Reciprocating Internal Combustion Engines

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University of Wisconsin-Madison

2012 Princeton-CEFRC
Summer Program on Combustion
Course Length: 9 hrs

(Wed., Thur., Fri., June 27-29)

Hour 5

Short course outine:

Engine fundamentals and performance metrics, computer modeling supported by in-depth understanding of fundamental engine processes and detailed experiments in engine design optimization.

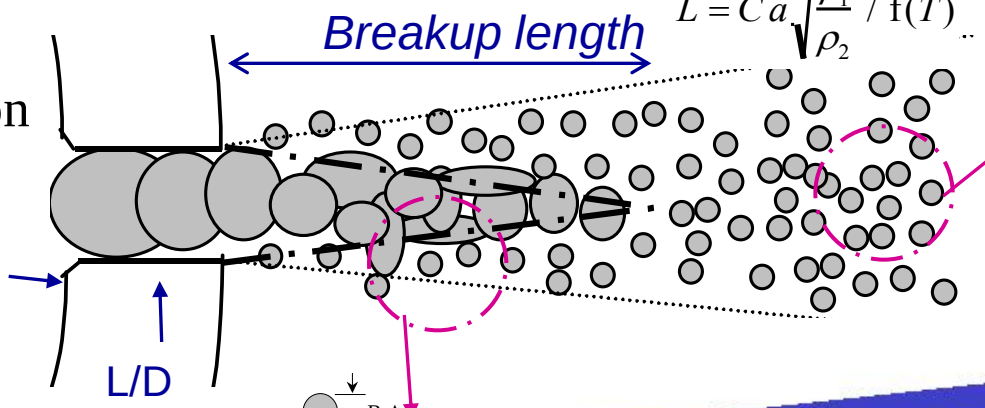
Day 1 (Engine fundamentals)
Hour 1: IC Engine Review, 0, 1 and 3-D modeling
Hour 2: Turbochargers, Engine Performance Metrics
Hour 3: Chemical Kinetics, HCCI & SI Combustion

Day 2 (Spray combustion modeling)
Hour 4: Atomization, Drop Breakup/Coalescence
Hour 5: Drop Drag/Wall Impinge/Vaporization
Hour 6: Heat transfer, NOx and Soot Emissions

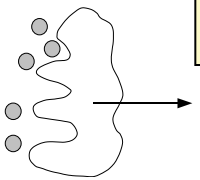
Day 3 (Applications)
Hour 7: Diesel combustion and SI knock modeling
Hour 8: Optimization and Low Temperature Combustion
Hour 9: Automotive applications and the Future

ERC Spray modeling

Blob injection model



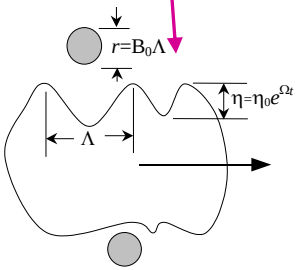
RT Model

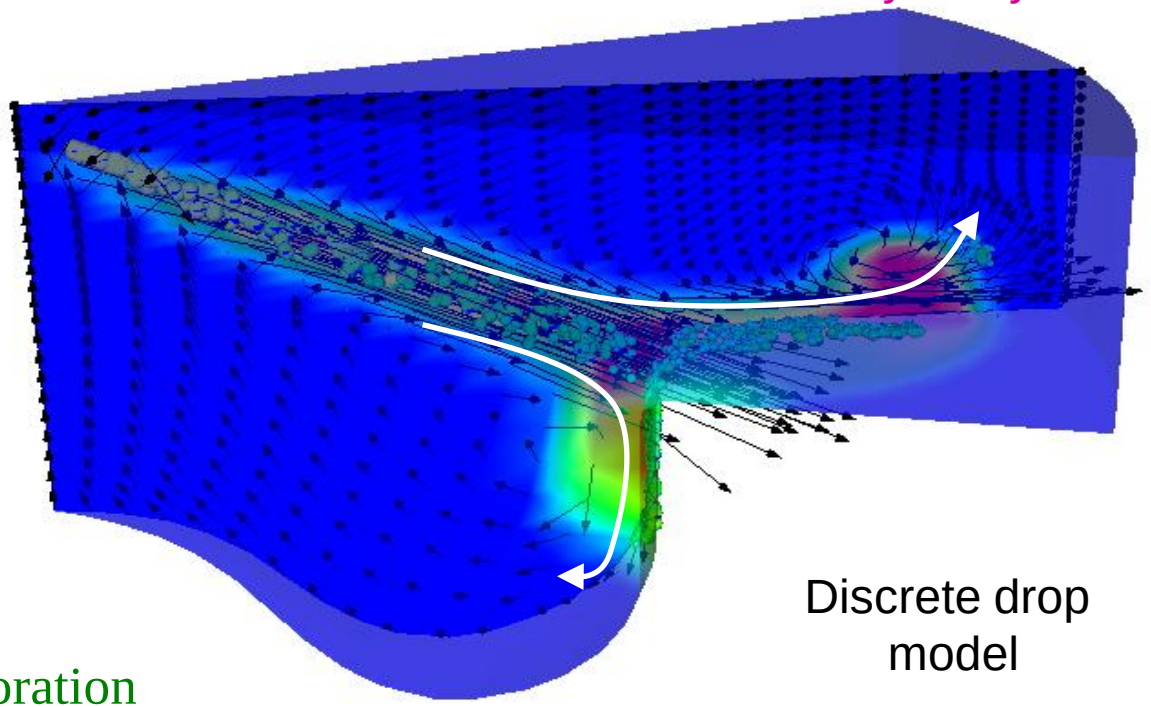


Beale &Reitz, 1999

Kelvin-Helmoltz
Rayleigh Taylor
Linearized instability analysis

KH Model





Discrete drop model

Spray Models
Nozzle flow/cavitation
Jet atomization
Drop breakup
} KH-RT
Drop collision/coalescence
Drop drag
Multi-component fuel evaporation
Spray-wall impingement

Droplet drag modeling

Liu, SAE 930072

Steady-state Stokes viscous drag, added-mass and Basset history integral

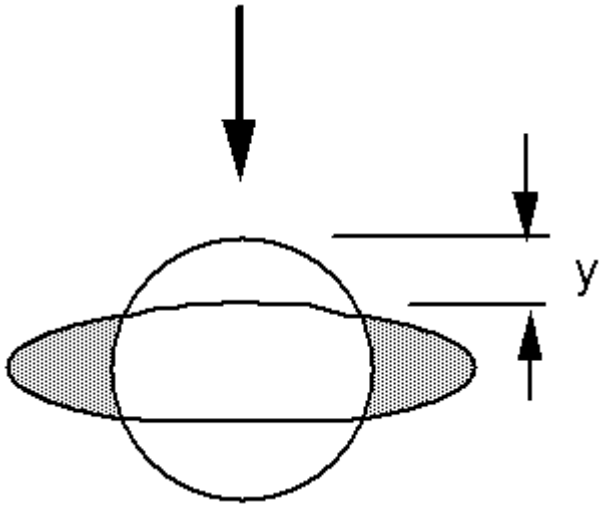
$$\mathrm{dv/dt} = \mathbf{F} = 6\pi r \mu_g \mathbf{v} + \tfrac{1}{2}\left(\tfrac{4}{3}\pi r^3 \rho_g\right)\frac{d\mathbf{v}}{dt} + 6r^2\sqrt{\pi\mu\rho_g}\int_0^t \frac{d\mathbf{v}/dt'}{\sqrt{t-t'}}dt'$$

General form

$$\rho_L V_d \, d\mathbf{v}/dt = C_D A_f \frac{\rho_g U^2}{2}\{\mathbf{U}/|\mathbf{U}|\}$$

$$C_d = \begin{cases} 24\,\mathrm{Re}_d^{-1}(1+\mathrm{Re}_d^{2/3}/6), & \mathrm{Re}_d < 1000 \\ 0.424, & \mathrm{Re}_d \geq 1000 \end{cases}$$

- Drop distortion (TAB model)



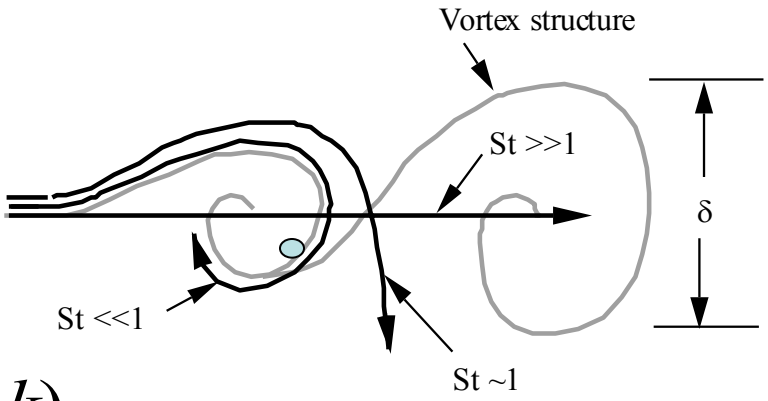
$$\ddot{y} = -5\frac{\mu_l}{\rho_l}\frac{\dot{y}}{r_d^2} - \frac{8\sigma y}{\rho_l r_d^3} + \frac{2}{3}\frac{\rho}{\rho_l}\frac{U_{rel}^2}{r_d^2}$$

