In-Cylinder Combustion of Bio-Diesel: Project Overview

Valmor de Almeida

Nuclear Science & Technology Division

Separations and Materials Research Group

24 January 2007

Spray Modeling & Simulation Group Meeting

Applied Math & Stat SUNY Stony Brook

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Outline

- **Motivation**
- **Goals**
- **Collaboration**
- **Modeling/simulation components**
- **Summary**

Bio-derived fuels could displace a significant fraction of U.S. oil consumption

2006 Presidential State of the Union Address: announced goal of reducing imports of foreign oil… and increase national competitiveness by use and development of advance energy technologies.

DOE to Invest $250 Million in New Bioenergy Centers Aug 2 06 press release

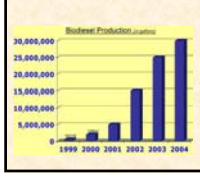
Basic Genomics Research on the Development of Biofuels to be Accelerated

JOLIET, IL – U.S. Department of Energy (DOE) Secretary Samuel W. Bodman announced today that DOE will spend $250 million to establish and operate two new Bioenergy Research Centers to accelerate basic research on the development of cellulosic ethanol and other biofuels. The Secretary made the announcement with Congressman Jerry Weller (IL-11th), local officials and biofuels stakeholders during a visit to Channahon, IL.

[illegible] programs to improve the technology and reduce the cost of biofuels production. The mission of these centers is to accelerate research that leads to breakthroughs in basic science to make biofuels a cost-effective alternative to fossil fuels."

ORNL LDRD 2006-2007

Alternative Liquid Fuels: Increased efficiency of combustion through optimization of vehicle technology for combustion of biofuels (LTC, HECC)



Double Biomass Production to 10 tons/acre

Improve Conversion Efficiencies

Double Fleet Fuel Efficiency

Currently idle land could fuel half of U.S. Passenger Fleet

30 Million Acres

Collaborative Team

http://dcpl.ornl.gov

Modeling and simulation of transport processes w/ emphasis on chemical systems

ORNL Research Staff:
Joanna McFarlane
Valmor de Almeida
Bill Steele

- Two national laboratories
- Two universities
- One DOE research center

http://www.erc.wisc.edu

Engine **R**esearch **C**enter

Coupled modeling and experimental program for IC engines

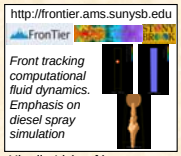
Rolf Reitz (prof.)
Youngchul Ra (post-doc)
Jessica Brakora (grad student)

http://feerc.ornl.gov

Detailed IC engines characterization facility

ORNL Research Staff:
Robert Wagner
Scott Sluder
Kalyan Chakravarthy
Stuart Daw

http://frontier.ams.sunysb.edu



Front tracking computational fluid dynamics. Emphasis on diesel spray simulation

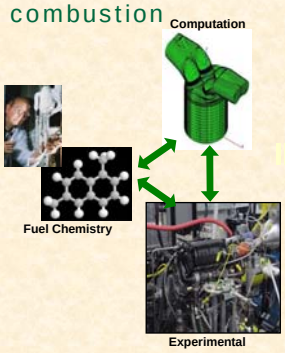
Xiaolin Li (prof.)
Jim Glimm (prof.)
Xingtao Liu (grad student)
Wurigen Bo (grad student)

http://www.lanl.gov/orgs/t/t3/codes

CFD Kiva-4 development for IC engines

LANL Research Staff:
David Torres

Goal:
To establish a new research capability for use of non-petroleum fuels in advanced combustion

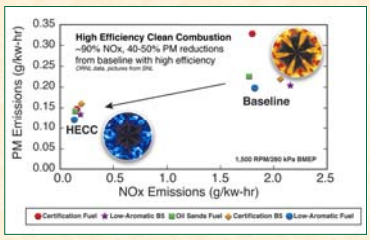


- Develop predictive tool to evaluate high-efficiency combustion of alternative fuels

- Combine capabilities in fuel chemistry and engineering computations with established strength in IC engine experimentation to create a unique R&D program

