Model Development of Fundamental Combustion Processes

Rainer Dahms, Jackie Chen (PIs)

Tuan Nguyen, Martin Rieth (Postdocs)

Sandia National Laboratories

FY 2019 DOE Vehicle Technologies Program Annual Merit Review
12:00 PM, Tue. 11 June 2019

Project ID# ACE125

Sponsor: **DOE Vehicle Technologies Program**
Program Managers: **Gurpreet Singh and Michael Weismiller**

Overview

Timeline

- Project provides fundamental research that supports DOE/ industry advanced engine development projects.
- Focused on next generation spray and combustion models providing more accurate predictive capability.
- Project directions and continuation are evaluated annually.

Budget

- Project funded by DOE/VT:
  - FY18 $ 390 K
  - FY19 $ 400 K
- Project lead: Sandia
  - PIs
    - Jackie Chen
    - Rainer Dahms

Barriers

Inability to accurately model engine combustion

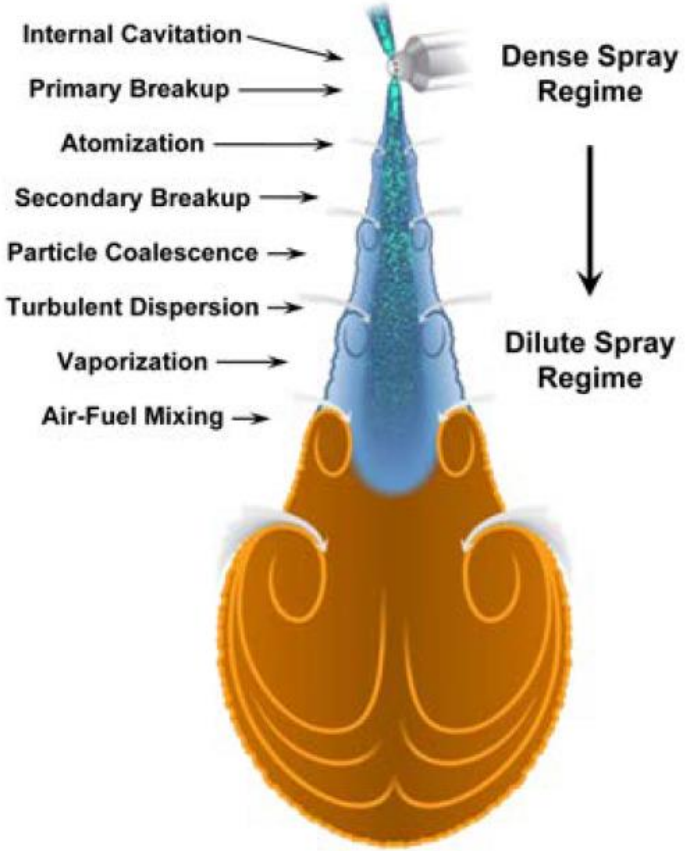
- Inability to predict spray and mixture formation
- Inability to model turbulence chemistry interaction
- CFD model improvement for engine design/optimization

Partners

- Engine Combustion Network
- Convergent Science
- TU Darmstadt
- DOE Exascale Computing Project
- LLNL

Objectives

Major objective: Develop predictive computational tools for engineering simulations



Liquid fuel injection
(Oefelein et al.,SAE 2012-01-1258)

Objectives

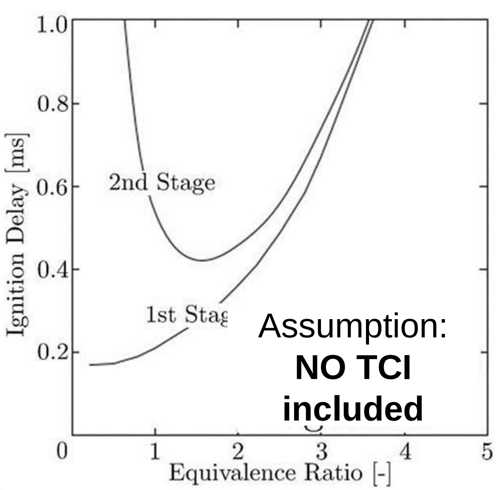
Major objective: Develop predictive computational tools for engineering simulations

- Better engine designs require accurate and predictive simulations
- Spray flame involves strongly coupled, multiscale/multiphysics phenomena
  - Fuel injection process
    - Mixing, liquid and vapor penetration affects mixture state at time of ignition
    - Surface wetting, efficiency and emissions of both diesel and gasoline engine
  - Combustion physics
    - Intense turbulence chemistry interaction (TCI)
    - Turbulent mixing affects formation of pollutant such as soot, NOx, CO
    - Complex multiphase/multicomponent mixture under high temperature from combustion affects heat and mass transfer rates between liquid and gas

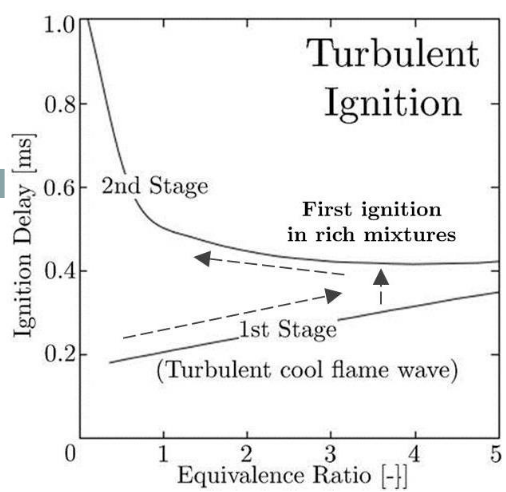
Objectives

Major objective: Develop predictive computational tools for engineering simulations

- Better engine designs require accurate and predictive simulations
- Spray flame involves strongly coupled, multiscale/multiphysics phenomena
  - Fuel injection process
    - > Mixing, liquid and vapor penetration affects mixture state at time of ignition
    - > Surface wetting, efficiency and emissions of both diesel and gasoline engine
  - Combustion physics
    - > Intense turbulence chemistry interaction (TCI)
    - > Turbulent mixing affects formation of pollutant such as soot, NOx, CO
    - > Complex multiphase/multicomponent mixture under high temperature from combustion affects heat and mass transfer rates between liquid and gas



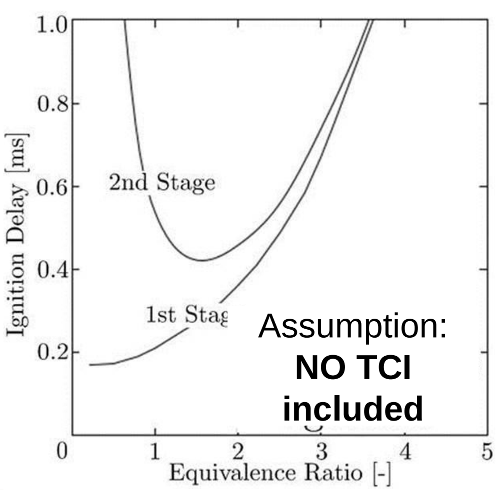
TCI



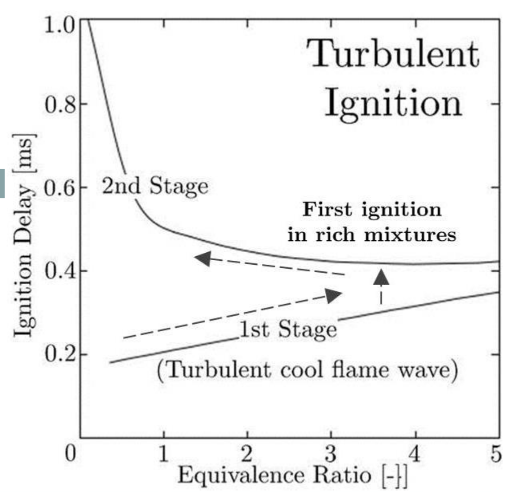
Objectives

Major objective: Develop predictive computational tools for engineering simulations

- Better engine designs require accurate and predictive simulations
- Spray flame involves strongly coupled, multiscale/multiphysics phenomena
  - Fuel injection process
    - Mixing, liquid and vapor penetration affects mixture state at time of ignition
    - Surface wetting, efficiency and emissions of both diesel and gasoline engine
  - Combustion physics
    - Intense turbulence chemistry interaction (TCI)
    - Turbulent mixing affects formation of pollutant such as soot, NOx, CO
    - Complex multiphase/multicomponent mixture under high temperature from combustion affects heat and mass transfer rates between liquid and gas



+ TCI



Current State-of-the-art Models

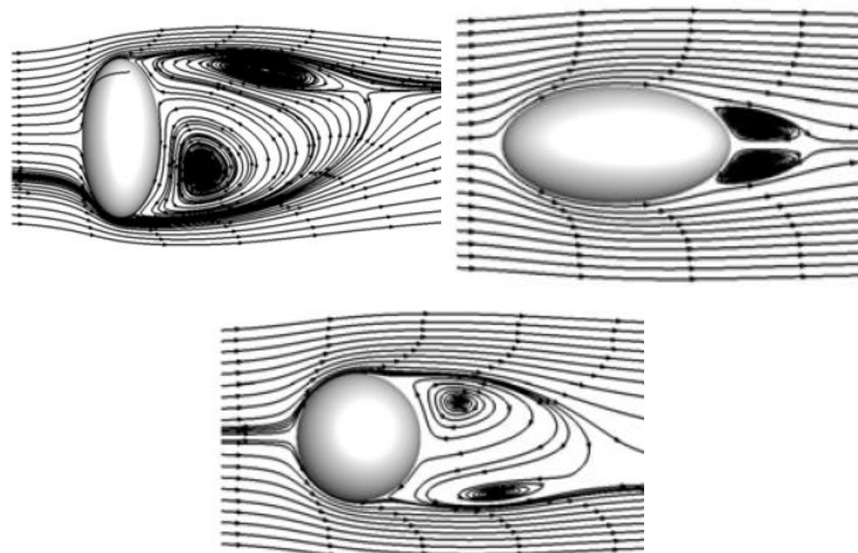
- Model free approach: Direct Numerical Simulation (DNS)
  - Resolve all time and length scales
  - Extremely high cell count -> computationally expensive
- Engineering simulations with coarse resolution needs accurate sub-grid models to account for unresolved phenomenon
- Uncertainties in numerical implementations, grid sizes, turbulence models lead to excessive model constant tuning
- Popular computationally efficient models often employs ideal/oversimplifying assumptions
  - Multi-zone (SAGE) combustion model
    - **Homogenous reactor: no explicit TCI**
  - Flamelet combustion model
    - **Based on ideal flame configurations: 1D laminar non premixed flame (diesel), 1D freely propagating premixed flame (gasoline)**
  - Two-phase (liquid-gas)**:** Lagrangian spray simulation
    - Liquid drops are treated as parcels/particles
    - Momentum/heat/mass transfers to gaseous flow fields are modeled
    - **Drops are spherical**

Model improvements based on rigorous asymptotic analysis, high-quality DNS, and experimental measurement

Development of Drop Model Based on Experimental Evidence

- Liquid drops under engine relevant conditions experience nonlinear oscillation and deformation
- New drop model take these effects into accounts
  - Drop oscillation and deformation, defined by a distortion factor, are modeled by the Taylor Analogy Breakup (TAB) approach
  - Empirical formulation for finite viscosity effect of spherical drops based on high-quality numerical data (Feng and Michaelides, 2001).
  - Regression model for drop distortion that predicts 99.8% of the variance of the drag coefficients (Richter and Nikrityuk ,2012).