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

Turbulence & Drop Dispersion

- Monte Carlo method

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$$



$$G(\mathbf{u}') = (4/3\pi k)^{-3/2} \exp(-3|\mathbf{u}'|^2/4k)$$

$S_t = \tau\,(\mathbf{u}-\mathbf{v})/2r$

$\tau = 2\rho_L r^2/9\mu_g$

Drop-eddy interaction time

Eddy life time

$$t_e = l/\sqrt{2k/3}$$

$$l = C_\mu^{3/4} k^{3/2}/\varepsilon$$

Residence time

$$t_p = l/|\bar{\mathbf{u}} - \mathbf{v}|$$

$$\delta = l$$

$$t_{\text{int}} = \min(t_e, t_p)$$

Gosman & Iaonnides, 1981

Spray Wall Impingement

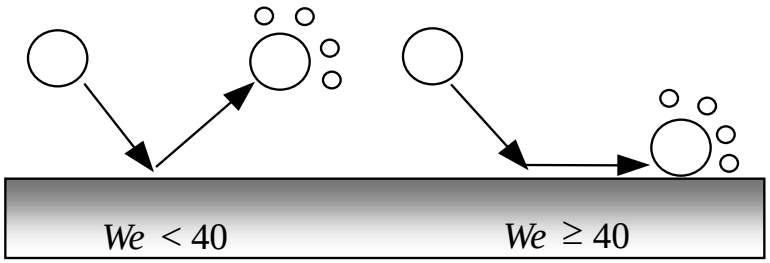
At low approach velocities (We) drops rebound elastically

With hot walls cushion of vapor fuel forms under the drop

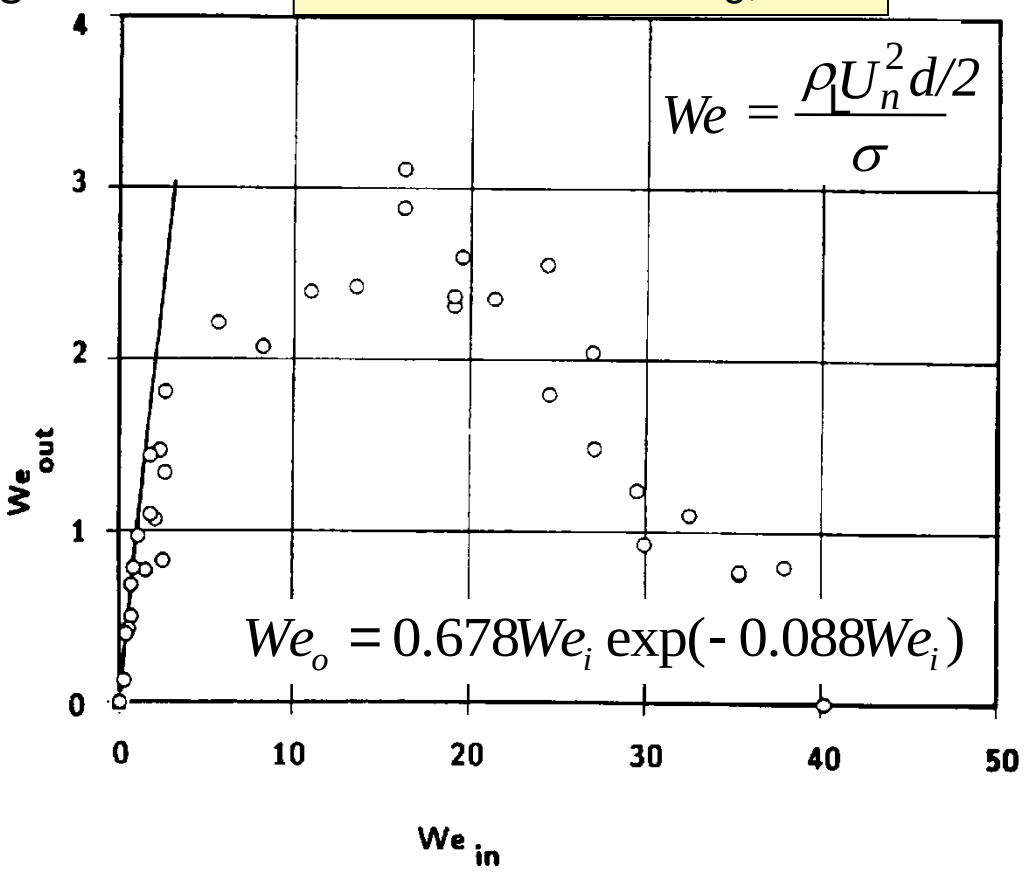
As approach velocity is increased, normal velocity component decreases and drop may break up

Beyond We = 40 liquid spreads into surface layer

At high temperatures film boiling takes place



Wachters & Westerling, 1966

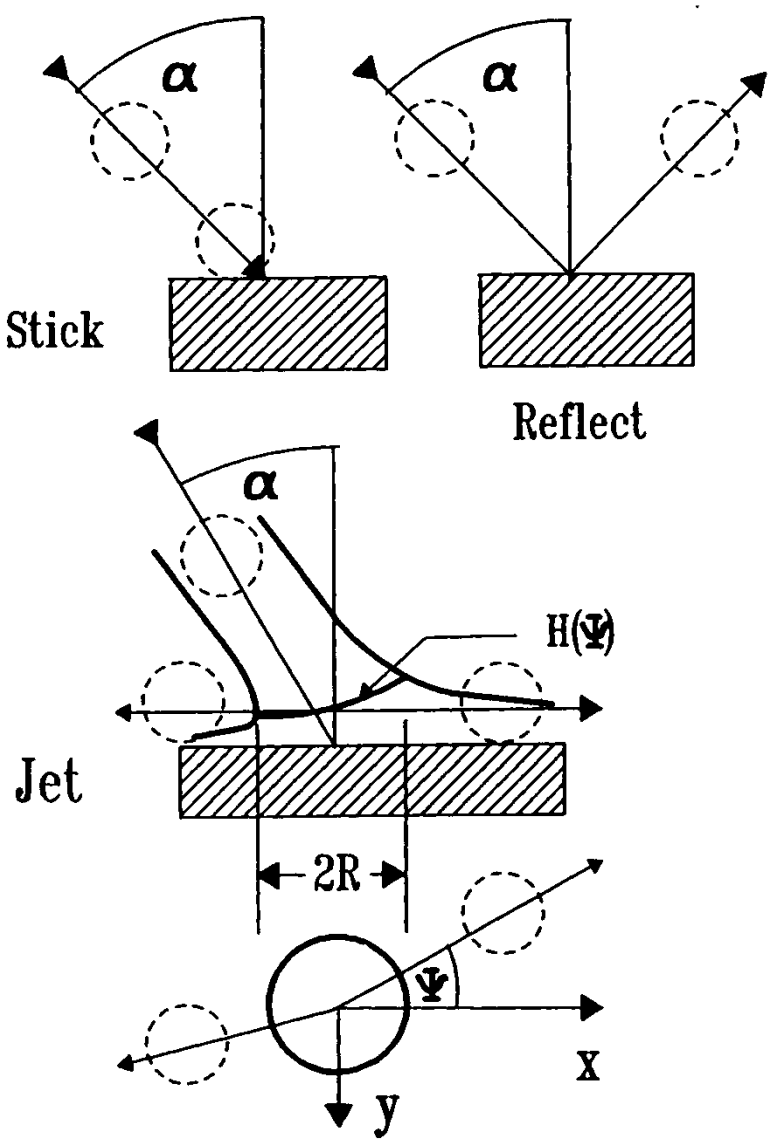


Dry Wall Impingement Models

Stick - drops stick to the wall

Reflect - drops rebound

Slide/Jet - incident drop leaves tangent to the surface



From mass and momentum conservation:

$$\psi = -\frac{\pi}{\beta}\ln\{1 - p(1-\exp(-\beta)\}$$

where $0 < p < 1$ random number

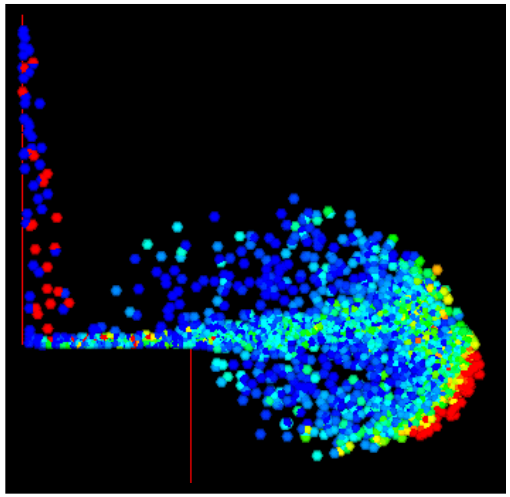
$$\sin\alpha = \left(\frac{\exp(\beta)+1}{\exp(\beta)-1}\right) / 1 + (\pi/\beta)^2$$