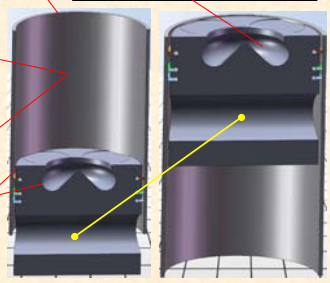
Advanced combustion modes will be used on some level in all future transportation engines

- Advanced combustion characterized by low temperature combustion (LTC) processes: low emissions and improved efficiency.
- Typically less stable than conventional forms of combustion (i.e., sensitive to air-fuel charge conditions including fuel properties).
- Several forms of LTC exist including Homogeneous Charge Compression Ignition (HCCI), Premixed Charge Compression Ignition (PCCI), etc.
- Modes are commonly referred to as High Efficiency Clean Combustion (HECC) in the literature.



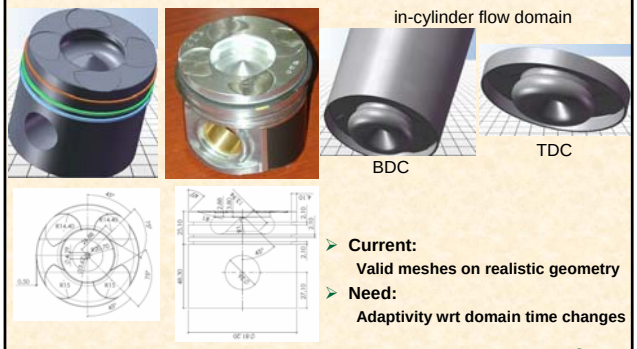
In-Cylinder Combustion: Advanced Modeling Components

- ***Realistic geometry***
  - *Moving parts (piston & valves)*
  - *Stationary parts (cylinder, injector, exhaust manifold)*
  - *Adaptive, unstructured meshing*
- ***3-D, transient fluid flow***
  - *Gas-phase multi-species*
  - *Turbulent*
  - *Reactive (exothermic)*
  - *Transport properties*
- ***Coupled detailed chemical reactions***
  - *Reaction mechanisms*
  - *Thermodynamic data*
- ***Boundary conditions***
  - *Turbulent film models*
- ***Experimental validation***
  - *Prototype engine*
  - *Modern automatic data acquisition*
- ***Spray fuel injection***
  - *Multi-component fuel*
  - *Gas-fuel interface prediction*
  - *Evaporation*
  - *Physical properties*



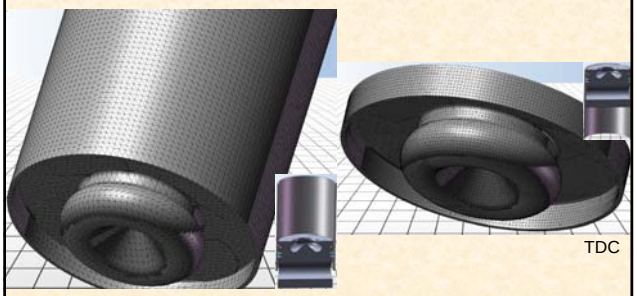
Realistic Geometry: GM 1.9 l Diesel Engine

- **Advances in CAD and combined meshing**



- **Current:**
  Valid meshes on realistic geometry
- **Need:**
  Adaptivity wrt domain time changes

- **(Re)Meshing and adaptivity**



- **Interpolation/re-mapping when needed**

- **Working on newly acquired parts**

cylinder head & exhaust manifold

valves

fuel injector

6 orifices ~150 μm

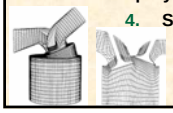
3-D Transient Fluid Flow Simulation

+ *Gas-phase multi-species*
+ *TurbulentReactive (exothermic)*
+ *Transport properties*

