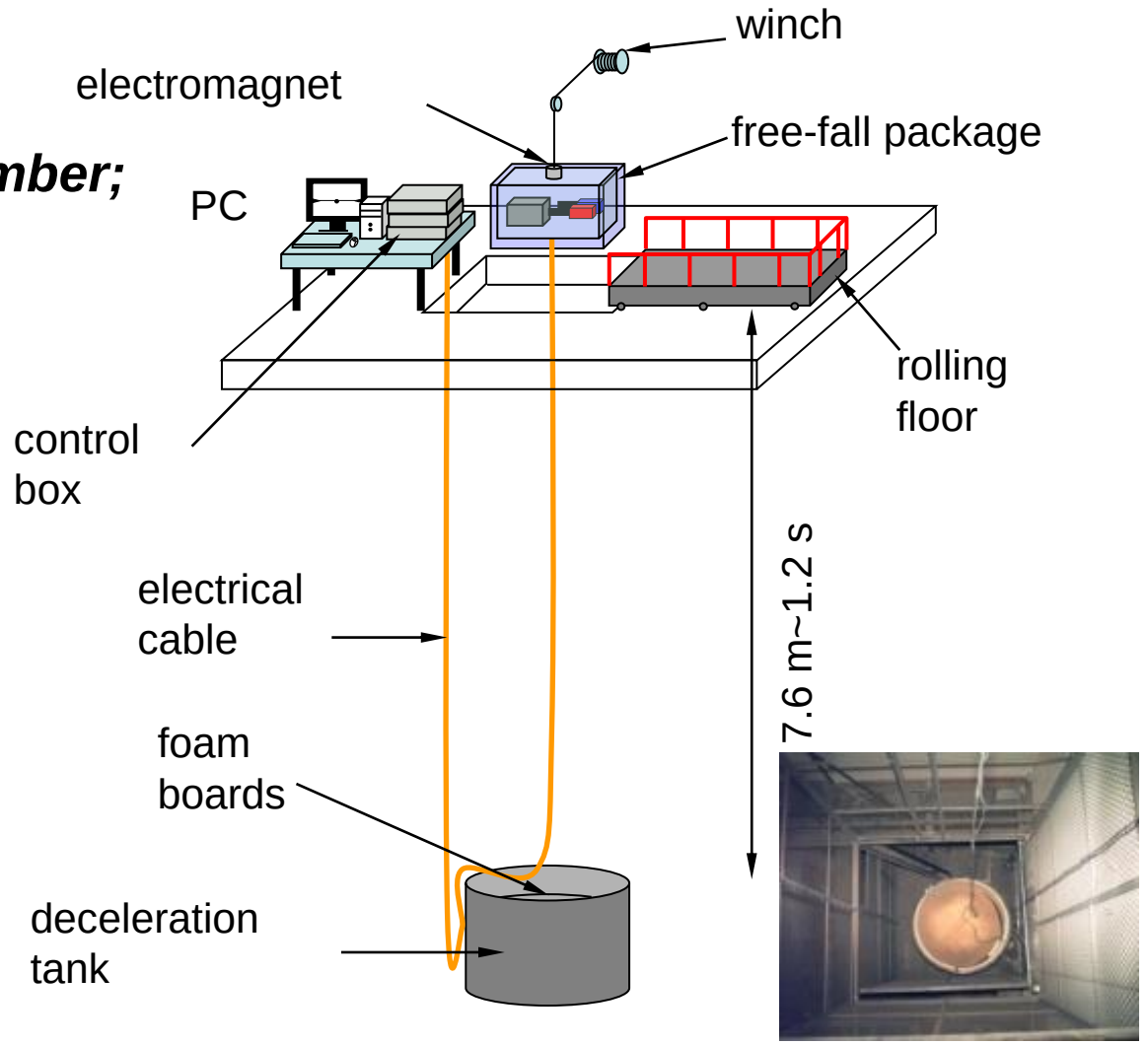
thank you

Experimental Hardware

experiments performed in free-fall

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

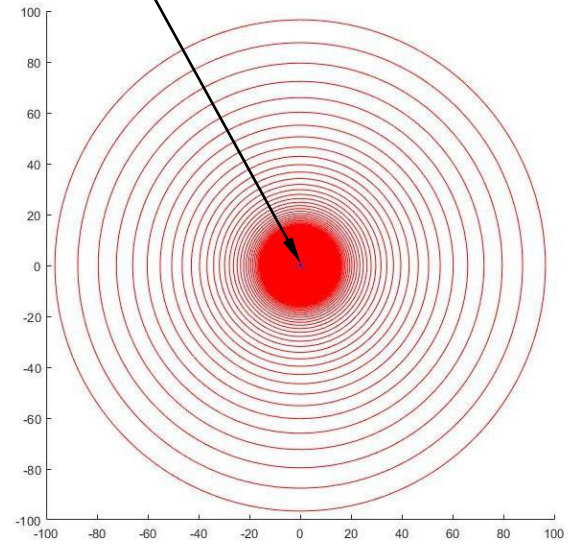
<u>minimize forced convection</u>:
stagnant ambience;
prevent droplet from moving
stagnant ambience;
(restrain droplet)