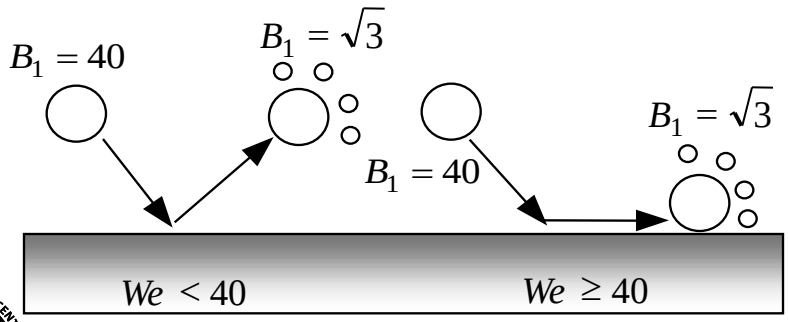
Naber & Reitz, SAE 880107

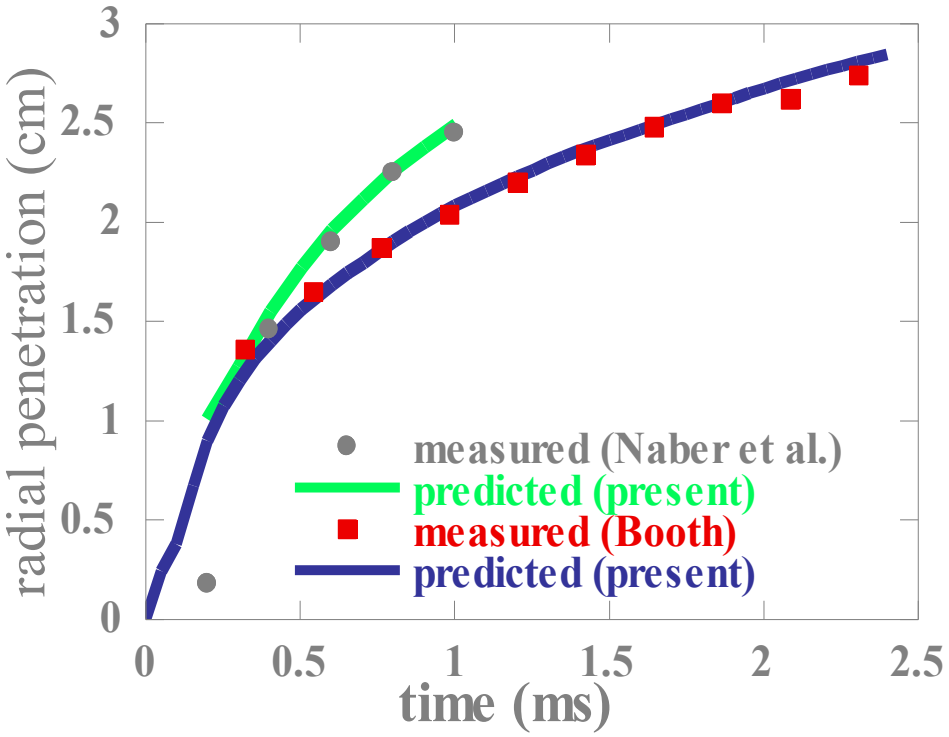
ERC Wall Impingement Model

- Rebound or slide based on We
- Enhanced breakup due to drop destabilization $B_1 = 1.73$

Senecal, SAE 971594



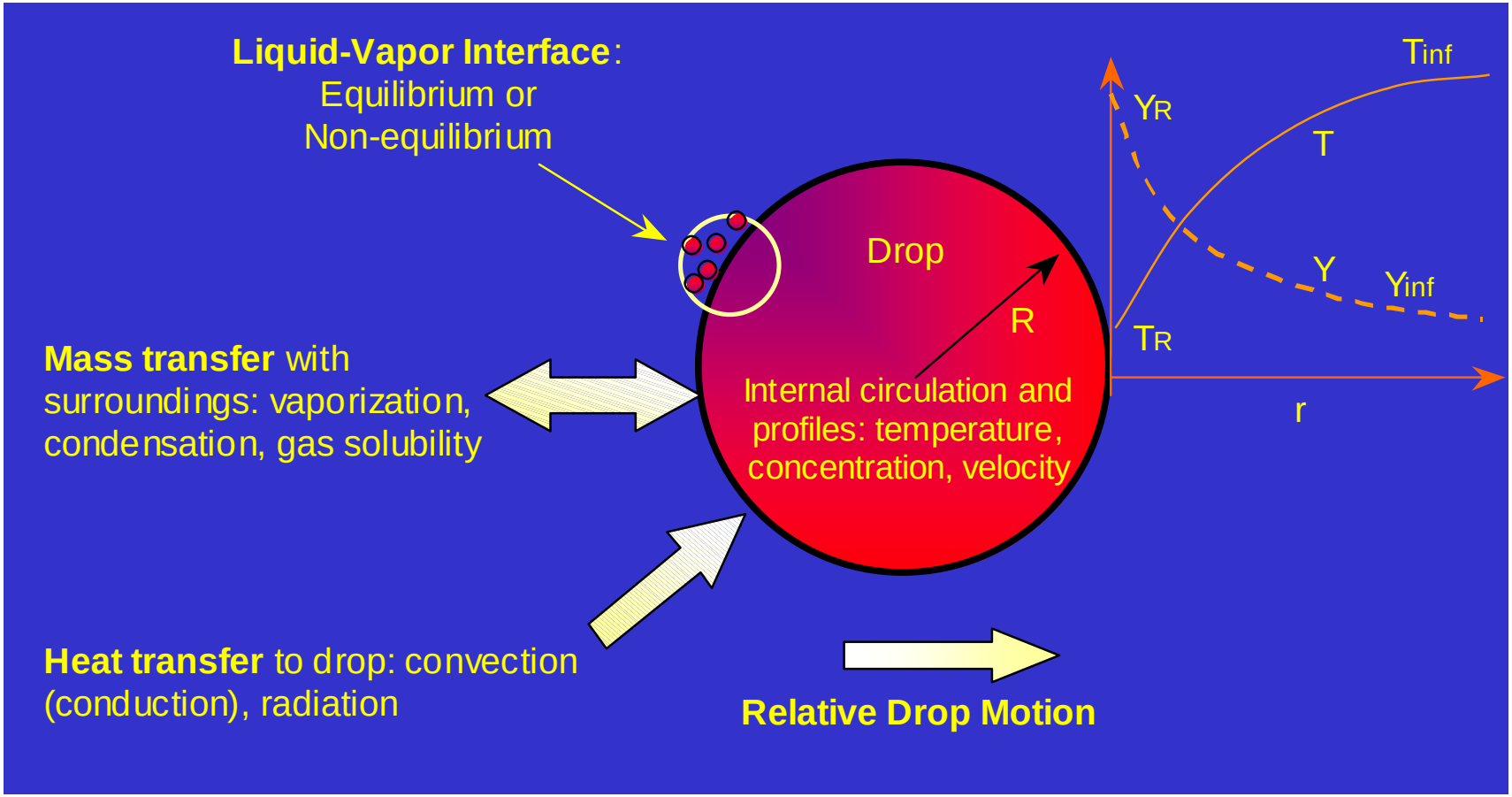




Drop Vaporization

Sirignano, 1999; Law 1976-77; Aggarwal SAE 2000-01-0588

- well understood for single component, low pressure
- D^2 Law



KIVA Vaporization Models

Amsden, 1989
Lefebvre, 1989

Frossling correlation

$$\mathbf{R} = dr/dt = -\rho DBSh/(2\rho_1 r)$$

Mass transfer number

$$B = (Y_1^* - Y_1)/(1 - Y_1^*)$$

Sherwood number

$$Sh = (2.0 + 0.6\,\mathrm{Re}_d^{1/2} Sc^{1/3})\frac{\ln(1+B)}{B}$$

Fuel mass fraction at drop surface

$$Y_1^* = W_1 / \{W_1 + W_0(\frac{p}{p_v(T_d)} - 1)\}$$

Vapor pressure P_v from thermodynamic tables

Drop Heat-up Modeling

Amsden, 1989
Lefebvre, 1989

Change in drop temperature from energy balance

$$\rho_d \frac{4}{3}\pi r^3 c_l \dot{T}_d - \rho_d 4\pi r^2 RL(T_d) = 4\pi r^2 Q_d$$

Rate of heat conduction to drop from

Ranz-Marshall correlation

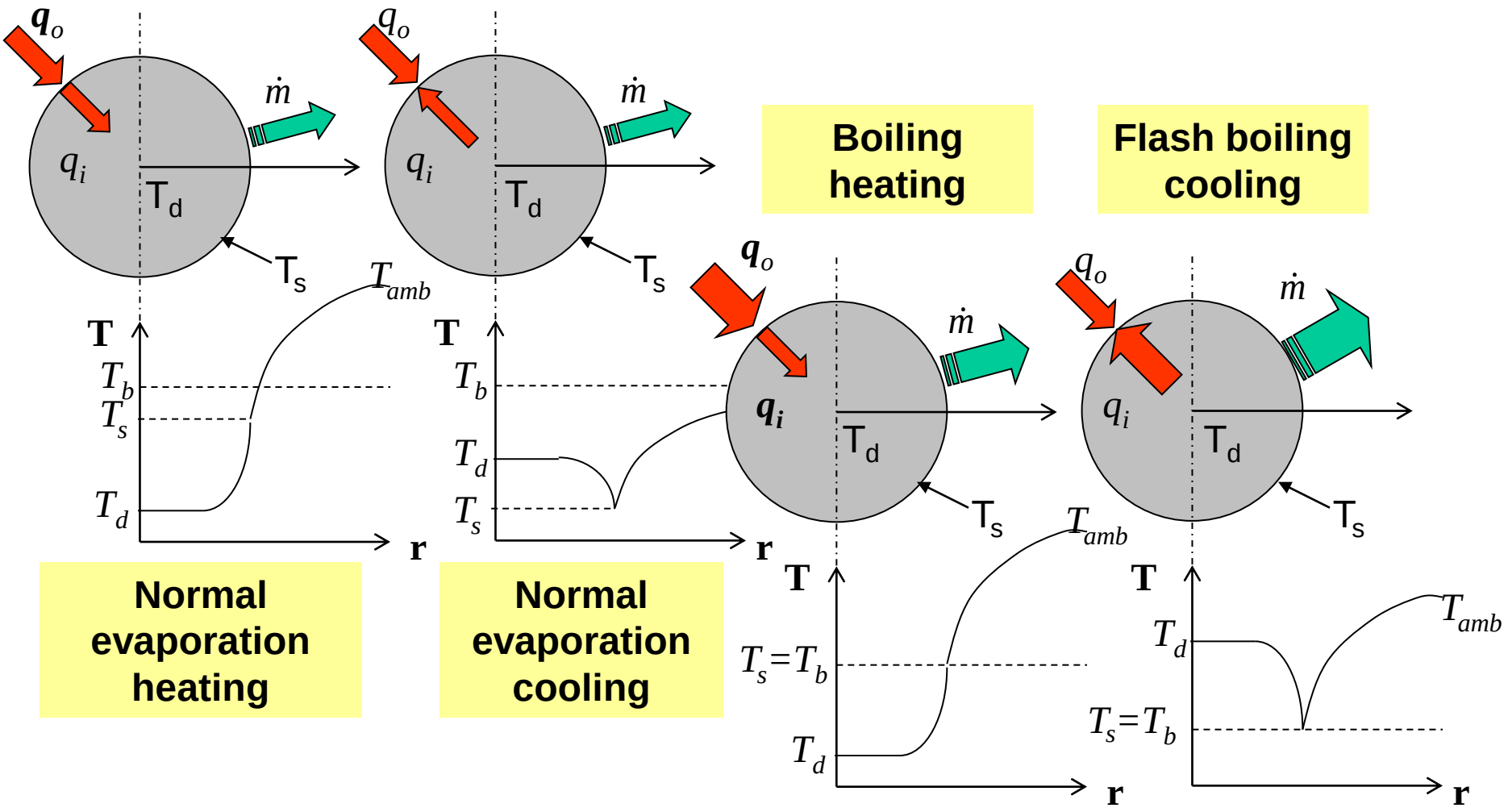
$$Q_d = \alpha(T_2 - T_1)Nu / (2\rho r)$$