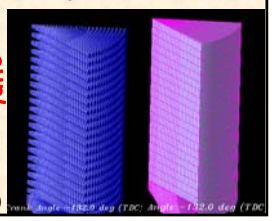
- **Kiva-3 (UW-ERC)**
  - **Sub-models: Spray, Soot, Liquid wall film, BC**
  - **ChemKin for detailed chemical reactions**
  - **Simple parallel processing (non-scalable beyond 8 processes)**
- **Kiva-4 (LANL)**
  - **Unstructured mesh, multicomponent fuel, parallel processing**
- **Both attempt to model and simulate in-cylinder:**

1. **Multi-species Turbulent Gas Flow**
2. **Chemical Reactions**
3. **Spray ("semi"-empirical)**
4. **Sub-models**

coupled



Kiva-3 (UW-ERC)



Conservation of Mass

$$\partial_t \rho_m + \mathrm{div}_x(\rho_m v) = \mathrm{div}_x\left(\rho D\, \nabla_x(\rho_m \rho^{-1})\right) + \dot{\rho}^c_m + \dot{\rho}^s \delta_{m1}$$

reaction coupling

spray evaporation coupling

$m = 1, 2, 3, \ldots, \#$ **of species**

default (12 species): fuel vapor, O_2, N_2, CO_2, H_2O, H, H_2, O, N, OH, CO, NO

$\rho_m(x,t)$: **mth-specie mass density**

$\dot{\rho}^c_m(x,t)$: **mth-specie rate from chemical reactions**

$\dot{\rho}^s(x,t)$: **fuel vapor rate from evaporation**

D: **single diffusion coefficient**

Momentum of the Gas Mixture

$$\partial_t(\rho v) + \mathrm{div}_x(\rho v \otimes v) = -\nabla_x p + \mathrm{div}_x \tau + f^s$$

spray momentum coupling

$\rho(x,t)$: density of the mixture

$v(x,t)$: mass average velocity

$f^s(x,t)$: spray force density

$p(x,t)$: thermodynamic pressure

$\tau(x,t)$: turbulent viscous stress tensor

$\tau(x,t) := \mu\left(\nabla_x v + (\nabla_x v)^T\right) + \lambda\, \mathrm{div}_x v I$

μ and λ: first and second turbulent viscosities

k–ϵ Turbulence Model

$$\rho\,\partial_t k + \rho\,\mathrm{div}_x(k v) = \mathrm{div}_x\left(\frac{\mu_t}{\sigma_k}\nabla_x k\right) + G_k - \rho\epsilon$$

$$\rho\,\partial_t \epsilon + \rho\,\mathrm{div}_x(\epsilon v) = \mathrm{div}_x\left(\frac{\mu_t}{\sigma_\epsilon}\nabla_x \epsilon\right) + \frac{\epsilon}{k}\left(C_{1\epsilon} G_k - C_{2\epsilon}\rho\epsilon\right)$$

$k(x,t)$: turbulent kinetic energy

$\epsilon(x,t)$: rate of dissipation of k

$C_{1\epsilon}$, $C_{2\epsilon}$, C_μ: calibration constants

σ_k, and σ_ϵ: turbulent Prandtl numbers

$\mu_t(x,t)$: turbulent viscosity field $:= \rho C_\mu \frac{k^2}{\epsilon}$

$G_k(x,t)$: production of k $:= 2\mu_t\,\mathrm{Sym}\,\nabla_x v$

Internal Energy of the Gas Mixture

$$\partial_t(\rho u) + \mathrm{div}_x(\rho v u) = -p\,\mathrm{div}_x v + \tau : \nabla_x u - \mathrm{div}_x q + \dot{Q}^c + \dot{Q}^s$$

$u(x,t)$: specific internal energy of the mixture

$q(x,t)$: heat flux by conduction and enthalpy diffusion

$q(x,t) := -K\nabla_x T - \rho D \sum_m h_m \nabla_x(\rho_m \rho^{-1})$

$\dot{Q}^c(x,t)$: rate of reaction heating

$\dot{Q}^s(x,t)$: heat from/to spray

Required Data

W_m: molecular weights

$c_{p,m}(T)$: specific heat capacities at cte pressure

$h_m(T)$: specific enthapies

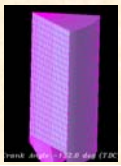
$\mu_{air}(T)$: dynamic viscosity of air