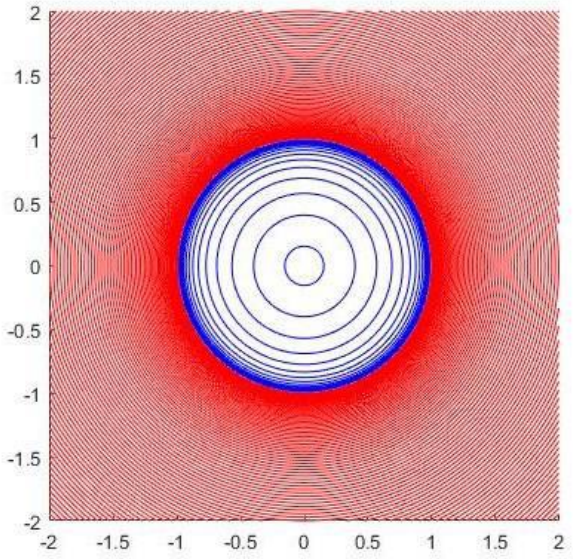


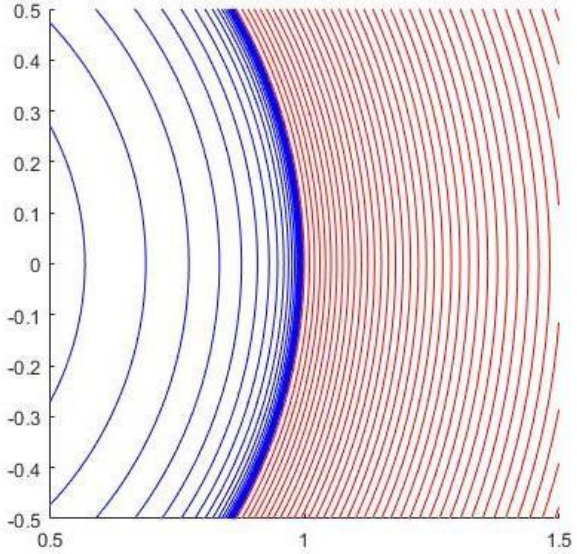
Computational Grid

-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)

droplet







Surrogate development process

***Constrained Optimization Approach**

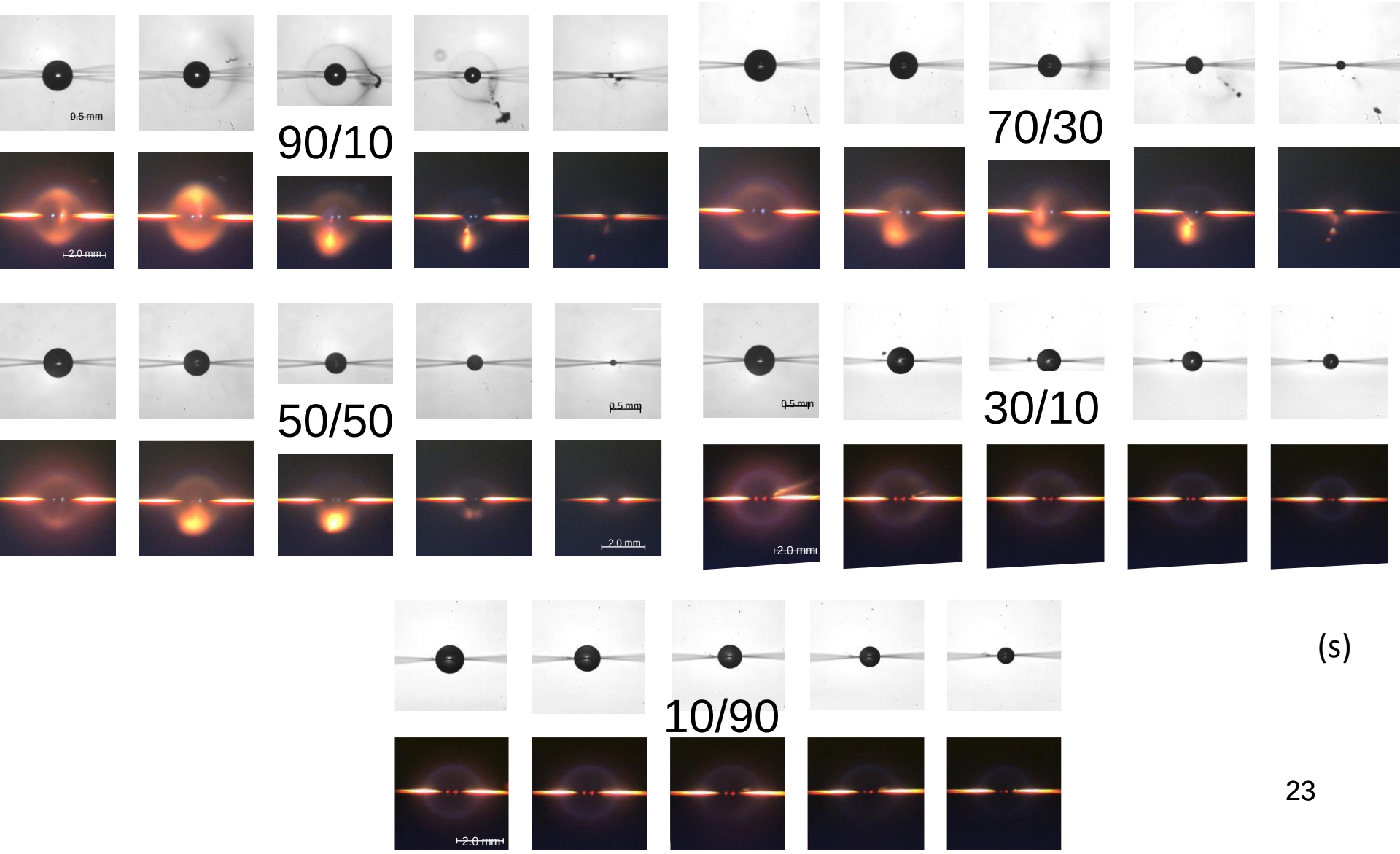
[Narayanaswamy, K., Pepiot, P, Pitsch, H., "A component library framework for deriving kinetic mechanisms for multi-component fuel surrogates: application for jet fuel surrogates," Comb. Flame 165, 288–309 (2016).]