where

$$Nu = (2.0 + 0.6\mathrm{Re}_d^{1/2}\,\mathrm{Pr}^{1/3})\frac{\ln(1+B)}{B}$$

Vaporization regimes

Ra & Reitz, 2003



Vaporization regimes

Normal evaporation

$$L(T_s)\dot{m} = q_i + q_o$$

Ra & Reitz, 2003

energy balance

$$\dot{m}L(T_s) = h_{i,eff}(T_d - T_s) + \frac{\kappa \bar{C}_P \dot{m}}{\exp\left[\frac{2r_o \bar{C}_P \dot{m}}{\lambda Nu} - \frac{[C_A](y_{F\infty} - y_{Fs})}{\lambda}\frac{Sh}{Nu}\right] - 1}(T_\infty - T_s)$$

mass balance

$$\dot{m} = g_m \ln(1 + B_M) = g_m \ln\left(1 + \frac{y_{Fs} - y_{F\infty}}{1 - y_{Fs}}\right)$$

$g_m = Sh\ \rho D/d$

$h_{o,eff}$

Flash Boiling evaporation (T_b from Clausius Clapeyron equation)

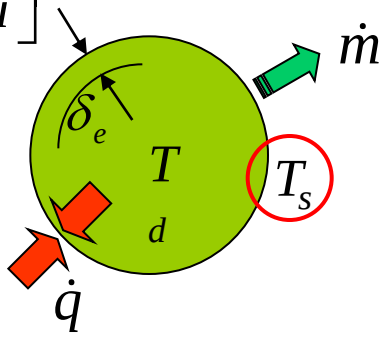
$$\dot{m}L(T_b) = (h_{i,eff} + \alpha_{sh})(T_d - T_b) + \frac{\kappa \bar{C}_P \dot{m}}{\exp\left[\frac{2r_o \bar{C}_P \dot{m}}{\lambda Nu} - \frac{[C_A](y_{F\infty} - 1)}{\lambda}\frac{Sh}{Nu}\right] - 1}(T_\infty - T_b)$$

$$\Delta T = T_d - T_b$$

Superheated droplet correlation (Adachi et al., 1997)

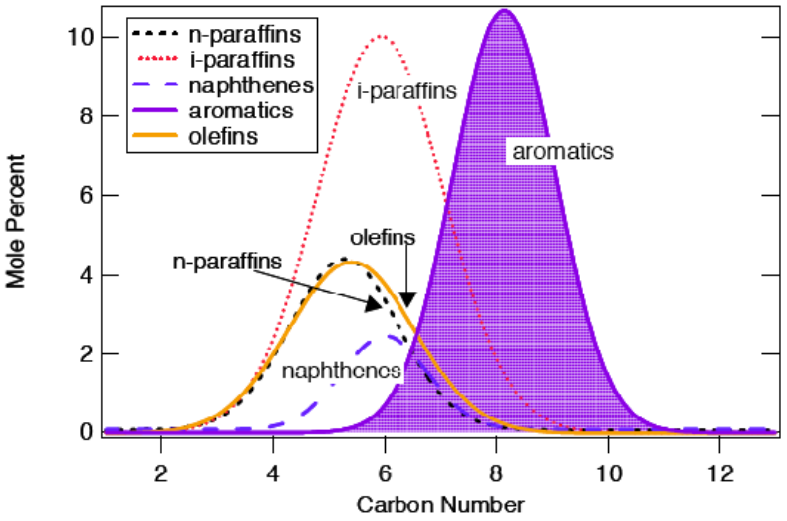
$$\alpha_{sh} = 0.76\Delta T^{0.26} \quad (0 \le \Delta T < 5)$$
$$= 0.027\Delta T^{2.33} \quad (5 \le \Delta T < 25)$$
$$= 13.8\Delta T^{0.39} \quad (25 \le \Delta T)$$

$$h_{i,eff} = \frac{\lambda}{\delta_e}, \quad \delta_e = \sqrt{\pi \alpha_{eff} t}$$



Multi-component fuel modeling

Gasoline



Common automotive fuels are multi-component

Components: Various molecular weights and chemical structures

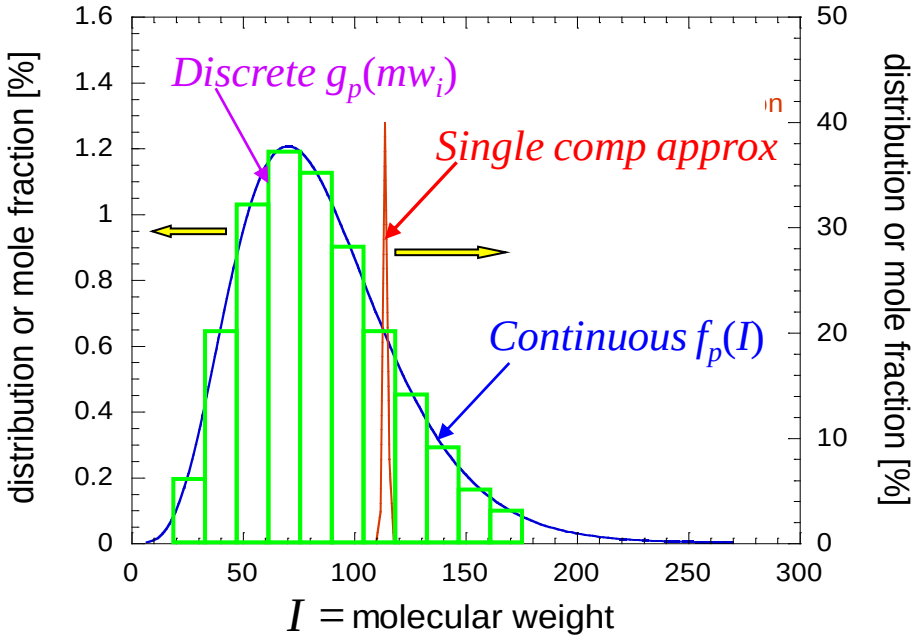
Three approaches;

i) single component approximation
ii) continuous multi-component
iii) discrete multi-component

Lippert & Reitz, 1997, Ra & Reitz 2003

Diesel

	diesel A	diesel B
Aromatic [%]	34	16
Sulfur [ppm]	10.5	7.3
Parafins [%]	33	42
Napthenes [%]	33	42
Olefin [%]	0.2	0.3
Cetane#	~43	~47
C/H ratio	7.014	6.393



Multi-component model formulation

Continuous Multi-Component

$p=l,v$

- Continuous system of a liquid phase + Semi-continuous mixture system of vapor phase fuel and ambient gas:

$$G_p(I) = {x_F}^p f_p(I) + \sum_{s=1}^{N} {x_s}^p \delta(I - I_s)$$

continuous phase | discrete phase

- Vapor phase transport equation,

$$\theta_p^n = \int_0^\infty I^n f_p(I) dI \qquad (n = 0, 1, 2, \cdots)$$

$$\frac{\partial}{\partial t}[\rho_f \theta_v^n] + \nabla \cdot [\rho_f \theta_v^n v] = -\nabla \cdot \int_0^\infty I^n J_I dI + S_g$$

- Assumed distribution function : Γ- func

$$f(I) = \frac{(I-\gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp[-\frac{(I-\gamma)}{\beta}]$$

$$\theta = \alpha\beta + \gamma, \quad \sigma^2 = \alpha\beta^2$$

Discrete Multi-Component

- Discrete system of a liquid phase + Discrete mixture system of vapor phase fuel and ambient gas:

$$G_p(I) = \sum_{F=1}^{N_F} {x_F}^p \delta(I - I_F) + \sum_{s=1}^{N_s} {x_s}^p \delta(I - I_s)$$

discrete phase of fuel | discrete phase of air/fuel mixture

- Vapor phase transport equation,

$$\frac{\partial}{\partial t}[\rho y_i] + \nabla \cdot [\rho y_i v] = \nabla \cdot (\rho D_i \nabla y_i) + s_{g,i}$$

$$\sum \Rightarrow$$

$$\frac{\partial}{\partial t}[\rho y_F] + \nabla \cdot [\rho y_F v] = \nabla \cdot (\rho \bar{D} \nabla y_F) + S_g$$