Video courtesy of Pickett and Skeen
n-hexadecane into 1000K, 43 bar pressure



Richter & Nikrityuk, 2012

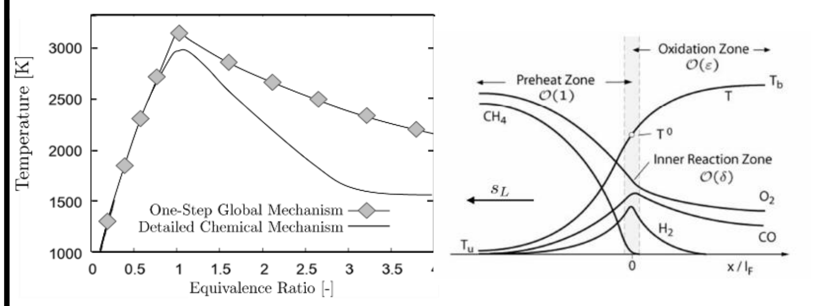
Realistic drops are non-spherical

TCI Characterization of The Multi-zone Combustion Model

- TCI characterizations of SAGE
  - Asymptotic analysis to show there is "implicit TCI" in the multi-zone combustion model
  - Quantify deficiencies of the implicit model
    - 1D flame simulations to compare results of the newly derive multi-zone TCI equation and the reference one TCI equation (Norbert Peters two-scale derivation of the flamelet approach)
    - Laminar flame speed calculation
    - Full CFD calculations with a detailed chemical mechanism

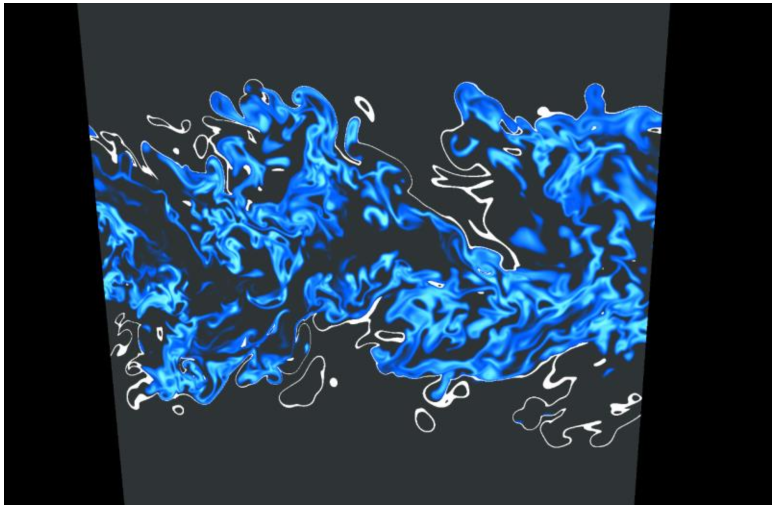
CFD must (at least) recover asymptotic at every point

Idealized Flame Structures

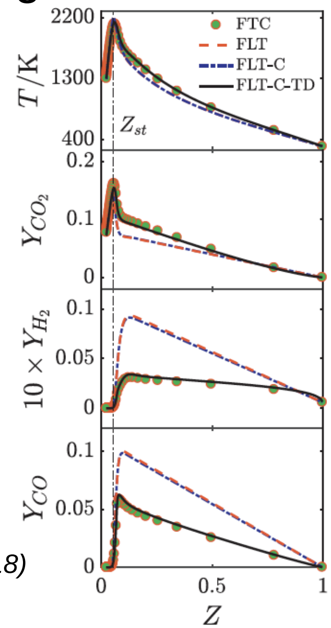


Neglect of Tangential Diffusion Lead to Errors in Flamelet Models

- Flamelet models, while computationally efficient, rely on many assumptions
  - Diesel engines: 1D laminar opposed jet diffusion flame solutions
    - TCI is accounted using presumed-shape Probability Density Function (PDF) -> preprocessed flamelet table
    - Species diffusion in the flamelet coordinate are represented by scalar dissipation rate (χ)
    - χ only significant in the coordinate normal to the flame front
- Multi-injection approach amplifies uncertainties and errors in the classic flamelet method
- DNS is the only way to study the intricate dynamics of the complex multi-stage ignition chemistry and its coupling with turbulent flow



Ketohydroperoxide ignition fronts in a diesel jet (Borghesi et al. 2018)



Comparison of curved flamelet with DNS at 1 atm

- FTC – DNS solution
- FLT – flamelet with normal diffusion
- FLT-C – flamelet with normal diffusion and curvature in normal direction
- FLT-C-TD –flamelet with normal diffusion, curvature in normal direction and tangential diffusion

Improve flamelet models utilizing high fidelity DNS data

Multi-Injection Flamelet Model

- PeleLM
  - Open source, exascale-ready AMR codes
  - 35 species reduced n-dodecane mechanism
  - ~1 μm cell size (to resolve ignition fronts)
- DNS of Spray A like conditions with multiple injections
  - Comparison with experimental results by Skeen & Pickett and study ignition delay sensitivity to mixing/chemical reaction interactions
  - Identify minimum set of control variables for split-injection ignition by sensitivity analysis (e.g. Z_1, Z_2, $C_{low\text{-}T}$, $C_{high\text{-}T}$, χ_1, χ_2, χ_{12}, age)

*AMR: adaptive mesh refinement

LES/multi-dimensional flamelet modeling outline

DNS

- DNS - ϕ^{DNS}
- Z_1, Z_2, and C

ϕ: thermo-physical quantities (e.g. species mass fractions)

Multi-Injection Flamelet Model

- PeleLM
  - Open source, exascale-ready AMR codes
  - 35 species reduced n-dodecane mechanism
  - ~1 μm cell size (to resolve ignition fronts)
- DNS of Spray A like conditions with multiple injections
  - Comparison with experimental results by Skeen & Pickett and study ignition delay sensitivity to mixing/chemical reaction interactions
  - Identify minimum set of control variables for split-injection ignition by sensitivity analysis (e.g. Z_1, Z_2, $C_{low\text{-}T}$, $C_{high\text{-}T}$, χ_1, χ_2, χ_{12}, age)
- Flamelet model development
  - Collect statistics of the relevant variables
    - Joint Probability Density Functions (PDFs) of the control variables
    - Pilot and main mixture fractions, progress and age variables
  - Generate flamelet tables from the statistics
  - LES simulations with new flamelet tables
  - Compare LES with DNS results

*AMR: adaptive mesh refinement

LES/multi-dimensional flamelet modeling outline

DNS

- DNS - ϕ^{DNS}
- Z_1, Z_2, and C

ϕ: thermo-physical quantities (e.g. species mass fractions)

Multi-Injection Flamelet Model

- PeleLM
  - Open source, exascale-ready AMR codes
  - 35 species reduced n-dodecane mechanism
  - ~1 μm cell size (to resolve ignition fronts)
- DNS of Spray A like conditions with multiple injections
  - Comparison with experimental results by Skeen & Pickett and study ignition delay sensitivity to mixing/chemical reaction interactions
  - Identify minimum set of control variables for split-injection ignition by sensitivity analysis (e.g. Z_1, Z_2, $C_{low\text{-}T}$, $C_{high\text{-}T}$, χ_1, χ_2, χ_{12}, age)
- Flamelet model development
  - Collect statistics of the relevant variables
    - > Joint Probability Density Functions (PDFs) of the control variables
    - > Pilot and main mixture fractions, progress and age variables
  - Generate flamelet tables from the statistics
  - LES simulations with new flamelet tables
  - Compare LES with DNS results

*AMR: adaptive mesh refinement

LES/multi-dimensional flamelet modeling outline

DNS

- DNS - ϕ^{DNS}
- Z_1, Z_2, and C

Z_1^{DNS}, Z_2^{DNS}, and C^{DNS} →

ϕ: thermo-physical quantities (e.g. species mass fractions)

Multi-Injection Flamelet Model

- PeleLM
  - Open source, exascale-ready AMR codes
  - 35 species reduced n-dodecane mechanism
  - ~1 μm cell size (to resolve ignition fronts)
- DNS of Spray A like conditions with multiple injections
  - Comparison with experimental results by Skeen & Pickett and study ignition delay sensitivity to mixing/chemical reaction interactions
  - Identify minimum set of control variables for split-injection ignition by sensitivity analysis (e.g. Z_1, Z_2, $C_{low\text{-}T}$, $C_{high\text{-}T}$, χ_1, χ_2, χ_{12}, age)
- Flamelet model development
  - Collect statistics of the relevant variables
    - Joint Probability Density Functions (PDFs) of the control variables
    - Pilot and main mixture fractions, progress and age variables
  - Generate flamelet tables from the statistics
  - LES simulations with new flamelet tables
  - Compare LES with DNS results

*AMR: adaptive mesh refinement

LES/multi-dimensional flamelet modeling outline

DNS

- DNS - ϕ^{DNS}
- Z_1, Z_2, and C

Z_1^{DNS}, Z_2^{DNS}, and C^{DNS} →

LES/Flamelet

$$\phi^{\mathrm{LES}} = \phi(\widetilde{Z_1}, \widetilde{Z_1''}, \widetilde{Z_2}, \widetilde{Z_2''}, \widetilde{C})$$

$$\phi^{\mathrm{LES}} = \phi(\widetilde{Z_1 + Z_2}, \widetilde{(Z_1 + Z_2)''}, \widetilde{C})$$

ϕ: thermo-physical quantities (e.g. species mass fractions)

Multi-Injection Flamelet Model

- PeleLM
  - Open source, exascale-ready AMR codes
  - 35 species reduced n-dodecane mechanism
  - ~1 μm cell size (to resolve ignition fronts)
- DNS of Spray A like conditions with multiple injections
  - Comparison with experimental results by Skeen & Pickett and study ignition delay sensitivity to mixing/chemical reaction interactions
  - Identify minimum set of control variables for split-injection ignition by sensitivity analysis (e.g. Z_1, Z_2, C_{low-T}, C_{high-T}, χ_1, χ_2, χ_{12}, age)

- Flamelet model development
  - Collect statistics of the relevant variables
    - > Joint Probability Density Functions (PDFs) of the control variables
    - > Pilot and main mixture fractions, progress and age variables
  - Generate flamelet tables from the statistics
  - LES simulations with new flamelet tables
  - Compare LES with DNS results

*AMR: adaptive mesh refinement

LES/multi-dimensional flamelet modeling outline

DNS

- DNS - ϕ^{DNS}
- Z_1, Z_2, and C

$Z_1^{\mathrm{DNS}},\ Z_2^{\mathrm{DNS}},\ \text{and}\ C^{\mathrm{DNS}}$ →

↔ $\phi^{\mathrm{DNS}}\ \text{vs.}\ \phi^{\mathrm{LES}}$

LES/Flamelet

$$\phi^{\mathrm{LES}} = \phi(\widetilde{Z_1}, \widetilde{Z_1''}, \widetilde{Z_2}, \widetilde{Z_2''}, \widetilde{C})$$

$$\phi^{\mathrm{LES}} = \phi(\widetilde{Z_1 + Z_2}, \widetilde{(Z_1 + Z_2)''}, \widetilde{C})$$

ϕ: thermo-physical quantities (e.g. species mass fractions)

Approach - Milestones

- ✓ **May 2018**
  Introduce a new model for turbulence-chemistry interactions in multi-zone approaches
- ✓ **July 2018**
  DNS simulation of multiple injections under Spray A condition
- ✓ **August 2018**
  Develop mixture fraction-age flamelet modeling approach
- ✓ **January 2019**
  Introduce a new model for oscillating dense-spray drop dynamics
- ✓ **March 2019**
  New drag models implemented in CONVERGE CFD via UDF implementations.