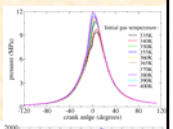
$c_{\epsilon 1}$, $c_{\epsilon 2}$, $c_{\epsilon 3}$,...: turbulence parameters

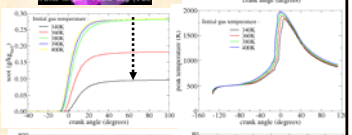
KIVA-3ERC in-cylinder combustion simulations for reference case

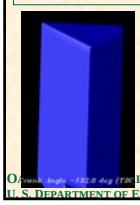
- **KIVA-3 UW ERC version running on ORNL cluster**
- **Simulation of diesel spray combustion on GM engine**
  - **ERC n-heptane reduced model (29 species, 54 reactions)**
- **Parametric studies w/ EGR temperature**
- **Simulation of HCCI mode**

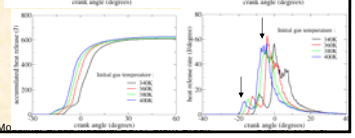
Youngchul Ra, U. Wisconsin ERC, Post –doc collaborator











Coupled Detailed Chemical Reactions

- *Reaction mechanisms*
- *Thermodynamic data*

$$\sum_m a_{m,r}\,\chi_m \rightleftarrows \sum_m b_{m,r}\,\chi_m \quad \forall \quad r \quad \text{reactions}$$

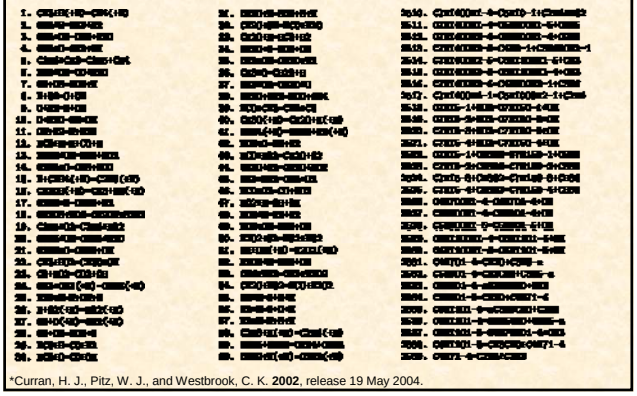
$a_{m,r}$, and $b_{m,r}$: stoichiometric coeffs.

χ_m: one mole of the mth species

- **Finite-rate chemistry**
  - **laminar**
  - **turbulent (KIVA 3V and later)**
- **Equilibrium**

Reaction mechanism example

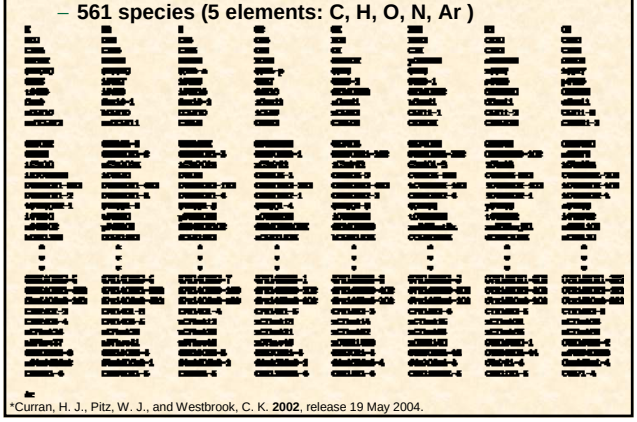
- **LLNL n-Heptane combustion detailed model***
  - **2539 reactions**



*Curran, H. J., Pitz, W. J., and Westbrook, C. K. **2002**, release 19 May 2004.

n-Heptane model cont.

- **LLNL detailed model***
  - **561 species (5 elements: C, H, O, N, Ar)**



*Curran, H. J., Pitz, W. J., and Westbrook, C. K. **2002**, release 19 May 2004.