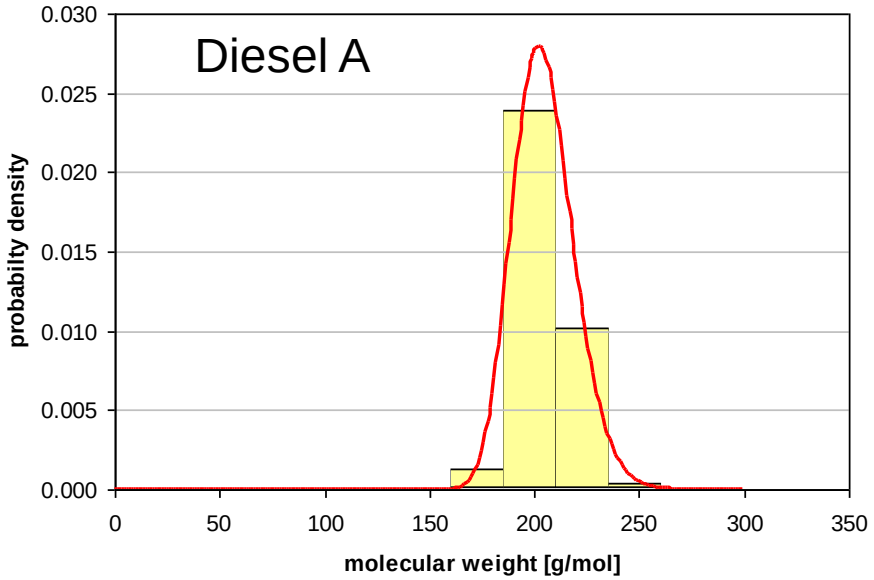
Ra & Reitz, 2003, 2009

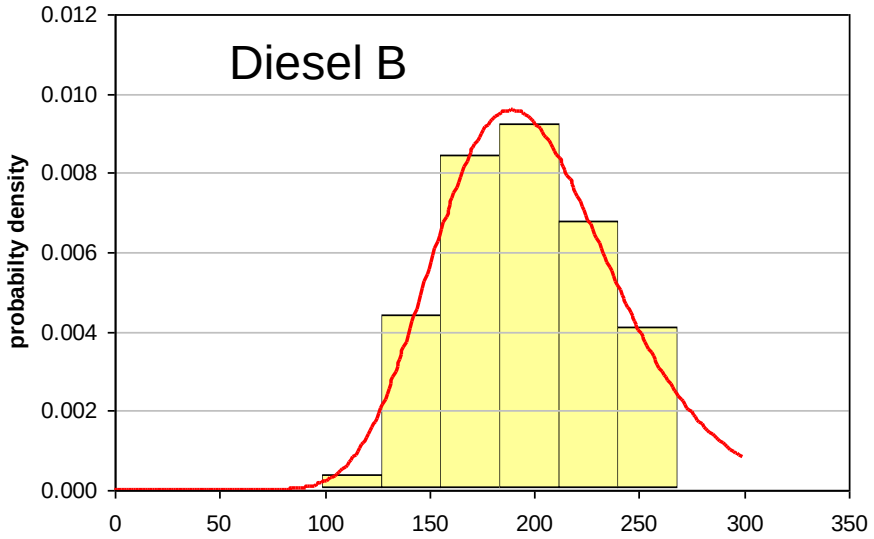
DMC Model Test

Modeled species contents*

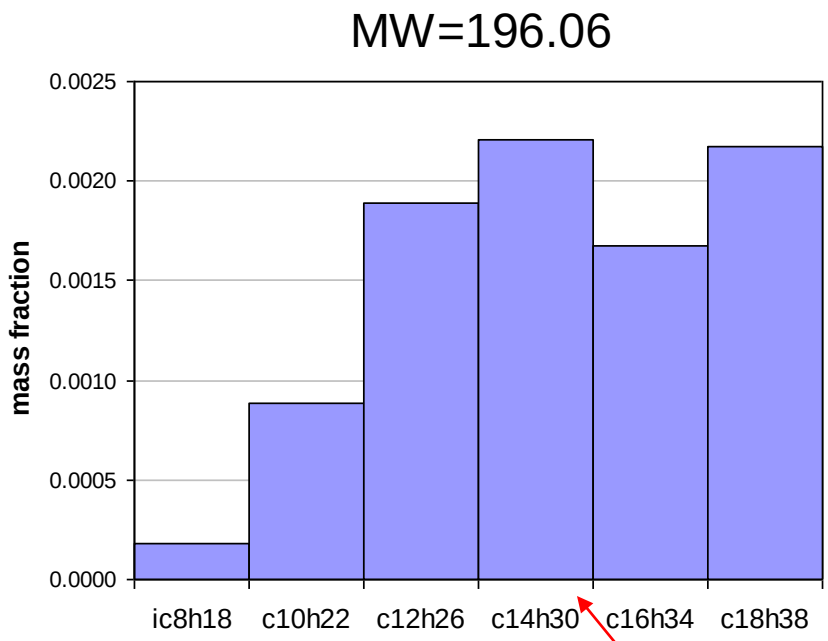
species	MW	Mass fraction
Diesel A (US narrow-cut Diesel)		
c14h30	198	0.6253
c12h26	170	0.0559
c16h34	226	0.3025
c18h38	254	0.0163
Diesel B (Euro Diesel)		
c14h30	198	0.2376
ic8h18	114	0.0153
c10h22	142	0.0807
c12h26	170	0.1863
c16h34	226	0.1984
c18h38	254	0.2817

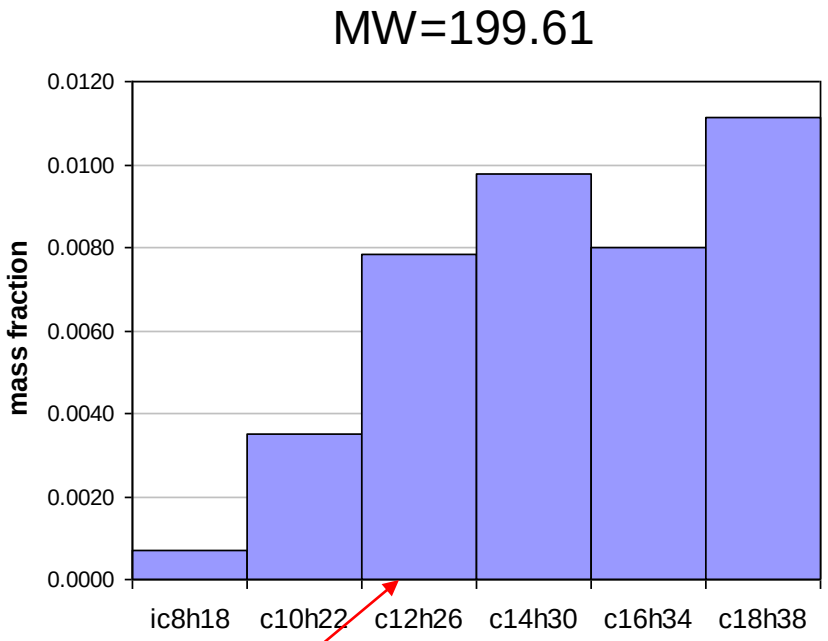
Ra & Reitz, 2009





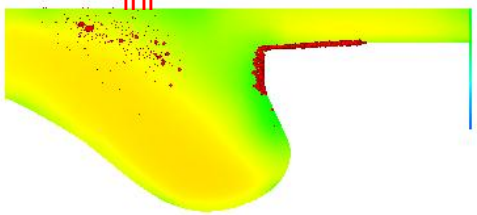
Component distributions

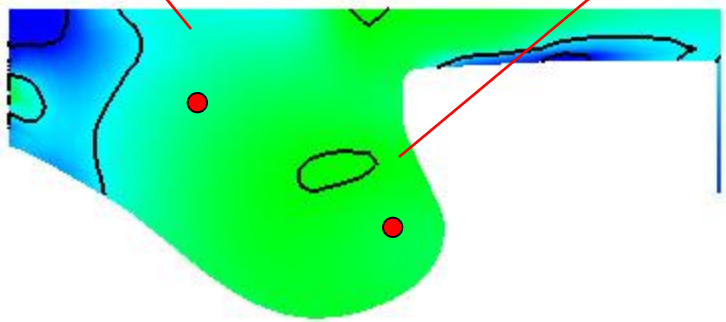


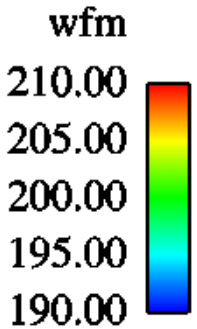


Diesel B

MW_{ini}=200





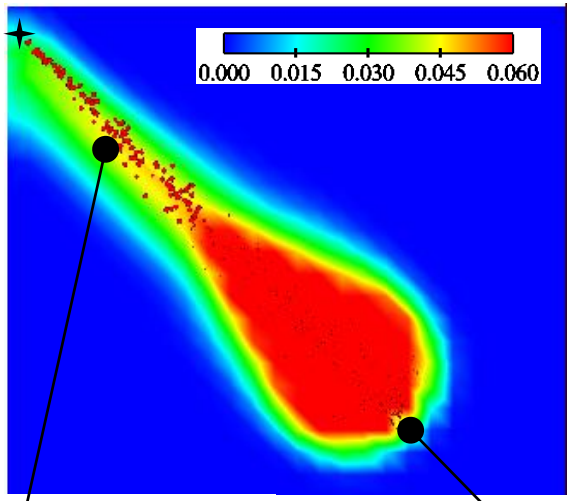


Ra & Reitz, 2009

CA=-14 (~ first ignition timing)