Example Case: SprayA Lagrangian Spray Simulations

- Commercial CFD drag model
  - Liu et al. (1993b)
  - Solid sphere -> distorted -> sharp disk
  - Drag coefficients: 0.047 (bubble), solid sphere (0.427)
- Case setup
  - Out-of-the-box non reacting Spray A configuration in Converge
  - $T_a = 900\ K,\ \ T_f = 363\ K$
  - $P_a = 6\ MPa,\ P_{\{inj\}} = 150\ Mpa$
  - Injection duration: 1.5 ms
  - Lagrangian+RANS model

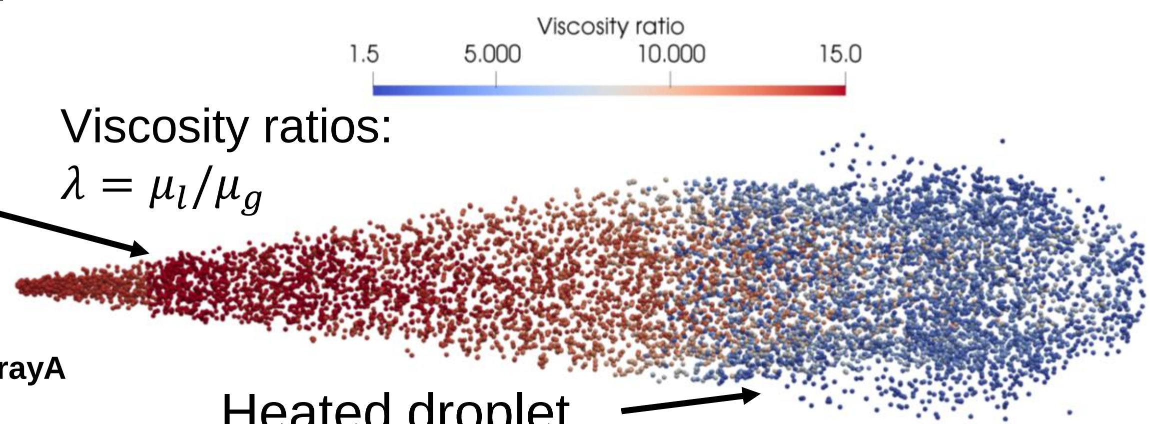
- Dahms and Oefelein (2016) model:
  - Drag coefficients are functions of drop Reynolds numbers and viscosity ratios.
  - Include distortion factor (account for non-spherical droplets)
  - Finite viscosity effect
- No constant tuning.

Example Case: SprayA Lagrangian Spray Simulations

- Commercial CFD drag model
  - Liu et al. (1993b)
  - Solid sphere -> distorted -> sharp disk
  - Drag coefficients: 0.047 (bubble), solid sphere (0.427)
- Case setup
  - Out-of-the-box non reacting Spray A configuration in Converge
  - $T_a = 900\ K,\ \ T_f = 363\ K$
  - $P_a = 6\ MPa,\ P_{\{inj\}} = 150\ Mpa$
  - Injection duration: 1.5 ms
  - Lagrangian+RANS model
- Dahms and Oefelein (2016) model:
  - Drag coefficients are functions of drop Reynolds numbers and viscosity ratios.
  - Include distortion factor (account for non-spherical droplets)
  - Finite viscosity effect
- No constant tuning.

Viscosity ratios:
$\lambda = \mu_l / \mu_g$

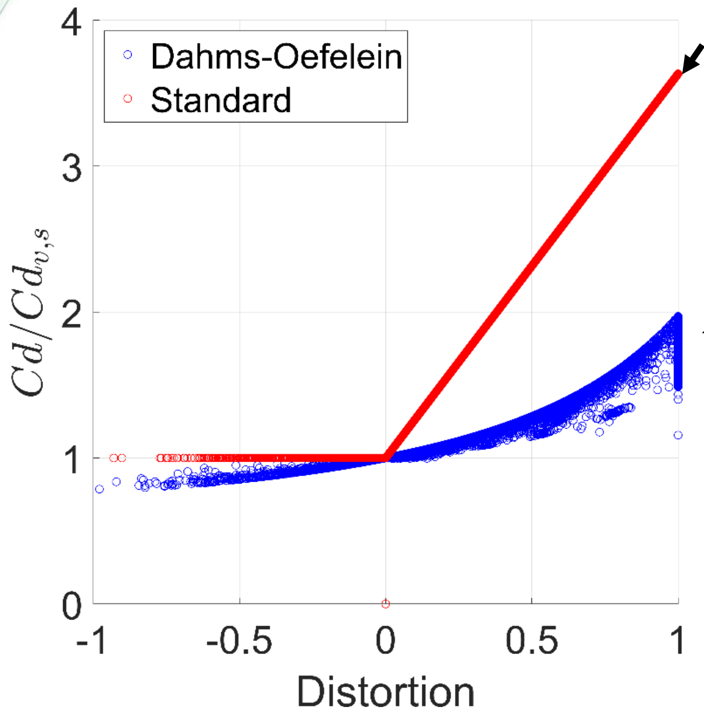
Cold liquid

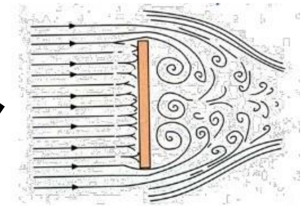


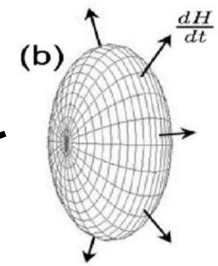
Heated droplet

Liquid parcel results of a SprayA Lagrangian simulation

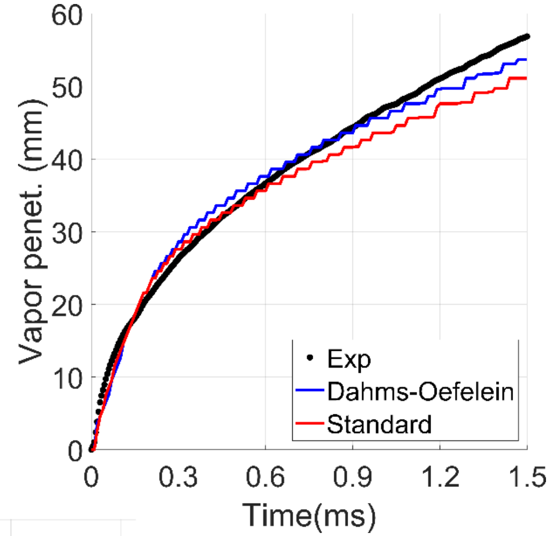
Simulation Results: Effect of Drag Prediction



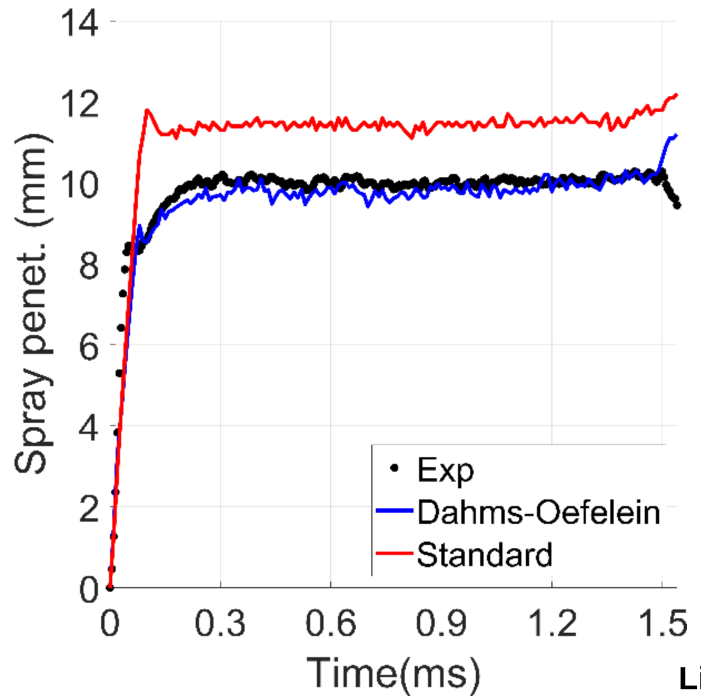




Normalized drag vs. distortion factor



Vapor penetration vs. time

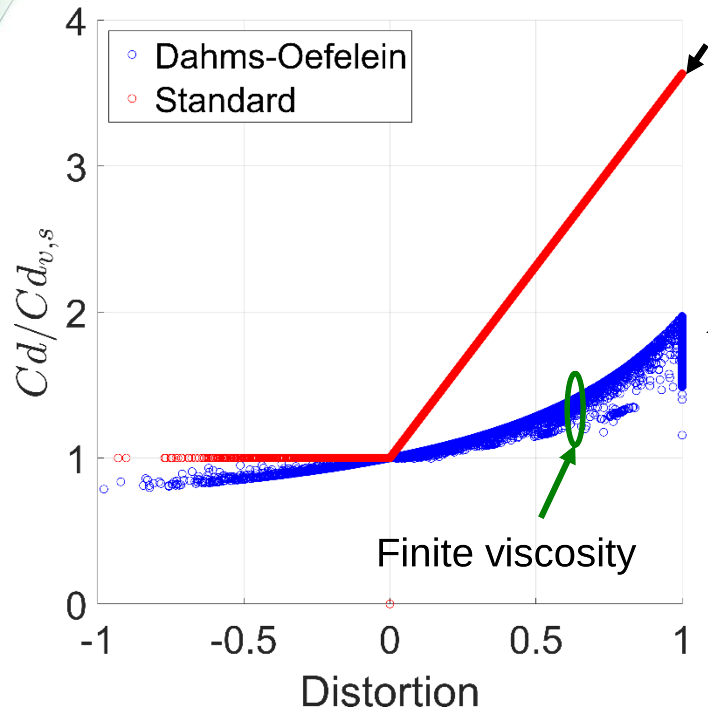


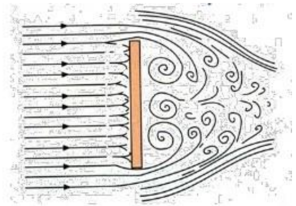
Liquid penetration vs. time

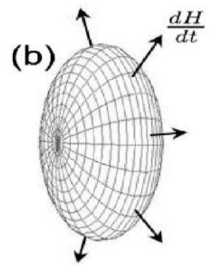
Correctly capturing drop shapes and finite viscosity effects leads to substantial change in drag prediction

Lower drag leads to significant change in liquid penetration prediction

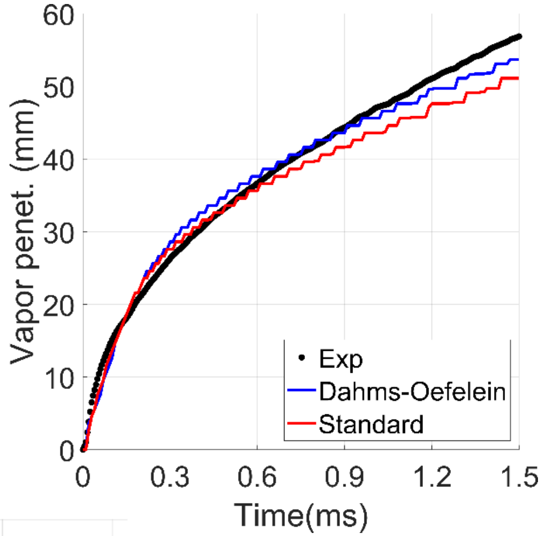
Simulation Results: Effect of Drag Prediction