***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.

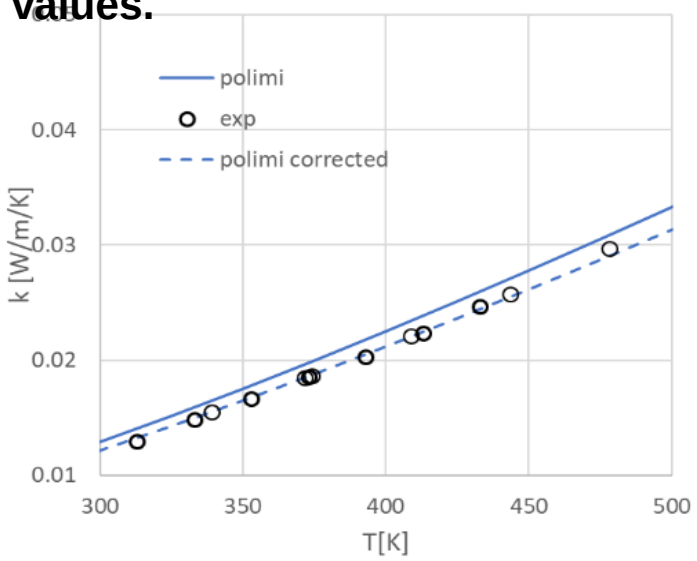
C.J. Mueller, W.J. Cannella, T.J. Bruno, B. Bunting, Heather D. Dettman, J.A. Franz, M.L. Huber, M.Natarajan, W.J. Pitz, M.A. Ratcliff, K.Wright, Methodology for formulating diesel surrogate fuels with accurate compositional, ignition quality and volatility characteristics, Energy&Fuels, 26, 3284-3303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