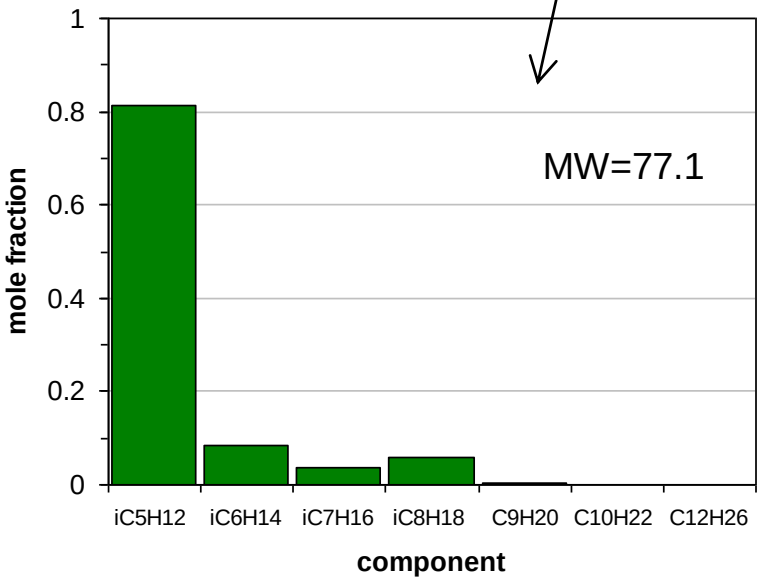
Multi-component spray vaporization

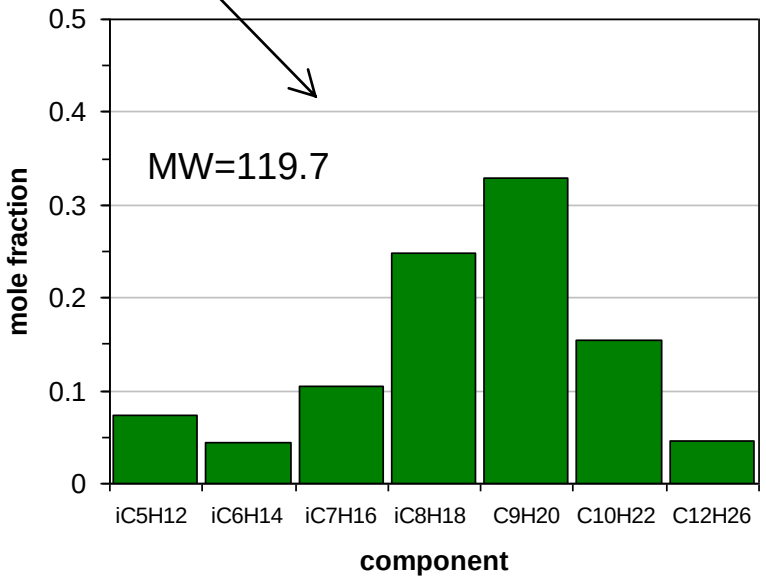
Ra & Reitz, 2009



Gasoline
Do=300 μm
Vinj=100 m/s

2.0 ms after SOI

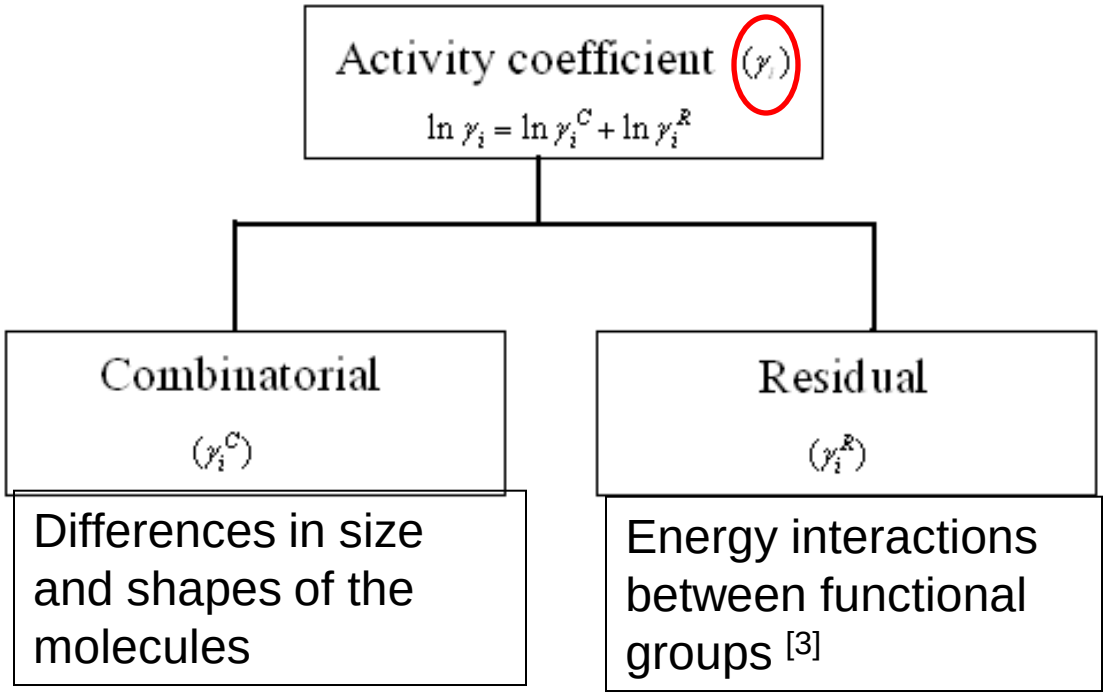




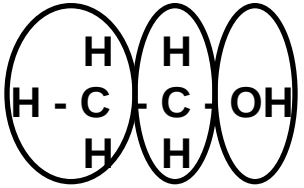
Non-ideal mixing using UNIFAC Method

Jiao, SAE 2011-01-0387

For mixtures composed of **polar components**, both initial and final boiling points in the distillation curve are not well predicted assuming **Ideal Mixing** (Raoult's Law) - misses the **azeotrope behavior of the mixture**.



$$x_i = \frac{P_{vap,i}}{P_m}\gamma_i x_{L,i}$$



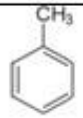
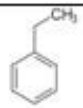
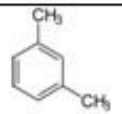
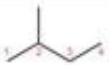
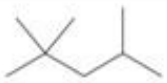
$P_{vap,i}$ Vapor pressure of pure comp. i ; P_m Total mixture pressure

$x_{L,i}$ Mole fraction of comp. i in liquid phase; x_i Mole fraction of comp. i in gas phase

Fredenslund, 1975

Ethanol/gasoline surrogate mixture

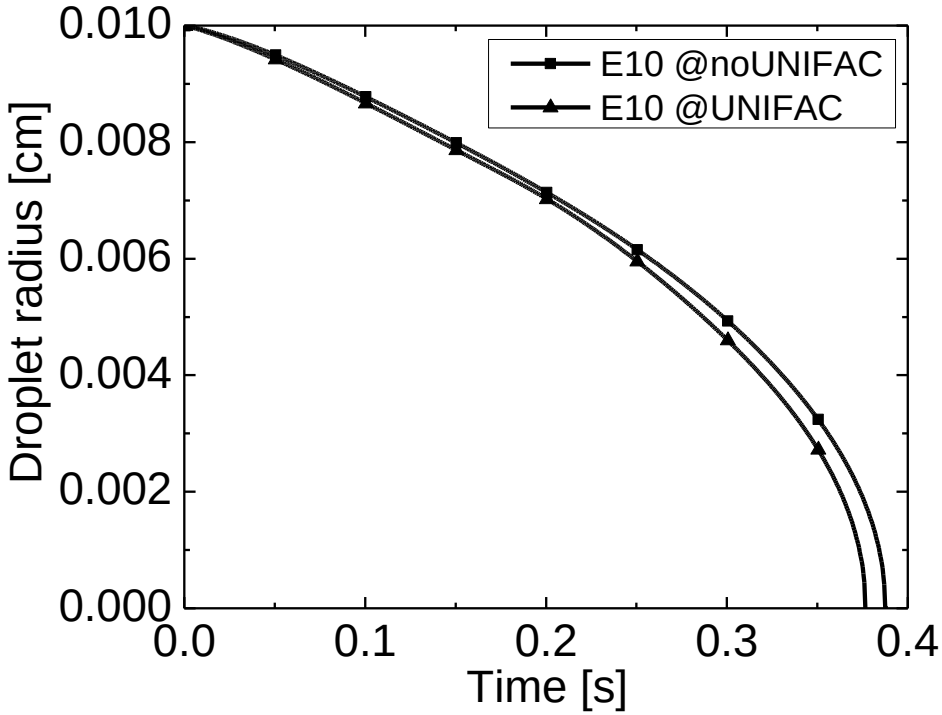
Pfahl,1996, Jiao, 2011

Component name	Mol %			Molecular Weight [g/mol]	b.p. [^{0}C]	Functional groups in UNIFAC
Cyclo-pentane	16.8	c5h10		70.1	49	5CH2
Toluene	9.7	c7h8		92.14	110.6	5ACH, 1ACCH3
Ethylbenzene	3.2	c8h10		106.167	136	5ACH,1ACCH2 1CH3
meta-Xylene	4.9	c8h10		106.167	139	4ACH, 2ACCH3
n-Pentane	3.0	nc5h12		72.15	36.1	2CH3,3CH2
n-Heptane	3.6	nC7h16		100.21	98.42	2CH3,5CH2
Isopentane	7.8	ic5h12		72.15	27.7	3CH3,1CH2 1CH
isoheptane	7.7	ic7h16		100.20	90.0	3CH3,3CH2, 1CH
iso-octane	2.5	ic8h18		114.23	99.3	5CH3,1CH2, 1CH,1C