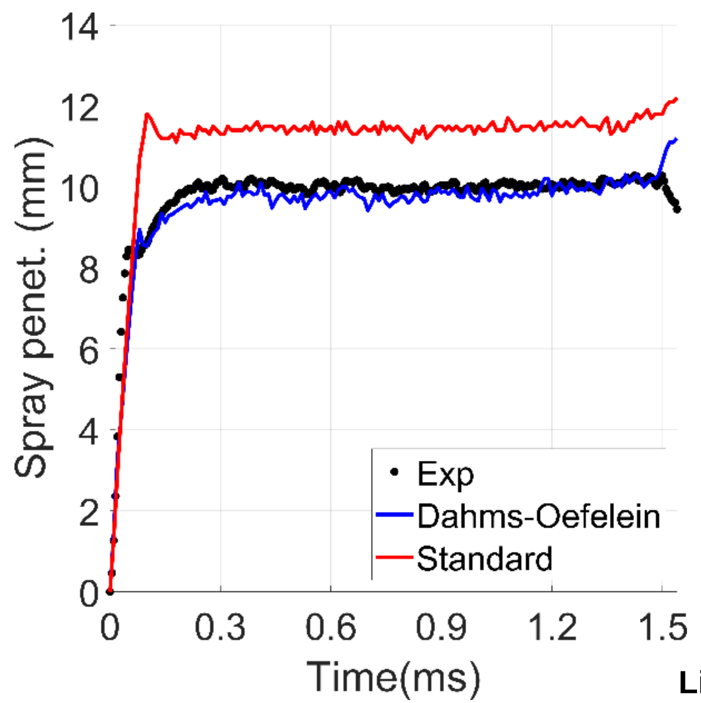




Normalized drag vs. distortion factor



Vapor penetration vs. time



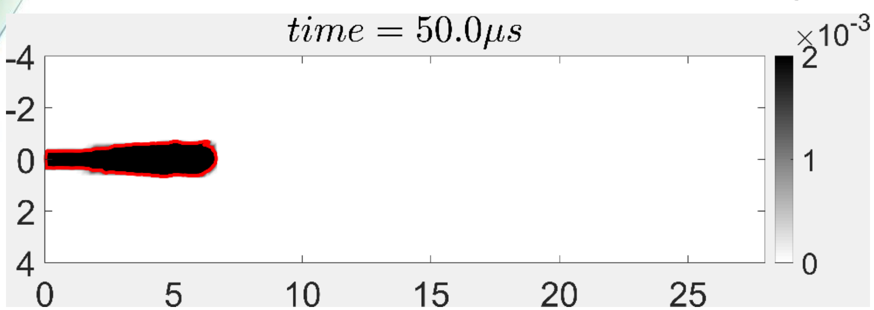
Liquid penetration vs. time

Correctly capturing drop shapes and finite viscosity effects leads to substantial change in drag prediction

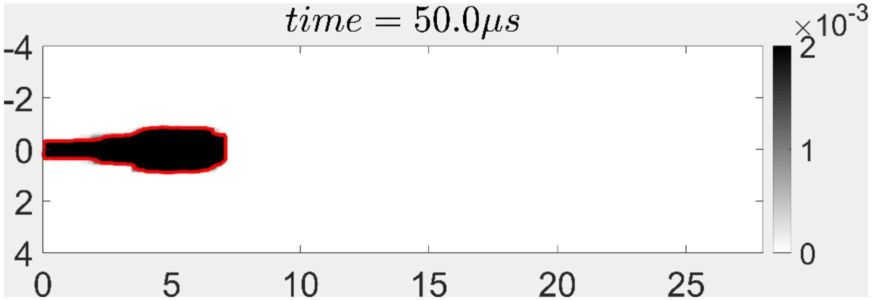
Lower drag leads to significant change in liquid penetration prediction

Simulation Results: Spray Characteristic Comparison

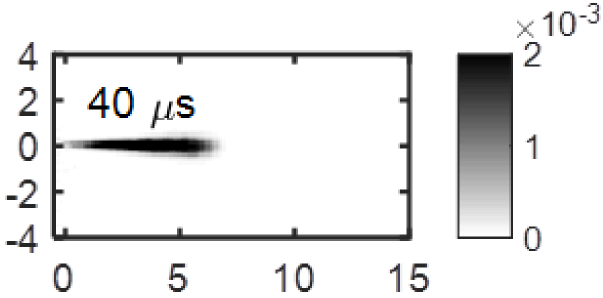
PLV: Projected Liquid Volume



Dahms-Oefelein



Standard

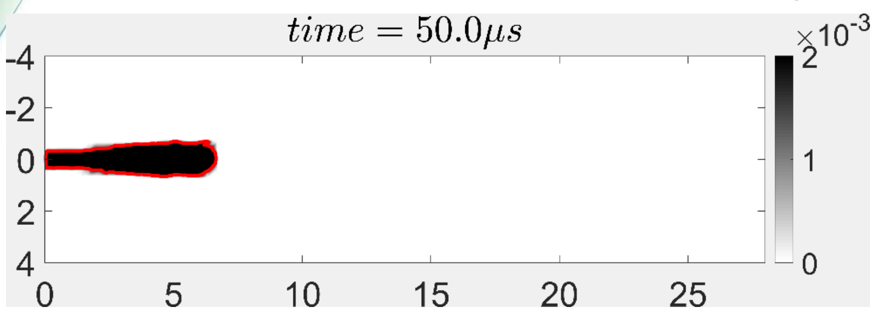


Experiment (Courtesy of Pickett and Skeen)

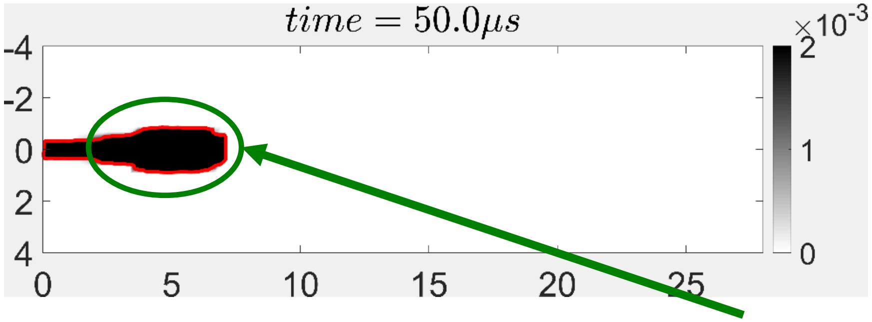
Differences in PLV suggest profound differences in the degree of wall wetting, even more than would be expected based on liquid penetration alone

Simulation Results: Spray Characteristic Comparison

PLV: Projected Liquid Volume

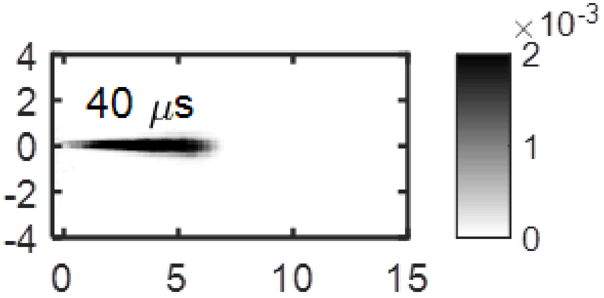


Dahms-Oefelein



Standard

Unphysical mushroom shape

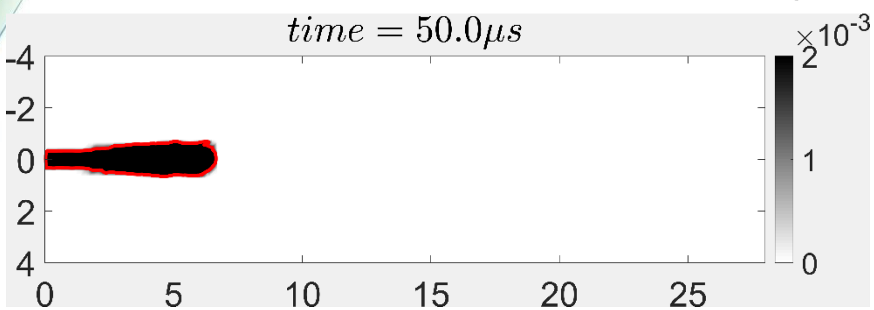


Experiment (Courtesy of Pickett and Skeen)

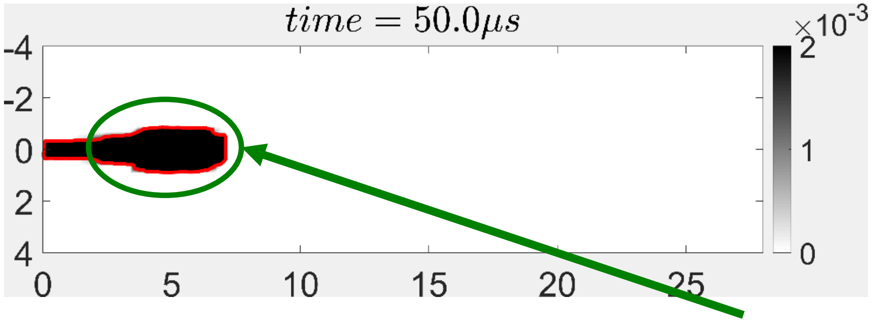
Differences in PLV suggest profound differences in the degree of wall wetting, even more than would be expected based on liquid penetration alone

Simulation Results: Spray Characteristic Comparison

PLV: Projected Liquid Volume

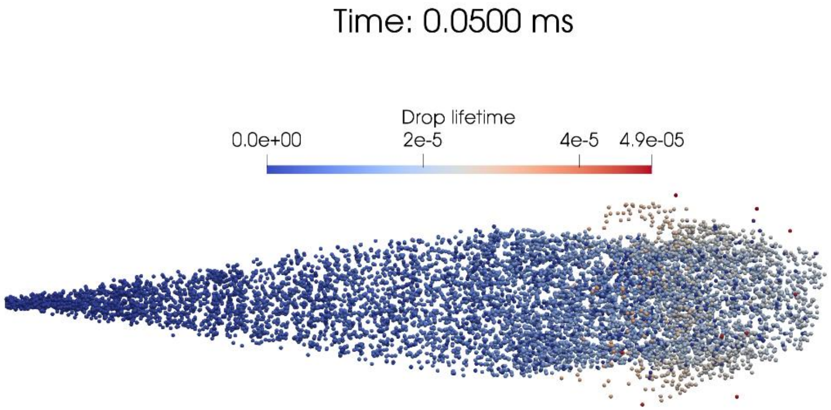


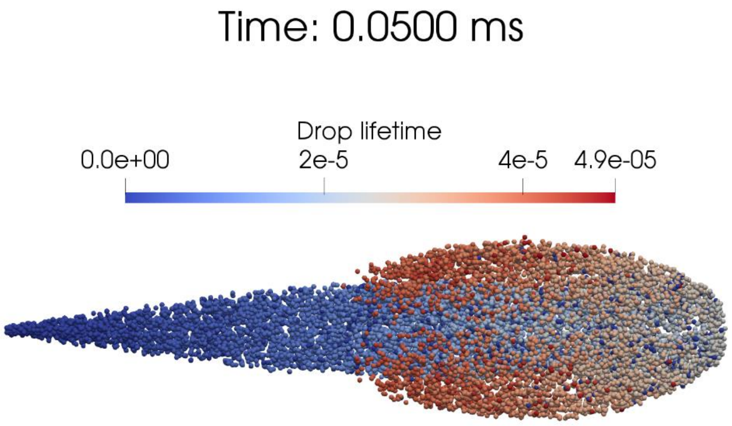
Dahms-Oefelein



Standard

Unphysical mushroom shape

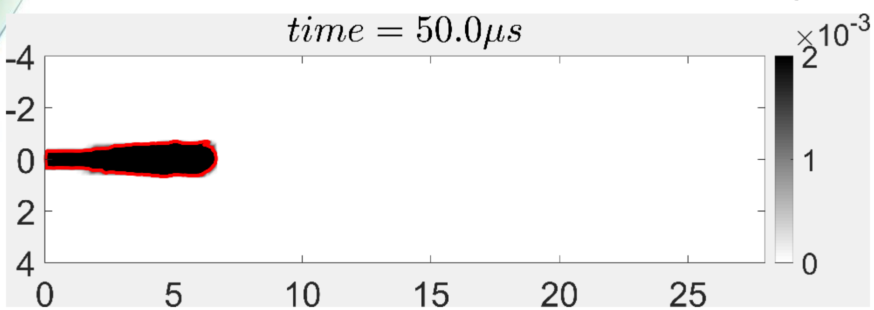




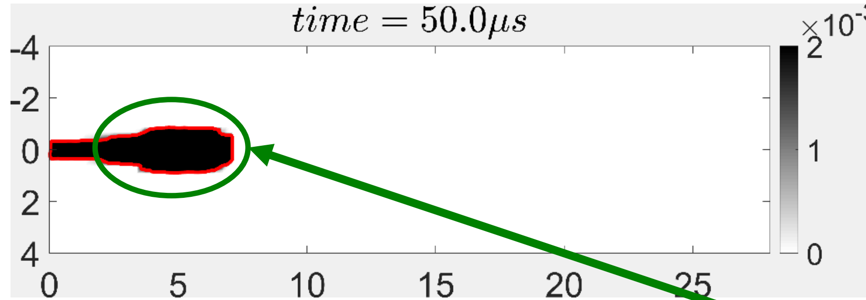
Differences in PLV suggest profound differences in the degree of wall wetting, even more than would be expected based on liquid penetration alone