Finite Rate Chemistry

$$\dot{\omega}_r = k_{f,r} \prod_m \left(\rho_m / W_m\right)^{a'_{m,r}} - k_{b,r} \prod_m \left(\rho_m / W_m\right)^{b'_{m,r}} \quad \forall \quad r$$

$\dot{\omega}_r$: molar density rate of the rth reaction

$k_{f,r}$, $k_{b,r}$: forward and backward rate constants

$a'_{m,r}$ and $b'_{m,r}$: forward and backward reaction orders

$$k_{f,r} = A_{f,r} T^{\beta_{f,r}} \exp\left(-E_{f,r}/RT\right)$$ Arrhenius form

$A_{f,r}$: pre-exponential factor

$\beta_{f,r}$: temperature exponent

$E_{f,r}$: activation energy

Coupling to Gas Flow

- **Mass conservation**

$$\dot{\rho}^c_m(x,t) = W_m \sum_r (b_{m,r} - a_{m,r})\, \dot{\omega}_r$$

- **Internal energy**

$$\dot{Q}^c(x,t) = \sum_r \left\{ \sum_m (a_{m,r} - b_{m,r})(\Delta h^0_f)_m \right\} \dot{\omega}_r$$

Required Data

$a_{m,r}$, and $b_{m,r}$: stoichiometric coeffs (all r and m).

$k_{f,r}$, $k_{b,r}$: forward and backward rate constants (all r)

$a'_{m,r}$ and $b'_{m,r}$: forward & backward reaction orders (all r & m)

$A_{f,r}$ and $A_{b,r}$: forward & backward pre-exponential factors (for all r)

$\beta_{f,r}$ and $\beta_{b,r}$: forward & backward temperature exponent (for all r)

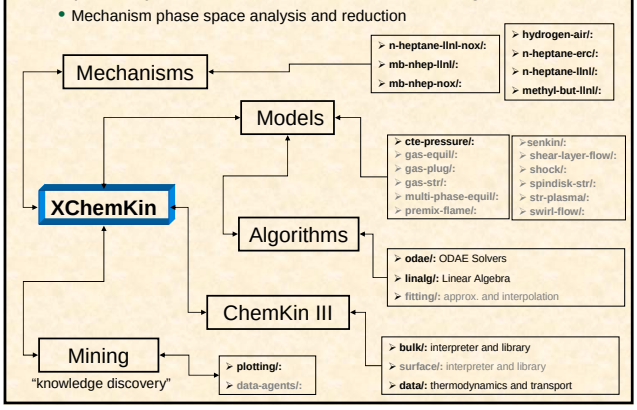
$E_{f,r}$ and $E_{b,r}$: forward & backward activation energy (for all r)

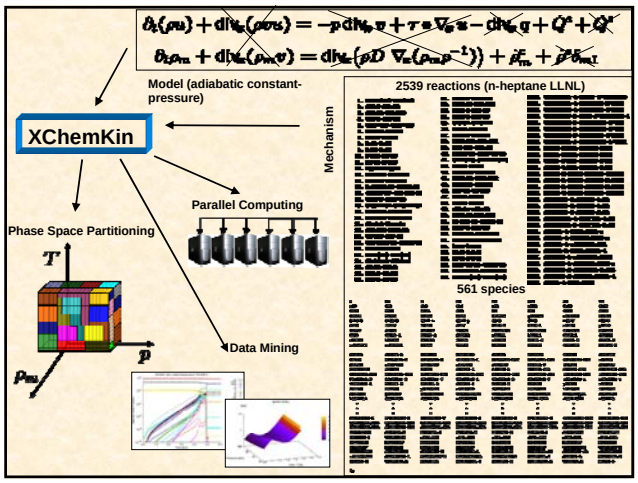
$(\Delta h^0_f)_m$: heat of formation for all m

K^r_c: equilibrium constant for all equilibrium r

XChemKin Architecture

- Exploratory tool for chemical kinetics modeling
  - Mechanism phase space analysis and reduction