Drop evaporation simulation

Jiao, SAE 2011-01-0387

- Droplet lifetime



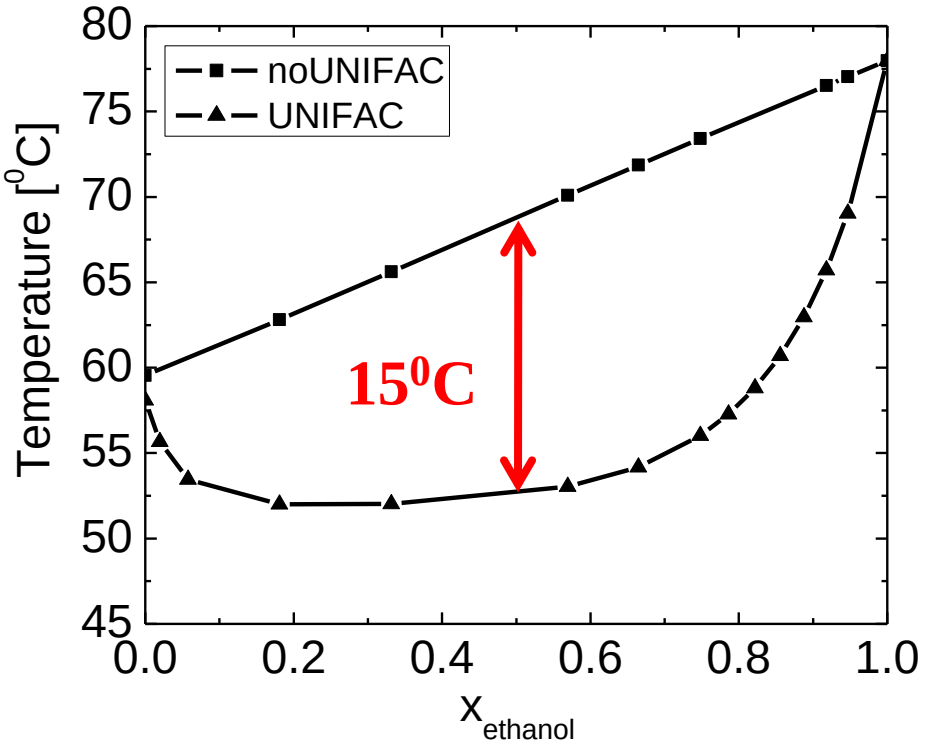
Adding ethanol decreases vapor pressure

- but with non-ideal effects, vapor pressure first increases

Adding ethanol broadens boiling temperature range

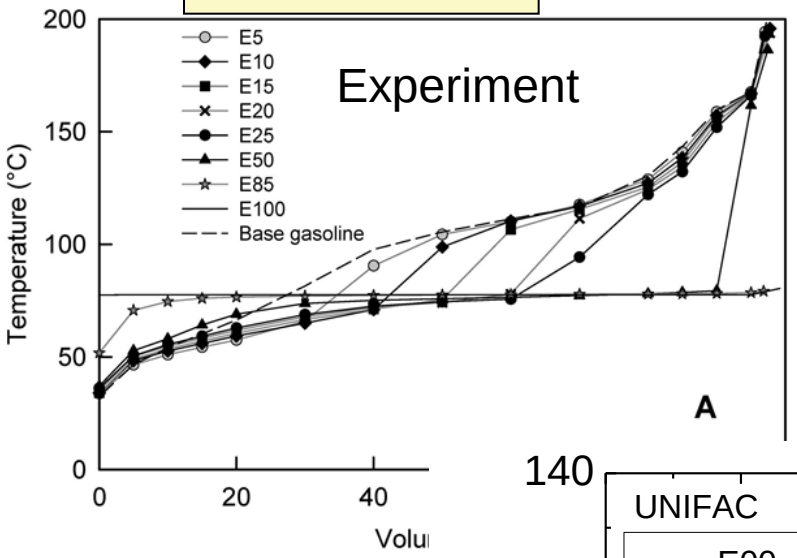
Phase diagram of mixture of ethanol and 9-component gasoline surrogate, P_{amb}=1bar

- Temp. vs. mole fraction

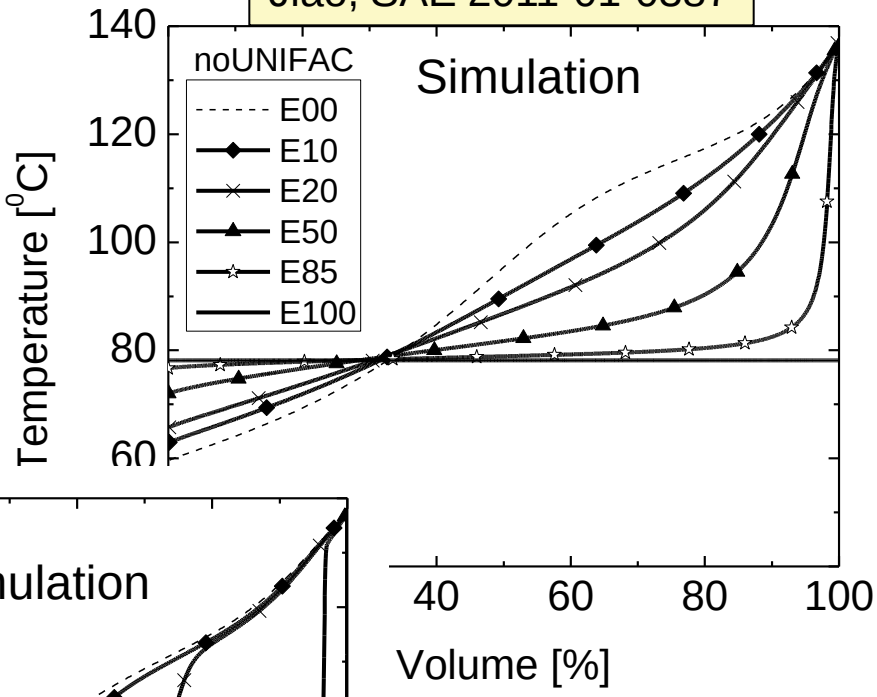


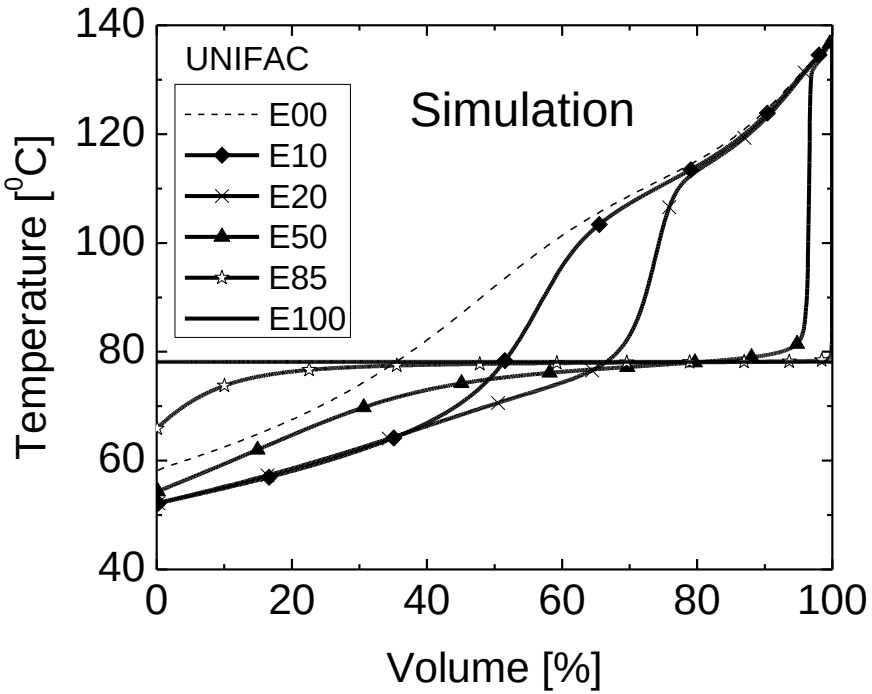
Distillation curve

Andersen, 2010



Jiao, SAE 2011-01-0387





E20 has the lowest initial boiling temperature

Hour 5: Drop Drag/Wall Impinge/Vaporization

	diesel	Jet-A	JP-8
cyC6	0.010000	0.022529	0.012529
c7h8	0.037698	0.035873	0.025873
c10h8	0.020000	0.009607	0.0
c10h18	0.0	0.0	0.030000
c10h22	0.113977	0.253797	0.721022
c12h26	0.124544	0.298704	0.118311
c14h10	0.0	0.0	0.0
c14h30	0.210805	0.202265	0.022265
c16h34	0.172593	0.060627	0.0
c18h38	0.085615	0.0	0.0
c20h42	0.084268	0.0	0.0
mxylene	0.010000	0.079442	0.0
mcymene	0.050355	0.0	0.0
c11h16	0.0	0.019881	0.0
tetralin	0.017362	0.017275	0.0
c12h18	0.017362	0.0	0.0
c13h20	0.045421	0.0	0.0
nc7h16	0.0	0.0	0.070000