Simulation Results: Spray Characteristic Comparison

PLV: Projected Liquid Volume

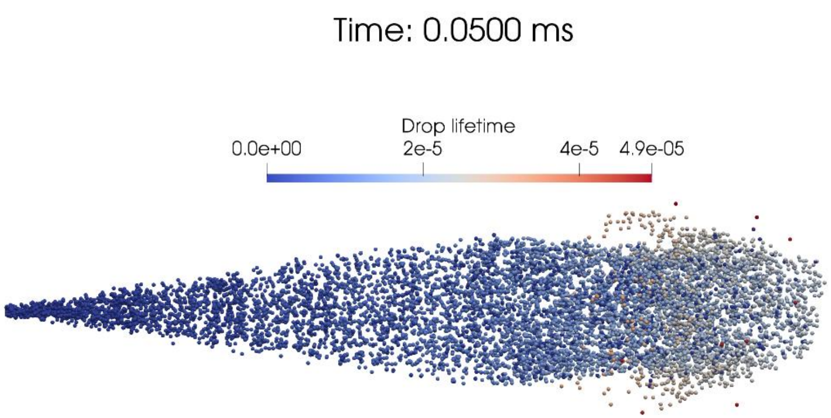


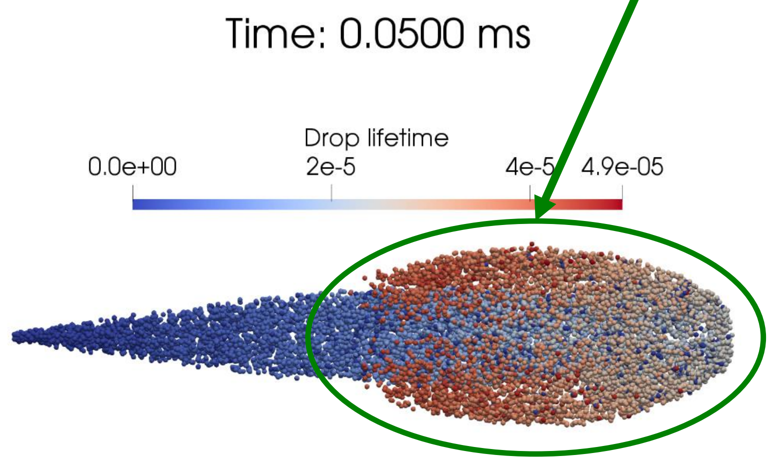
Dahms-Oefelein



Standard

Unphysical mushroom shape





Differences in PLV suggest profound differences in the degree of wall wetting, even more than would be expected based on liquid penetration alone

TCI Characterization of the Multi-zone Combustion Model

Assumptions
Species/temperature diffusion determined by model
Variance implies "production=dissipation"
Constant conditional gradients in mixture fraction space

- Start: Definition of multi-zone reactor model:

$$\frac{dY_{ij}}{dt} = \frac{\dot{m}_{ij}}{\rho_i}$$

- End:

$$\rho \frac{(dY_i)}{dt} = \rho \frac{(\Delta Z)^2}{m_i Le_i} \left(\sum_{k=1}^{2} (-1)^k \, \dot{m}_{i,k} \right) + \dot{m}_i$$

Multi-zone TCI eqs.

Full 3D reactive Navier-Stokes eqs. → Asymptotic solution →

$$\rho \frac{(dY_i)}{dt} = \rho \frac{\chi}{2Le_i} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{m}_i$$

Reference TCI eqs.

- Implicit TCI means
  - Performance based on grid size, numeric, etc.
  - Neglect of turbulent mixture state fluctuations
  - Neglect of molecular transport in TCI
    - True even at high fidelity LES
  - "Production = Dissipation" (local equilibrium)
    - Problematic for non-equilibrium

Vanish

In the limit of Δx, Δt -> 0 (DNS)
Diminishing χ (HCCI)

Multi-zone model implicitly contains TCI

- Caution: not to confuse with flamelet models (e.g., G-eqn, RIF, M-RIF)

TCI Characterization of the Multi-zone Combustion Model

Assumptions
Species/temperature diffusion determined by model
Variance implies "production=dissipation"
Constant conditional gradients in mixture fraction space

- Start: Definition of multi-zone reactor model:

$$\frac{dY_{ij}}{dt} = \frac{\dot{m}_{ij}}{\rho_i}$$

- End:

$$\rho \frac{(dY_i)}{dt} = \rho \frac{(\Delta Z)^2}{m_i Le_i} \left(\sum_{k=1}^{2} (-1)^k \, \dot{m}_{i,k} \right) + \dot{m}_i$$

Multi-zone TCI eqs.

Full 3D reactive Navier-Stokes eqs. → Asymptotic solution

$$\rho \frac{(dY_i)}{dt} = \rho \frac{\chi}{2Le_i} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{m}_i$$

Reference TCI eqs.

- Implicit TCI means
  - Performance based on grid size, numeric, etc.
  - Neglect of turbulent mixture state fluctuations
  - Neglect of molecular transport in TCI
    - True even at high fidelity LES
  - "Production = Dissipation" (local equilibrium)
    - Problematic for non-equilibrium

Vanish

In the limit of Δx, Δt -> 0 (DNS)
Diminishing χ (HCCI)

Multi-zone model implicitly contains TCI

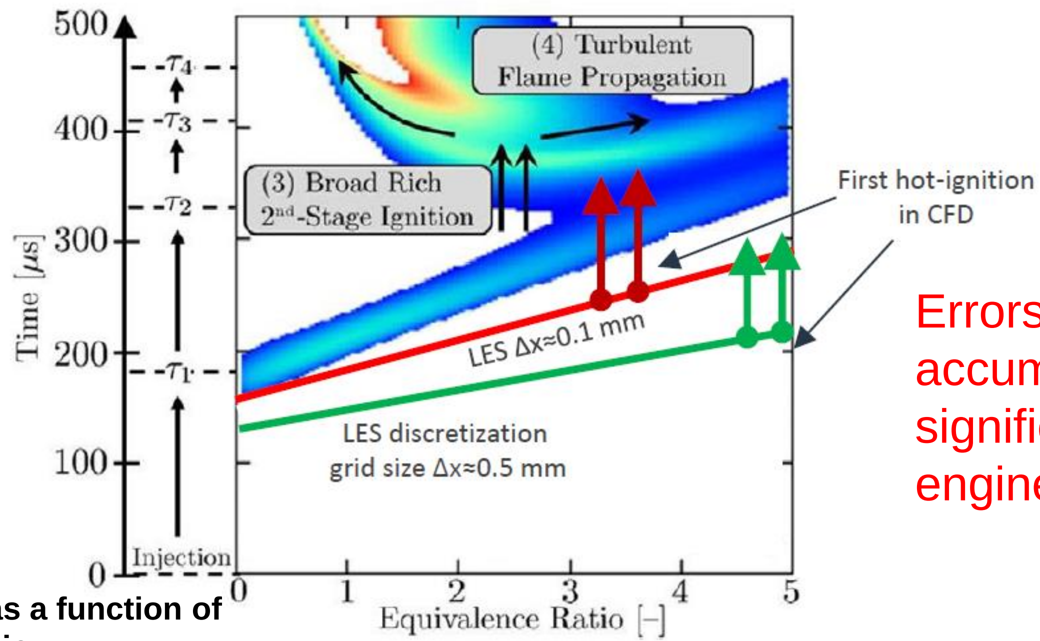
- Caution: not to confuse with flamelet models (e.g., G-eqn, RIF, M-RIF)

Preliminary Results: Performance of "Multi-zone TCI Equations.

- Differences between "multi-zone TCI" and reference TCI equations using SprayA reacting case

(a) LLNL reduced n-dodecane mechanism (250 species), (b) LES turbulence model, (c) ideal gas law and LLNL transport data, (d) grid size ~ 100 µm, (e) time-step 1e-6 sec, (f) 2^{nd} order central in space, (g) 2^{nd} order RK in time, (h) local conditions at tip of injection in SprayA (Dahms et al., PROCI 2017)

CFD Solver Configuration → **Multi-Zone TCI Solver** → **Unsteady TCI fidelity determination + detailed error assessment**

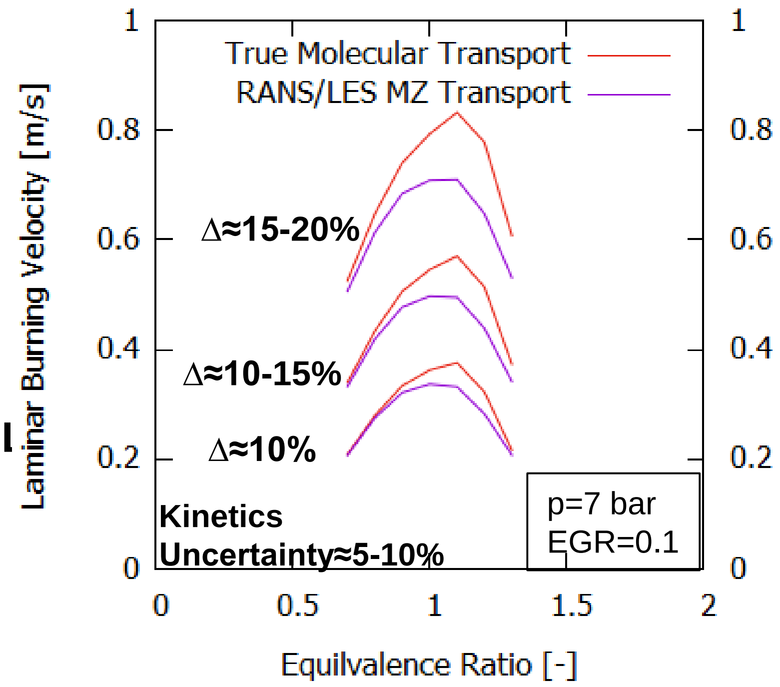


Ignition delay as a function of equivalence ratio

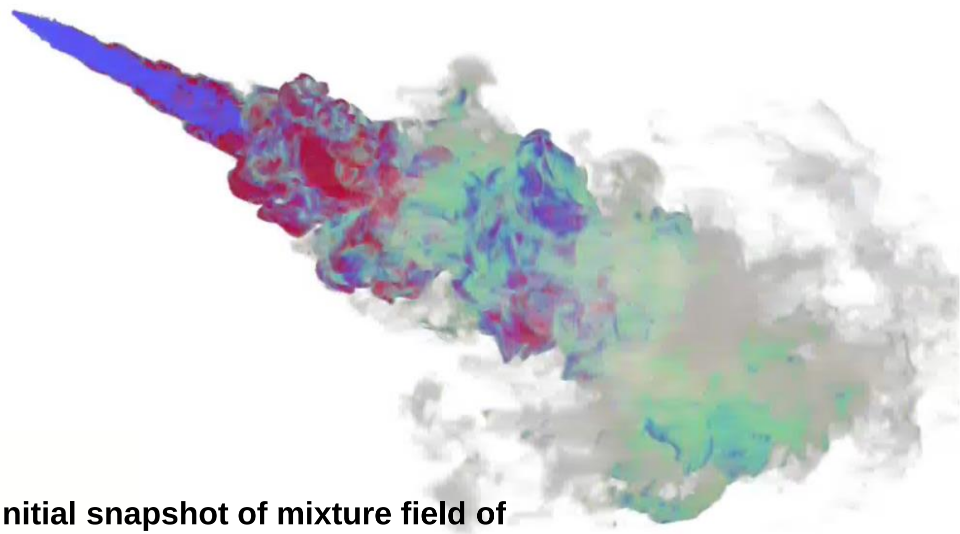
Errors in TCI modeling accumulate over time and significantly degrade final engine-CFD results