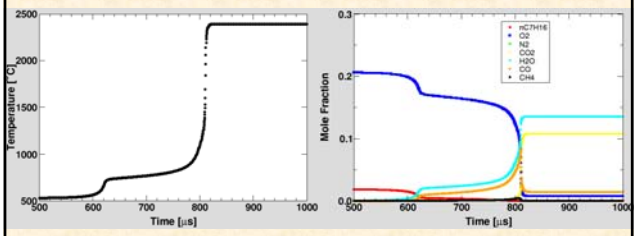




n-Heptane combustion

Results with LLNL Detailed Model

- **50 atm, 800 K, stoichiometric mixture**
  - **CHEMKIN III, VODE (Δt = 0.25 ms)**



- **Total auto-ignition delay at ~810 μs**
- **Cold flame delay at ~620 μs**

n-Heptane data

- **UW ERC reduced model**
  - **29 species (4 elements)**

[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
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  - **52 reactions**

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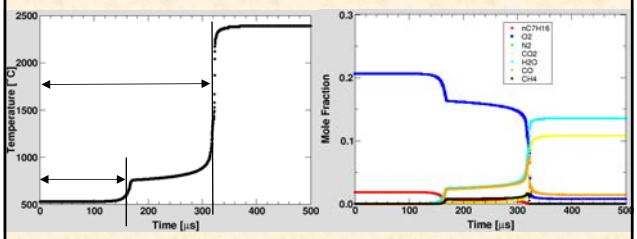
52. [illegible]

n-Heptane combustion

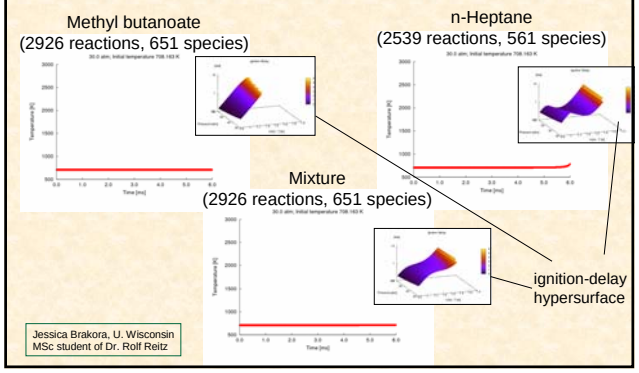
Results with ERC Reduced Model

- **50 atm, 800 K, stoichiometric mixture**
  - **CHEMKIN III, VODE (Δt = 0.25 ms)**



- **Total auto-ignition delay at ~320 μs**
- **Cold flame delay at ~160 μs**

XChemKin analysis captures differences in ignition delay arising from fuel composition



Jessica Brakora, U. Wisconsin
MSc student of Dr. Rolf Reitz

Spray Fuel Injection

Two-phase Fluid Mechanics with Sharp Interface Governing Equations

Momentum balance $\partial_t(\rho_\alpha \boldsymbol{v}_\alpha) + \mathrm{div}_{\boldsymbol{x}}(\rho_\alpha \boldsymbol{v}_\alpha \otimes \boldsymbol{v}_\alpha) = \mathrm{div}_{\boldsymbol{x}} \boldsymbol{T}_\alpha + \boldsymbol{b}_\alpha$

Mass balance $\partial_t \rho_\alpha + \mathrm{div}_{\boldsymbol{x}}(\rho_\alpha \boldsymbol{v}_\alpha) = 0$

Internal energy balance

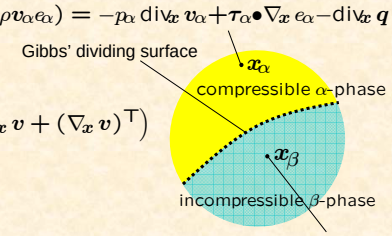
$$\partial_t(\rho e_\alpha) + \mathrm{div}_{\boldsymbol{x}}(\rho \boldsymbol{v}_\alpha e_\alpha) = -p_\alpha \,\mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{v}_\alpha + \boldsymbol{\tau}_\alpha \bullet \nabla_{\boldsymbol{x}}\, e_\alpha - \mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{q}$$