burning histories of heptane/isobutanol droplets

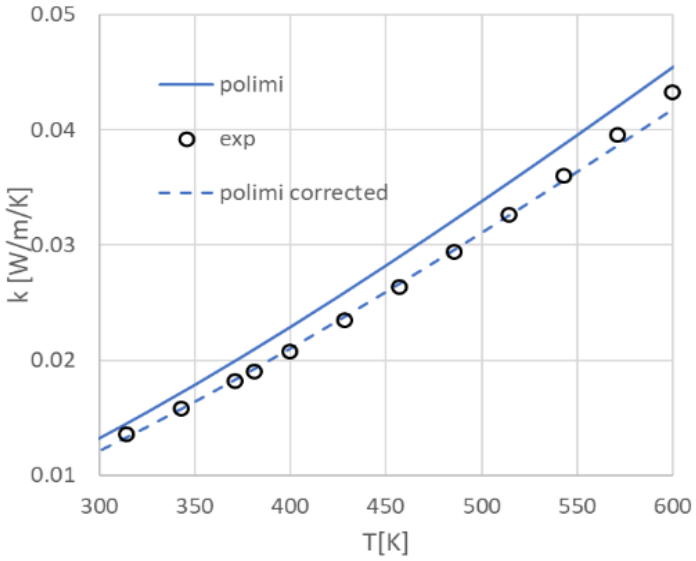


Simulation

- **Thermal properties have strong influence on simulations.**
- **Chapman-Enskog kinetic theory conductivity prediction, corrected for polyatomic gases with the Eucken approach used to simulate conductivities.**
- **Kinetic theory prediction is accurate for spherical-like molecules but can deviate significantly for cylindrical-like aggregates since there is no basis to assume an isotropic interaction potential.**
- **Published thermal conductivity values were 7-8% lower than values incorporated in the original OpenSMOKE++ framework.**
- **The predicted values were corrected by a factor of 0.9 to better match published values.**



Iso-butanol Thermal Conductivity



Heptane Thermal Conductivity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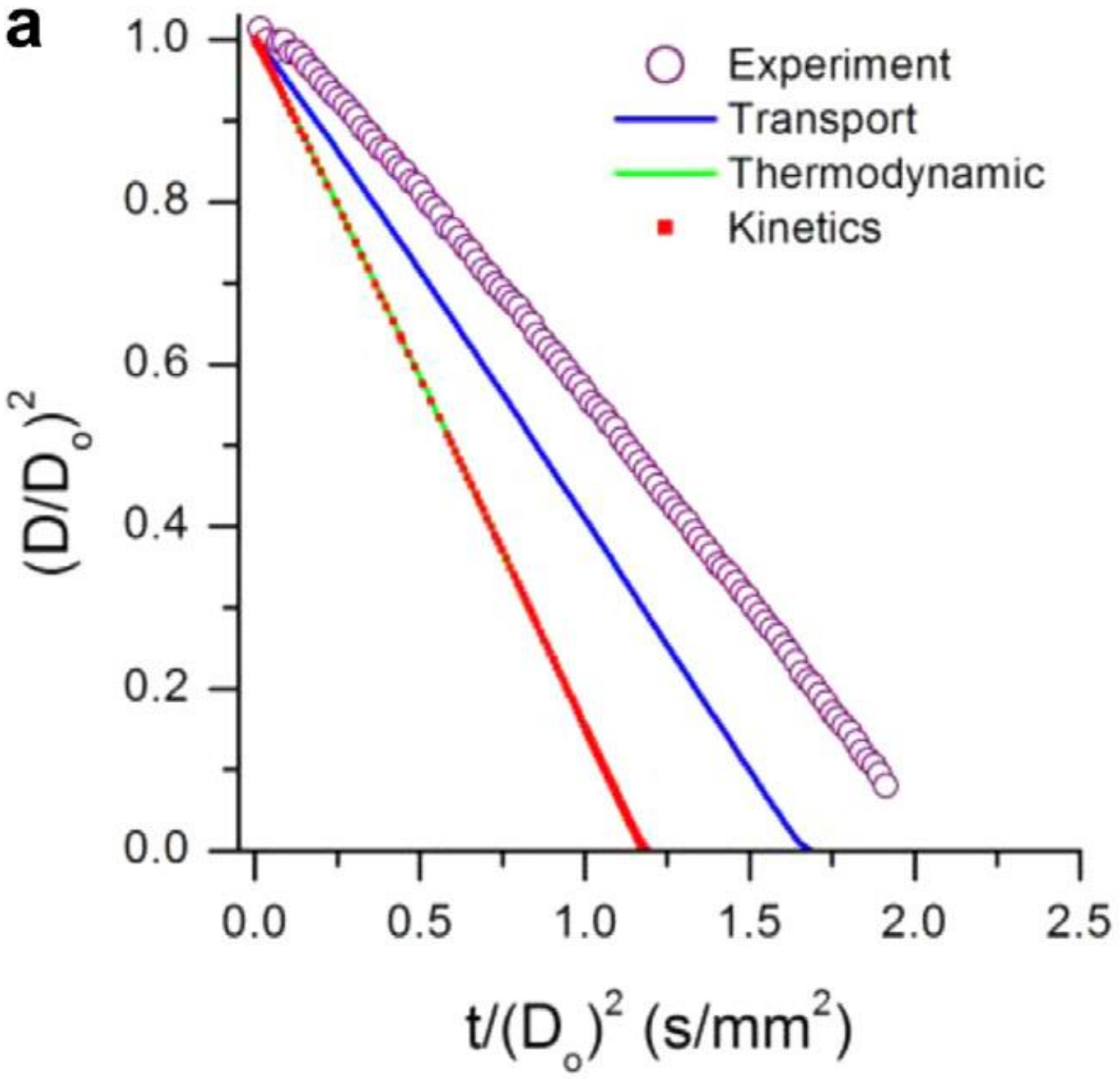
1868


a
Experiment
Transport
Thermodynamic
Kinetics
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)