Preliminary Results: Importance of TCI in Comparison with Kinetics

- **1-D laminar burning velocities**
  - **336 n-dodecane mechanism**
  - **Reference calculation by S. LaPointe (LLNL)**
  - **CFD: kernel transition to fully-developed flame**
- **Full CFD calculations**
  - **Porting LNLL 2302 species mechanism to CONVERGE CFD by Goutham Kukkadapu (LLNL)**



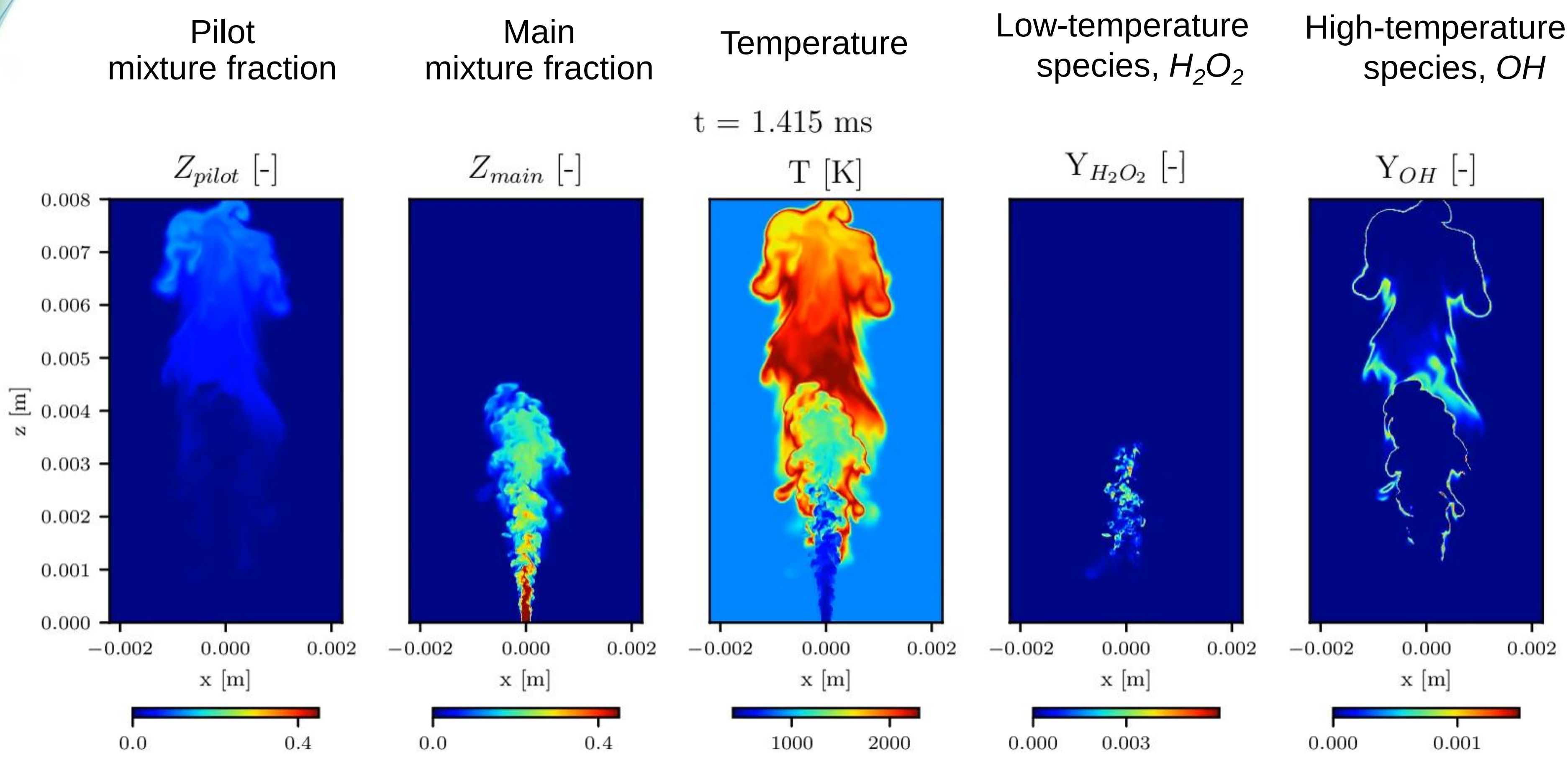
Laminar burning velocity as a function of equivalence ratio



Initial snapshot of mixture field of the full SprayA CFD calculation with multi-zone combustion model

Errors from TCI >= uncertainties in kinetics
Kinetic fidelity is lost using the multi-zone model

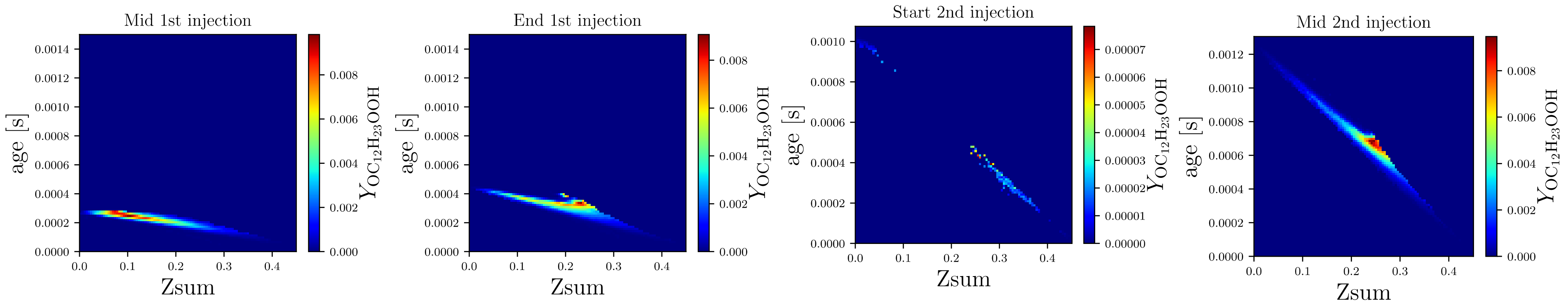
Direction Numerical Simulation of SprayA with Multi-injections



Multi-injection ignition sequence shows strong coupling between turbulence and ignition kinetics

Importance of Age Variable in Flamelet Modeling for Multi-Injection

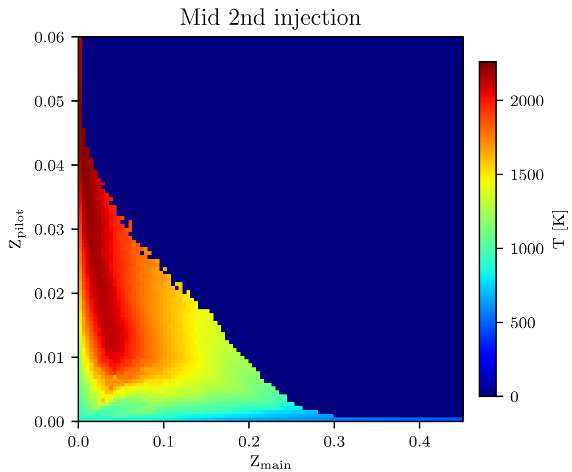
- ‘Age’ is a measure of the residence time of a fluid parcel; age transport equation is similar to mixture fraction with an integer counter, useful for modeling transient phenomena, e.g. ignition
- Multi-injection flamelets require multi-dimensional flamelets with an additional mixture fraction coordinate for each injection (Hasse / Cook / Doran)
- Recast multiple-mixture fraction approach (with dimensions of number of injections) by a single two-dimensional age-mixture fraction flamelet (Richardson/Doran)
- Requires the dissipation rate of ‘age’ and its cross-dissipation with mixture fraction obtained from DNS

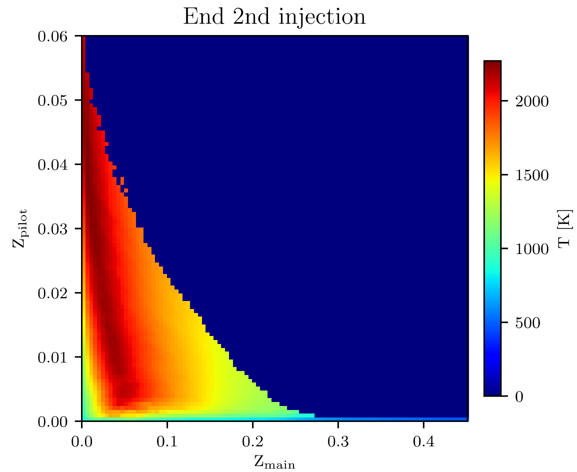


Ketohydroperoxide, a low temperature ignition marker, conditioned on (Z_{sum}, *age*)

Low temperature combustion depends on age.
Age variable is essential for the new flamelet model

Statistics of Control Variables for Modeling and Validation



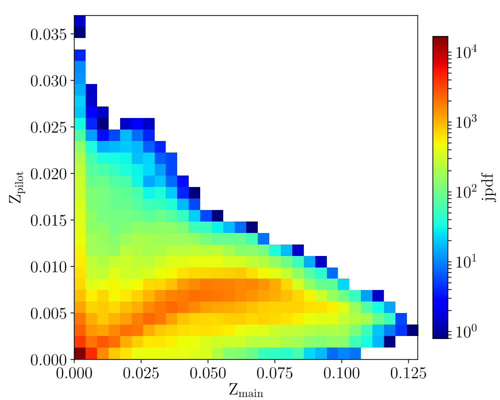


- DNS statistics provide both modeling and validation metrics
- Scalar dissipation rate PDFs for both injections are log normal, contrary to the popular Dirac δ assumption
- Cross scalar dissipation rate exhibits stretched exponential distribution

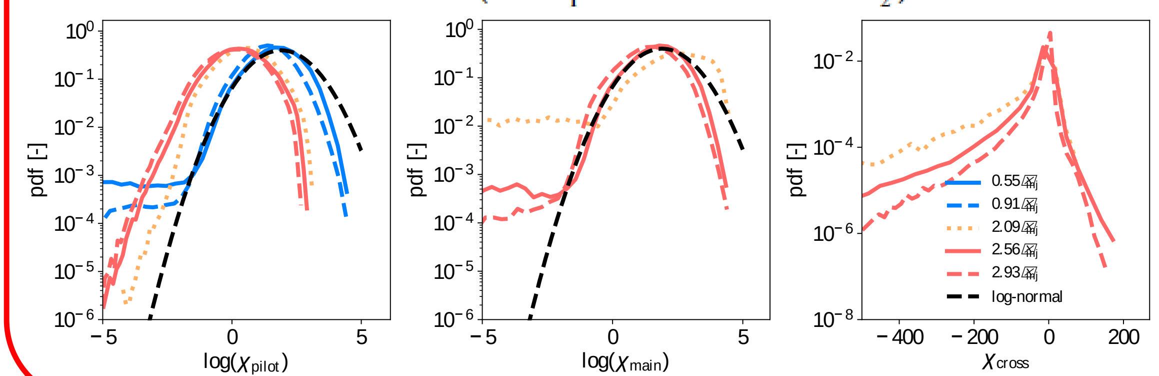
Validation metric: temperature conditioned on the two mixture fractions

Modeling statistics

$$\dot{Q}_{1+2} = \iint^{1} \dot{Q}(Z_1, Z_2) P(Z_1, Z_2) \mathrm{d}Z_1 \, \mathrm{d}Z_2$$