Constitutive equations

$$\boldsymbol{T} := -p\boldsymbol{I} + \boldsymbol{\tau}$$

$$\boldsymbol{\tau} := \lambda\, \mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{v}\boldsymbol{I} + \mu\left(\nabla_{\boldsymbol{x}} \boldsymbol{v} + (\nabla_{\boldsymbol{x}} \boldsymbol{v})^\top\right)$$

$$\boldsymbol{q} := -K\, \nabla_{\boldsymbol{x}}\, T$$



Equation of state (EOS)

$$p_\alpha = f(\rho_\alpha, e_\alpha)$$

Momentum balance $\rho_\beta \partial_t \boldsymbol{v}_\beta + \rho_\beta\, \mathrm{div}_{\boldsymbol{x}}(\boldsymbol{v}_\beta \otimes \boldsymbol{v}_\beta) = \mathrm{div}_{\boldsymbol{x}} \boldsymbol{T}_\beta + \boldsymbol{b}_\beta$

Mass balance $\mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{v}_\beta = 0$

Sharp interface equations. cont.

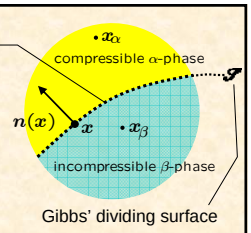
Impermeable interface

$$[\![\, \boldsymbol{v} \cdot \boldsymbol{n} \,]\!] := (\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta) \cdot \boldsymbol{n} = 0$$

Interfacial momentum balance

$$\mathbf{div}_{\mathscr{S}}\, \mathbf{T} + [\![\, \boldsymbol{T}\boldsymbol{n} \,]\!] = \mathbf{0}$$

where $[\![\, \boldsymbol{T}\boldsymbol{n} \,]\!] := (\boldsymbol{T}_\alpha - \boldsymbol{T}_\beta) \cdot \boldsymbol{n}$



Interfacial energy balance

$$[\![\, \boldsymbol{q} \cdot \boldsymbol{n} \,]\!] = 0$$

Geometric Non-linearity

Constitutive equation

$$\mathbf{T} := \sigma \mathbf{I} \qquad \mathbf{div}_{\mathscr{S}}\, \mathbf{T} = \mathbf{div}_{\mathscr{S}}(\sigma \mathbf{I}) = 2\mathscr{H}\sigma\boldsymbol{n}$$

Typical independent assumption

Continuous tangential component of the velocity field on $\mathscr{S}$

Current Approximations using Kiva-4 and Frontier

Momentum balance $\partial_t(\rho_\alpha \boldsymbol{v}_\alpha) + \mathrm{div}_{\boldsymbol{x}}(\rho_\alpha \boldsymbol{v}_\alpha \otimes \boldsymbol{v}_\alpha) = \mathrm{div}_{\boldsymbol{x}} \boldsymbol{T}_\alpha + \boldsymbol{b}_\alpha$

Mass balance $\partial_t \rho_\alpha + \mathrm{div}_{\boldsymbol{x}}(\rho_\alpha \boldsymbol{v}_\alpha) = 0$

Internal energy balance

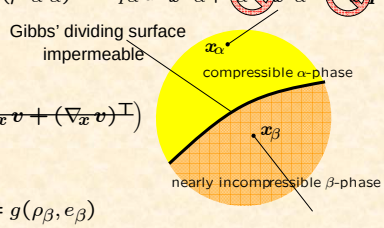
$$\partial_t(\rho e_\alpha) + \mathrm{div}_{\boldsymbol{x}}(\rho \boldsymbol{v}_\alpha e_\alpha) = -p_\alpha \,\mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{v}_\alpha + \boldsymbol{\tau}_\alpha \bullet \nabla_{\boldsymbol{x}}\, e_\alpha - \mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{q}$$