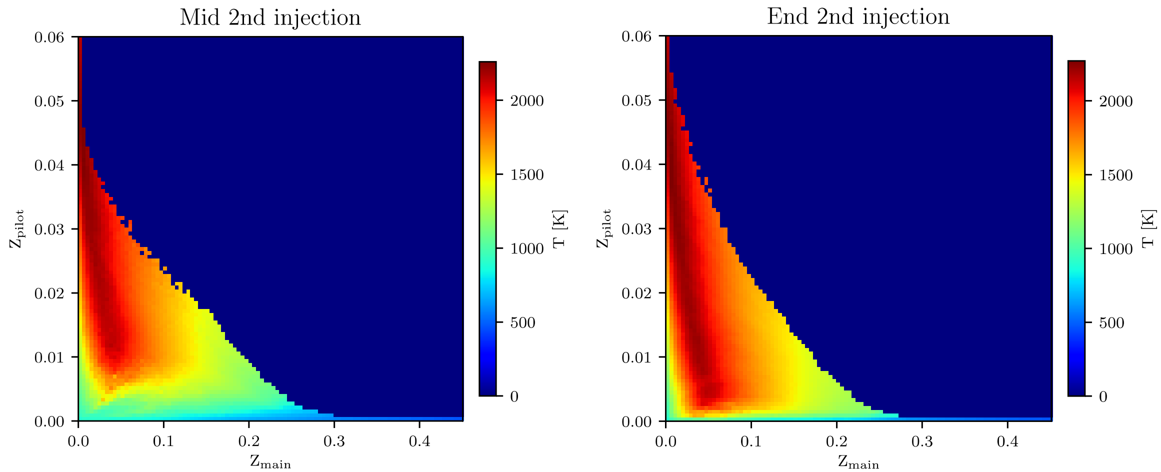


$$\rho \frac{\partial Y_k}{\partial t} = \rho \left(\frac{\chi_1}{2} \frac{\partial^2 Y_k}{\partial Z_1^2} + \chi_{12} \frac{\partial^2 Y_k}{\partial Z_1 \partial Z_2} + \frac{\chi_2}{2} \frac{\partial^2 Y_k}{\partial Z_2^2} \right) + \rho \dot{\omega}_k$$



Joint PDFs of the two mixture fractions

Statistics of Control Variables for Modeling and Validation

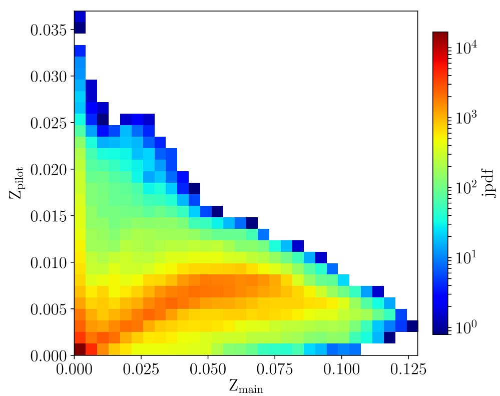


- DNS statistics provide both modeling and validation metrics
- Scalar dissipation rate PDFs for both injections are log normal, contrary to the popular Dirac δ assumption
- Cross scalar dissipation rate exhibits stretched exponential distribution

Validation metric: temperature conditioned on the two mixture fractions

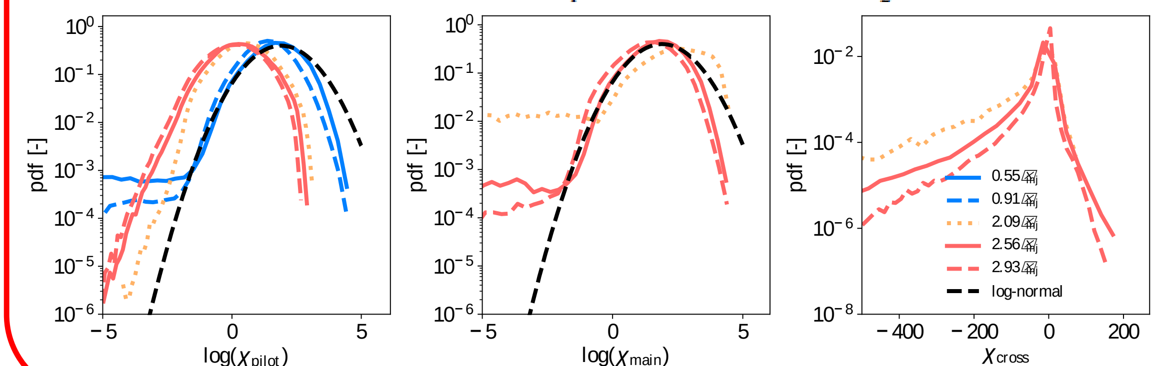
Can LES simulation with the new flamelet model recover this behavior ?

$$\dot{Q}_{1+2} = \iint^{1} \dot{Q}(Z_1, Z_2) P(Z_1, Z_2) \mathrm{d}Z_1 \, \mathrm{d}Z_2$$



Joint PDFs of the two mixture fractions

$$\rho \frac{\partial Y_k}{\partial t} = \rho \left(\frac{\chi_1}{2} \frac{\partial^2 Y_k}{\partial Z_1^2} + \chi_{12} \frac{\partial^2 Y_k}{\partial Z_1 \partial Z_2} + \frac{\chi_2}{2} \frac{\partial^2 Y_k}{\partial Z_2^2} \right) + \rho \dot{\omega}_k$$



Responses to previous year reviewer comments

- N/A

Collaborations and Coordination with Other Institutions

- TCI and drop modeling
  - Lawrence Livermore National Labs for chemical kinetics
  - ECN researchers for extensive validations
  - CONVERGE UDFs implementation -> quick, widespread use of the new models by engine community

- Multiple-injection modeling
  - Flamelet modeling efforts led by Christian Hasse (TU Darmstadt)
  - DOE ASCR Exascale Computing Project
    - PI: Jackie Chen
    - 5 DOE Labs collaborations
    - Tianfeng Lu at U. Connecticut for automated chemistry generation and reduction
    - High fidelity DNS open source research codes (PeleC and PeleLM)
    - ECN researchers for experimental validations
    - Similar computations performed for UAV (Army UAS program) for different fuels and conditions

Remaining Challenges/Barriers

- Drop modeling
  - Distorted drops lead to increase in surface area -> enhance evaporation
  - Validity in the liquid core becomes questionable
  - Lagrangian simulations cannot capture near nozzle physics
  - Drop distortion model for high Weber number
  - Model formulations and correlation for drop Reynolds <1000 -> large fast moving drops questionable

- Turbulence Chemistry Interaction
  - For large chemical mechanism -> HPC resources
  - Identify deficiencies in the limit of premixed flame (SI relevant)
  - Multi-component transport in CFD calculations to recover kinetics fidelity

- Multi-injection modeling
  - Effect of dwell time on the PDFs of mixture fraction(s), progress variable, and age?
  - What is the joint PDF of control variables?
  - Are the control variables statistically independent?
  - How accurate are the conditional means and variances for different species when flamelet tables are constructed from ideal configurations (laminar opposed jet flames, freely propagating flames ..etc..) compared to DNS data

Proposed Future Research (FY19-FY21)

- Development and validation of improved drop models
  - Complete implementation of the drop evaporation model based on the drag model framework
  - Apply the fully coupled drag and evaporation model to study both diesel and gasoline liquid injection process
  - Perform Eulerian Lagrangian Spray Atomization (ELSA) calculation
    - Hybrid Volume of Fluids to capture near nozzle dense liquid core physics and Lagrangian spray simulation with improved drop model for computational efficiency
    - Potentially provide full physics of liquid fuel injection while maintaining reasonable computation cost
- Quantification of errors associated with implicit TCI
  - High fidelity CFD calculations
    - Same numerical set up: grid sizes, turbulence models, full kinetics
    - Quantities key differences compared to reference TCI solutions for further engineering model development
  - Using similar techniques and assumptions, quantify implicit TCI in multi-zone combustion model relevant in Spark Ignition (SI) engines (G-equation)
  - Revisit reference TCI solutions (effect of tangential diffusion)
- Development and Validation of Improved Multi Injection Modeling
  - DNS calculations for different dwell times and ambient temperature
  - Implementation of Lagrangian spray model into PeleLM
  - Study film combustion
  - Explore different strategies for flamelet table generation
  - Perform LES calculations with the new flamelet models and validate against DNS data

Any proposed future work is subject to change based on funding levels.

Presentation Summary

- Project relevant to development of predictive computational models for engineering engine combustion simulations
  - Development of a new drag model motivated by experimental observation
  - Validation with a SprayA nonreacting case shows significant improvements in liquid length penetration even for engineering calculations (RANS model)
  - Asymptotic analysis shows the presence of an “implicit TCI” in the popular multi-zone (SAGE) combustion model
  - Quantify the effects of CFD configurations combined with the multi-zone TCI equations to correctly predict cool flame dynamics
  - Multi-zone model degrades kinetics fidelity even in an ideal 1D laminar calculations
  - Demonstrate the importance of tangential diffusion in diesel engine combustion
  - Provide systematic approach utilizing DNS data to develop a flamelet combustion model that can capture correctly the physics of transient highly curved ignition fronts

Technical Backup Slides

Multi-zone TCI equations derivations

- **Peters 2000: Two-scale asymptotic analysis of reactive Navier-Stokes eqs.**

Full 3D reactive Navier-Stokes eqs. → Asymptotic solution

$$\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2\, Le_i} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{m}_i$$

$$\rho \frac{\partial T}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} + \rho \frac{\chi}{2\, c_p} \left(\sum_{i=1}^{n} \frac{c_{p,i}}{Le_i} \frac{\partial Y_i}{\partial Z} + \frac{\partial c_p}{\partial Z} \right) \frac{\partial T}{\partial Z} + \frac{1}{c_p} \left(\frac{\partial p}{\partial t} - \sum_{i=1}^{n} \dot{m}_i\, h_i \right)$$

- **True solution of Navier-Stokes eqs. for TCI (!) when asymptotic are valid**
  → *"Fast chemistry requirement" (t_D/t_C>>1)*
- **"Fast chemistry" requirement seems to limit first-principle value**
  - Reactions must occur in thin layers only
  - Hot burning flames (Peters 1984, 2000)
  - ➢ *Renders it questionable for engine flows (!)*
- **Detailed analysis of t_D/t_C for engine flows**
  - Using strictly derived species-specific diffusion times
  - t_D/t_C always >> 1 for engine flows (!)

Improved flamelet modeling: tangential diffusion + curvature effects

- Flamelet models typically ignore scalar gradients/fluxes that are not normal to the flame
- Neglect of tangential diffusion and curvature affects can significantly impact flame/ignition structure and may impact macro-parameters such as lift-off and combustion phasing

Flamelet space (Z, s_2, s_3)

$$\rho \frac{\partial T}{\partial \tau} + \Lambda^{T}_{\mathrm{LT}} = \Lambda^{T}_{\mathrm{norm}} + \Lambda^{T}_{\mathrm{TD}} + \Lambda^{T}_{\mathrm{curv}} + \Lambda^{T}_{\mathrm{src}}$$

$$\rho \frac{\partial Y_k}{\partial \tau} + \Lambda^{Y_k}_{\mathrm{LT}} = \Lambda^{Y_k}_{\mathrm{norm}} + \Lambda^{Y_k}_{\mathrm{TD}} + \Lambda^{Y_k}_{\mathrm{curv}} + \Lambda^{Y_k}_{\mathrm{src}}$$

Improved flamelet modeling: tangential diffusion + curvature effects

Physical space (x_1, x_2, x_3)

$$\frac{\partial \rho\phi}{\partial t} + \nabla(\rho\phi) = \nabla \cdot (\rho D \nabla \phi) + \dot{\omega}^{\phi}_{\mathrm{src}}$$

- Flamelet models typically ignore scalar gradients/fluxes that are not normal to the flame
- Neglect of tangential diffusion and curvature affects can significantly impact flame/ignition structure and may impact macro-parameters such as lift-off and combustion phasing

Flamelet space (Z, s_2, s_3)