Constitutive equations

$$\boldsymbol{T} := -p\boldsymbol{I} + \boldsymbol{\tau}$$

$$\boldsymbol{\tau} := \lambda\, \mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{v}\boldsymbol{I} + \mu\left(\nabla_{\boldsymbol{x}} \boldsymbol{v} + (\nabla_{\boldsymbol{x}} \boldsymbol{v})^\top\right)$$

$$\boldsymbol{q} := -K\, \nabla_{\boldsymbol{x}}\, T$$



Equations of state (EOS)

$$p_\alpha = f(\rho_\alpha, e_\alpha); \;\; p_\beta = g(\rho_\beta, e_\beta)$$

Momentum balance $\partial_t(\rho_\beta \boldsymbol{v}_\beta) + \mathrm{div}_{\boldsymbol{x}}(\rho_\beta \boldsymbol{v}_\beta \otimes \boldsymbol{v}_\beta) = \mathrm{div}_{\boldsymbol{x}} \boldsymbol{T}_\beta + \boldsymbol{b}_\beta$

Mass balance $\partial_t \rho_\beta + \mathrm{div}_{\boldsymbol{x}}(\rho_\beta \boldsymbol{v}_\beta) = 0$

Sharp interface approx. cont.

Impermeable interface

$$[\![v \cdot n]\!] := (v_\alpha - v_\beta) \cdot n = 0$$

Interfacial momentum balance

$$\mathrm{div}_{\mathscr{S}} \mathbf{T} + [\![Tn]\!] = 0$$

where $[\![Tn]\!] = [\![pn]\!] + [\![\tau n]\!]$

Interfacial energy balance

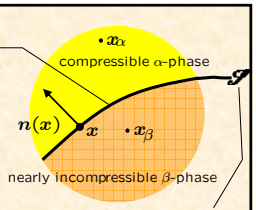
$$[\![q \cdot n]\!] = 0$$

Constitutive equation

$$\mathbf{T} := \sigma \mathbf{I}$$

Independent assumption

Discontinuous tangential component of the velocity field on $\mathscr{S}$



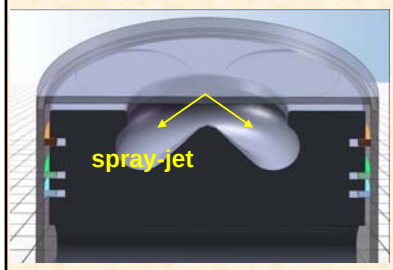
Gibbs' dividing surface impermeable

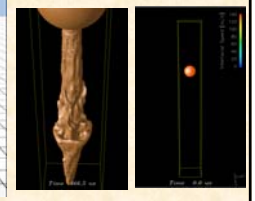
Geometric Non-linearity

$$\mathrm{div}_{\mathscr{S}} \mathbf{T} = \mathrm{div}_{\mathscr{S}}(\sigma \mathbf{I}) = 2\mathscr{H}\sigma n$$

Advanced Spray Modeling & Simulation

- **Path forward:**
  - **Jet and drop studies**

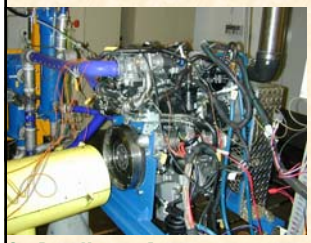




- **First-principles continuum mechanics jet break-up modeling and simulation w/ micro-scale resolved front tracking**

Experimental Validation

- **GM 1.9 l Diesel Engine (DOE NTRC at ORNL)**
  - **Four-stroke, turbocharged, light-duty**
  - **In-line, four cylinders**
  - **High-speed cranckshaft > 1500 RPM**
  - **Direct fuel injection into piston bowl**
  - **Bio-diesel**
  - **Research engine at UW and SNL**
  - **Instrumented**
    - **Cylinder pressure, temperature**
    - **Heat release**
    - **After-gas treatment**



Summary

- **Bio-fuel is in the national political agenda for energy security**
- **There is a gap (opportunity) in modeling and simulation of sprays in the (realistic) combustion regime**
  - **Need micro-scale resolution and prediction of jet breakup event**
  - **Need tight coupling with chemistry of evaporation and combustion**
  - **Need state-of-the-art computing infrastructure (hardware and software)**
- **Important for this group to become leaders in developing unique modeling & simulation capability**