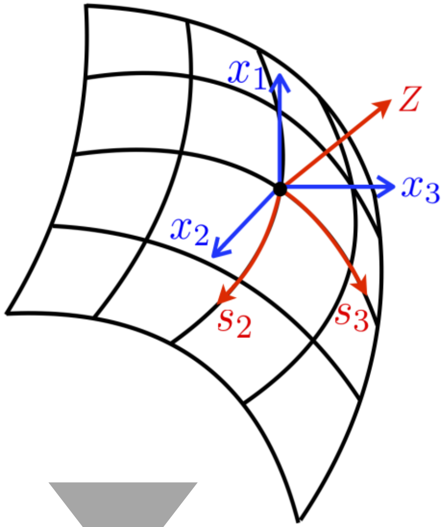
$$\rho\frac{\partial T}{\partial \tau} + \Lambda^{T}_{\mathrm{LT}} = \Lambda^{T}_{\mathrm{norm}} + \Lambda^{T}_{\mathrm{TD}} + \Lambda^{T}_{\mathrm{curv}} + \Lambda^{T}_{\mathrm{src}}$$

$$\rho\frac{\partial Y_k}{\partial \tau} + \Lambda^{Y_k}_{\mathrm{LT}} = \Lambda^{Y_k}_{\mathrm{norm}} + \Lambda^{Y_k}_{\mathrm{TD}} + \Lambda^{Y_k}_{\mathrm{curv}} + \Lambda^{Y_k}_{\mathrm{src}}$$

Improved flamelet modeling: tangential diffusion + curvature effects

Physical space (x_1, x_2, x_3)

$$\frac{\partial \rho\phi}{\partial t} + \nabla(\rho\phi) = \nabla \cdot (\rho D \nabla \phi) + \dot{\omega}^{\phi}_{\mathrm{src}}$$



- Flamelet models typically ignore scalar gradients/fluxes that are not normal to the flame
- Neglect of tangential diffusion and curvature affects can significantly impact flame/ignition structure and may impact macro-parameters such as lift-off and combustion phasing

Flamelet space (Z, s_2, s_3)

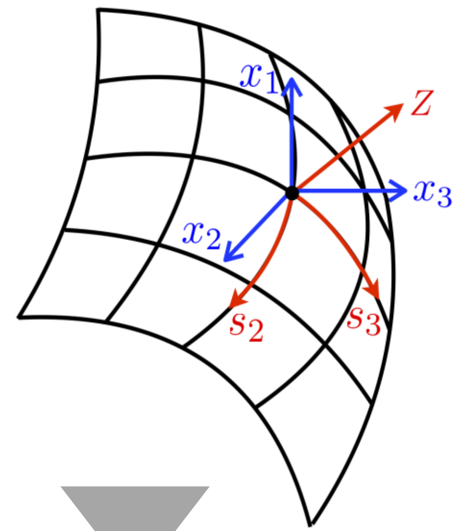
$$\rho\frac{\partial T}{\partial \tau} + \Lambda^{T}_{\mathrm{LT}} = \Lambda^{T}_{\mathrm{norm}} + \Lambda^{T}_{\mathrm{TD}} + \Lambda^{T}_{\mathrm{curv}} + \Lambda^{T}_{\mathrm{src}}$$

$$\rho\frac{\partial Y_k}{\partial \tau} + \Lambda^{Y_k}_{\mathrm{LT}} = \Lambda^{Y_k}_{\mathrm{norm}} + \Lambda^{Y_k}_{\mathrm{TD}} + \Lambda^{Y_k}_{\mathrm{curv}} + \Lambda^{Y_k}_{\mathrm{src}}$$

Improved flamelet modeling: tangential diffusion + curvature effects

Physical space (x_1, x_2, x_3)

$$\frac{\partial \rho \phi}{\partial t} + \nabla(\rho \phi) = \nabla \cdot (\rho D \nabla \phi) + \dot{\omega}^{\phi}_{\mathrm{src}}$$



- Flamelet models typically ignore scalar gradients/fluxes that are not normal to the flame
- Neglect of tangential diffusion and curvature affects can significantly impact flame/ignition structure and may impact macro-parameters such as lift-off and combustion phasing

Flamelet space (Z, s_2, s_3)

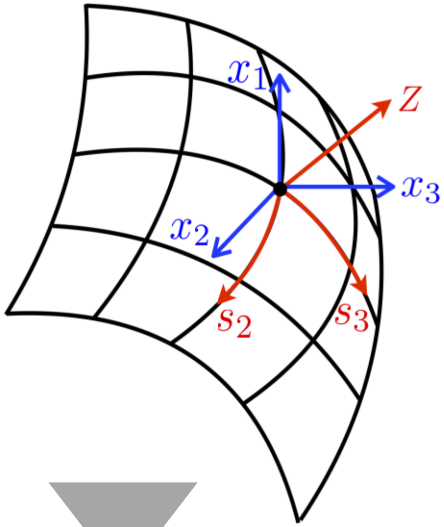
$$\rho \frac{\partial T}{\partial \tau} + \Lambda^{T}_{\mathrm{LT}} = \Lambda^{T}_{\mathrm{norm}} + \Lambda^{T}_{\mathrm{TD}} + \Lambda^{T}_{\mathrm{curv}} + \Lambda^{T}_{\mathrm{src}}$$

$$\rho \frac{\partial Y_k}{\partial \tau} + \Lambda^{Y_k}_{\mathrm{LT}} = \Lambda^{Y_k}_{\mathrm{norm}} + \Lambda^{Y_k}_{\mathrm{TD}} + \Lambda^{Y_k}_{\mathrm{curv}} + \Lambda^{Y_k}_{\mathrm{src}}$$

Improved flamelet modeling: tangential diffusion + curvature effects

Physical space (x_1, x_2, x_3)

$$\frac{\partial \rho \phi}{\partial t} + \nabla(\rho \phi) = \nabla \cdot (\rho D \nabla \phi) + \dot{\omega}^{\phi}_{\mathrm{src}}$$



- Flamelet models typically ignore scalar gradients/fluxes that are not normal to the flame
- Neglect of tangential diffusion and curvature affects can significantly impact flame/ignition structure and may impact macro-parameters such as lift-off and combustion phasing

Flamelet space (Z, s_2, s_3)

$$\rho \frac{\partial T}{\partial \tau} + \Lambda^{T}_{\mathrm{LT}} = \Lambda^{T}_{\mathrm{norm}} + \Lambda^{T}_{\mathrm{TD}} + \Lambda^{T}_{\mathrm{curv}} + \Lambda^{T}_{\mathrm{src}}$$

$$\rho \frac{\partial Y_k}{\partial \tau} + \Lambda^{Y_k}_{\mathrm{LT}} = \Lambda^{Y_k}_{\mathrm{norm}} + \Lambda^{Y_k}_{\mathrm{TD}} + \Lambda^{Y_k}_{\mathrm{curv}} + \Lambda^{Y_k}_{\mathrm{src}}$$

Extract statistics on $P(Z_1,Z_2;t)$ and χ_{ij} to support engineering modeling

Doran, Pitsch and Cook 2013

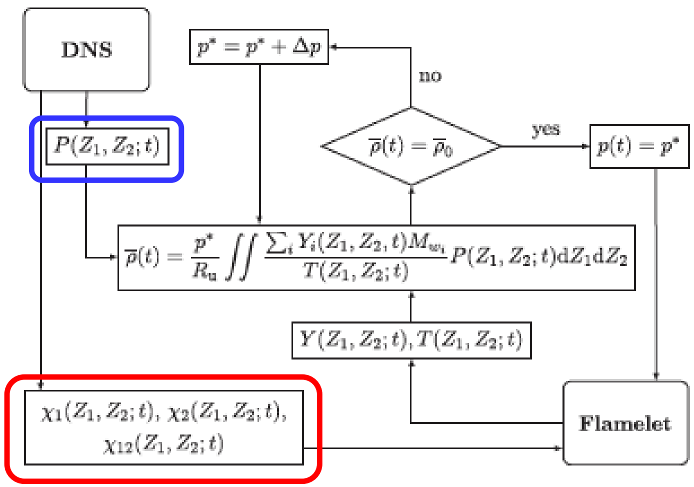
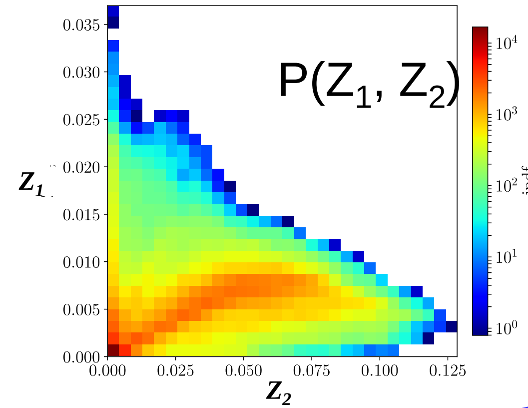
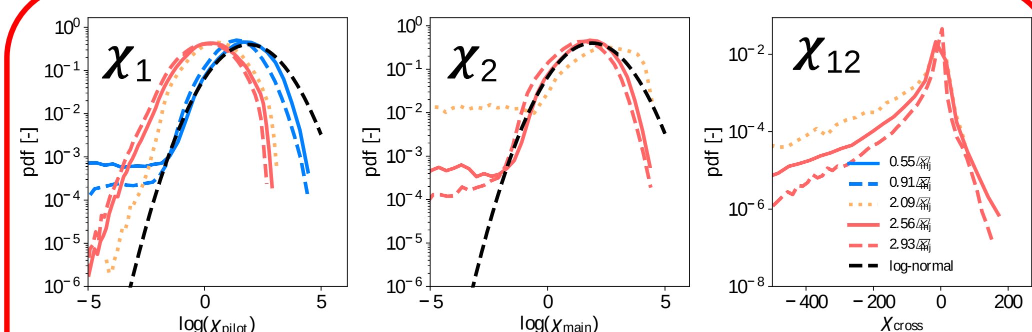


Fig. 2. Computation of flamelet using data from DNS studies for validation purposes.

$$\dot{Q}_{1+2} = \iint_{\epsilon}^{1} \dot{Q}(Z_1,Z_2) P(Z_1,Z_2) \mathrm{d}Z_1 \, \mathrm{d}Z_2$$





$$\rho \frac{\partial Y_k}{\partial t} = \rho \left(\frac{\chi_1}{2} \frac{\partial^2 Y_k}{\partial Z_1^2} + \chi_{12} \frac{\partial^2 Y_k}{\partial Z_1 \partial Z_2} + \frac{\chi_2}{2} \frac{\partial^2 Y_k}{\partial Z_2^2} \right) + \rho \dot{\omega}_k$$

Drag Model Implementation

Particle equation of motion

$$\frac{dx_p}{dt} = u_p$$

$$\frac{du_p}{dt} = \frac{3}{4} C_d Re \frac{\mu}{(\rho_p d_p^2)} (u - u_p)$$

Standard model

$$C_d = C_{d,s}(1 + 2.632y)$$

$$C_{d,s} = \frac{24}{Re}\left(1 + \frac{1}{6} Re^{\left\{\frac{2}{3}\right\}}\right)$$

Re: Reynolds number
u: velocity vector
μ: molecular dynamic viscosity
ρ: Density
y: distortion factor
r/d: radius/diameter
C_b: modeling constant
Subscript
p: particle/parcel

Dahms-Oefelein model

$$C_d = C_{d,vis}\left(\frac{0.21 + \frac{20}{Re}\left(\frac{l}{d_p}\right)^{0.58} + \frac{6.9}{\sqrt{Re}}\left(\frac{l}{d_p}\right)^{-1.4}}{0.21 + \frac{20}{Re} + \frac{6.9}{\sqrt{Re}}}\right)$$

$$l = 2\, r_p(1 - C_b y)$$

$$C_{d,vis} = \frac{2-\lambda}{2} C_{d,b} + \frac{4\lambda}{6+\lambda} C_{d,2} \quad (0 \le \lambda \le 2;\ 5 < Re < 1000)$$

$$C_{d,vis} = \frac{4}{\lambda + 2} C_{d,2} + \frac{\lambda - 2}{\lambda + 2} C_{d,s} \quad (2 \le \lambda \le \infty;\ 5 < Re < 1000)$$

$$C_{d,b} = \frac{48}{Re}\left(1 + \frac{2.21}{\sqrt{Re}} - \frac{2.14}{Re}\right)$$

$$C_{d,2} = 17 Re^{-\frac{2}{3}}$$

$$C_{d,s} = \frac{24}{Re}\left(1 + \frac{1}{6} Re^{\left\{\frac{2}{3}\right\}}\right)$$

$$\lambda = \frac{\mu_l}{\mu_g}$$