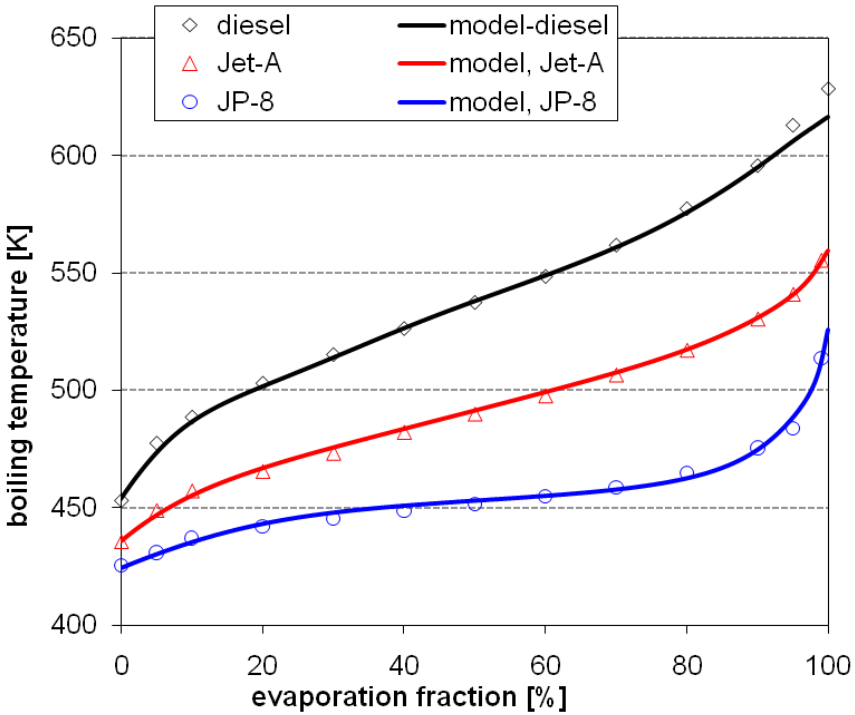
alkanes

aromatics

cycloalkanes

PAH

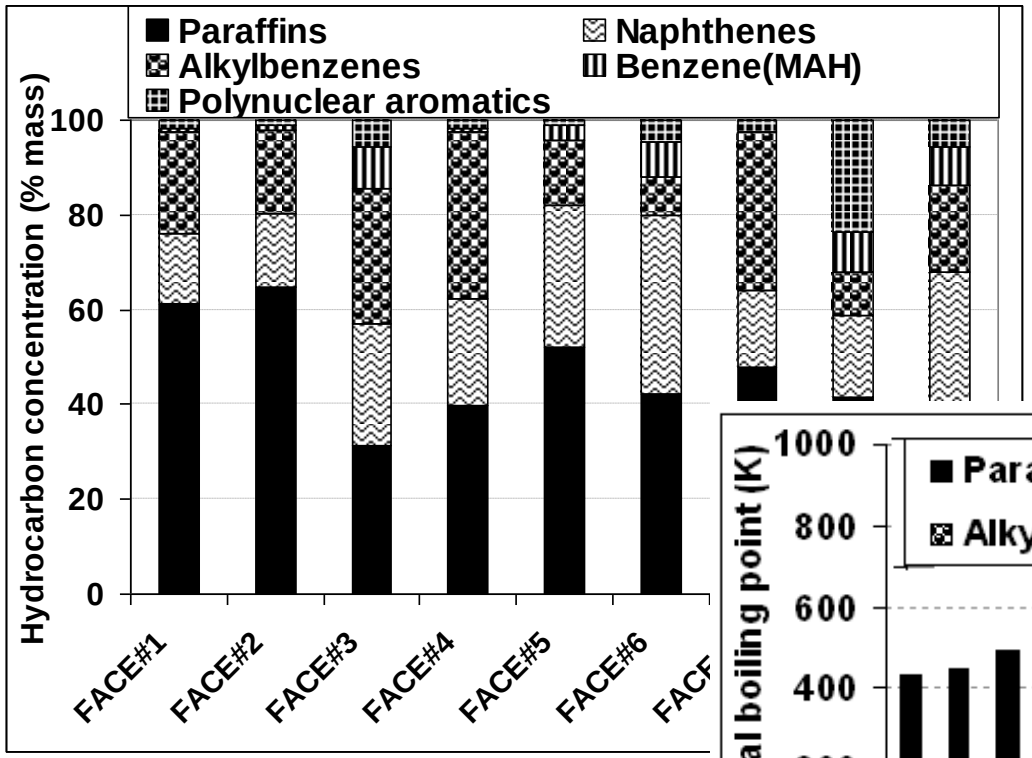
Surrogate fuels - 18 component model



	Diesel	Model-Di	Jet-A	Model-JetA	JP-8	Model-JP8
Density [g/cm^3]	0.8478	0.7800	0.8101	0.7638	0.7547	0.7333
Viscosity [cSt]	2.71	2.05	1.55	1.36	1.15	1.01
Surface tension [dynes/cm]	30	26.91	29.1	25.53	25.2	23.64
LHV [kJ/kg]	42526	42527.7	43305	43306.6	44185	44199.4
Saturates [%]		81.4	84.4	83.7	94.7	94.1
Aromatics [%]		17.6	14.0	14.1	1.2	2.2
Olefins [%]			1.6		4.1	
Naphthenes [%]		1.0		2.2		3.7
C/H ratio	6.852	6.102	6.534	5.997	5.95	5.565
Molecular weight [g/mol]	190	177	160	152	150	139

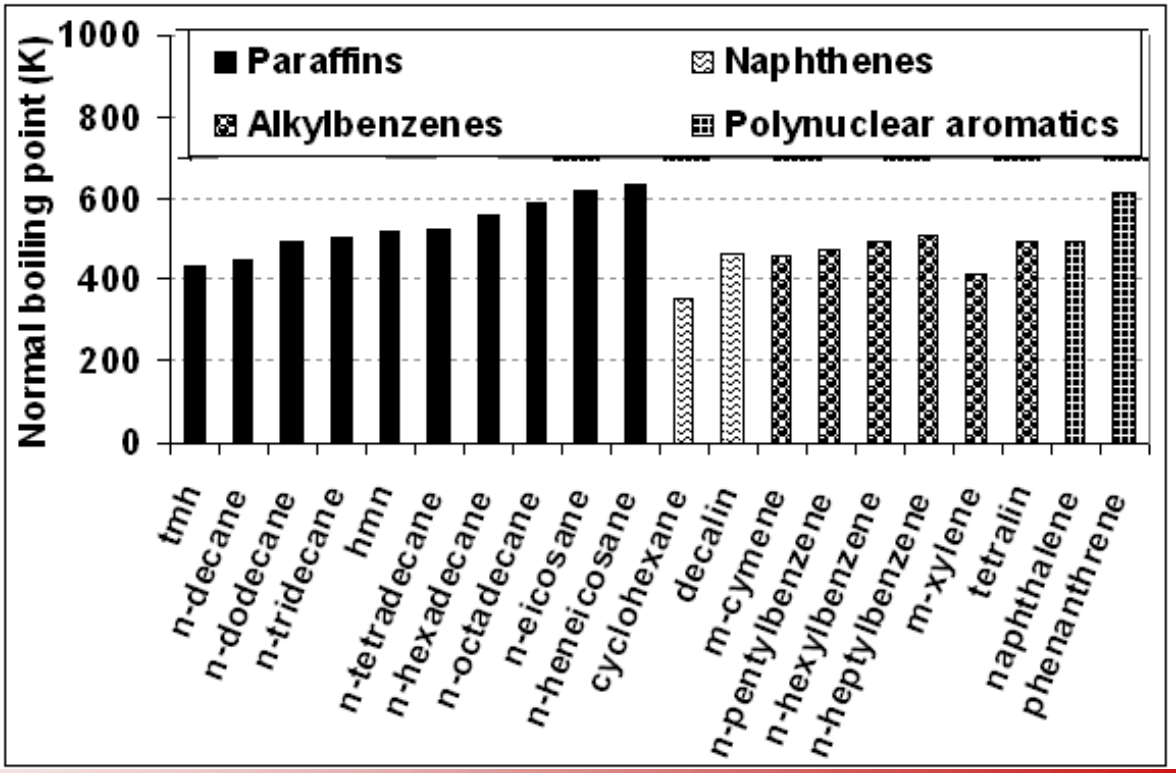
← corrected

Diesel Hydrocarbon Class Distributions and Surrogates



Anand, 2011

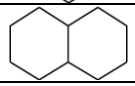
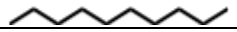
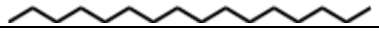
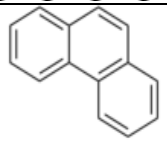
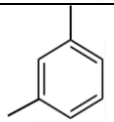
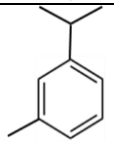
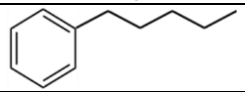
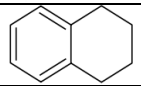
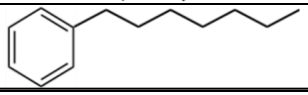
20 species physical property surrogate database



FUELS for Advanced Combustion Engines (FACE)

Measured hydrocarbon class distributions

Chemical Structure and Activity Coefficients of Face #9 Surrogates

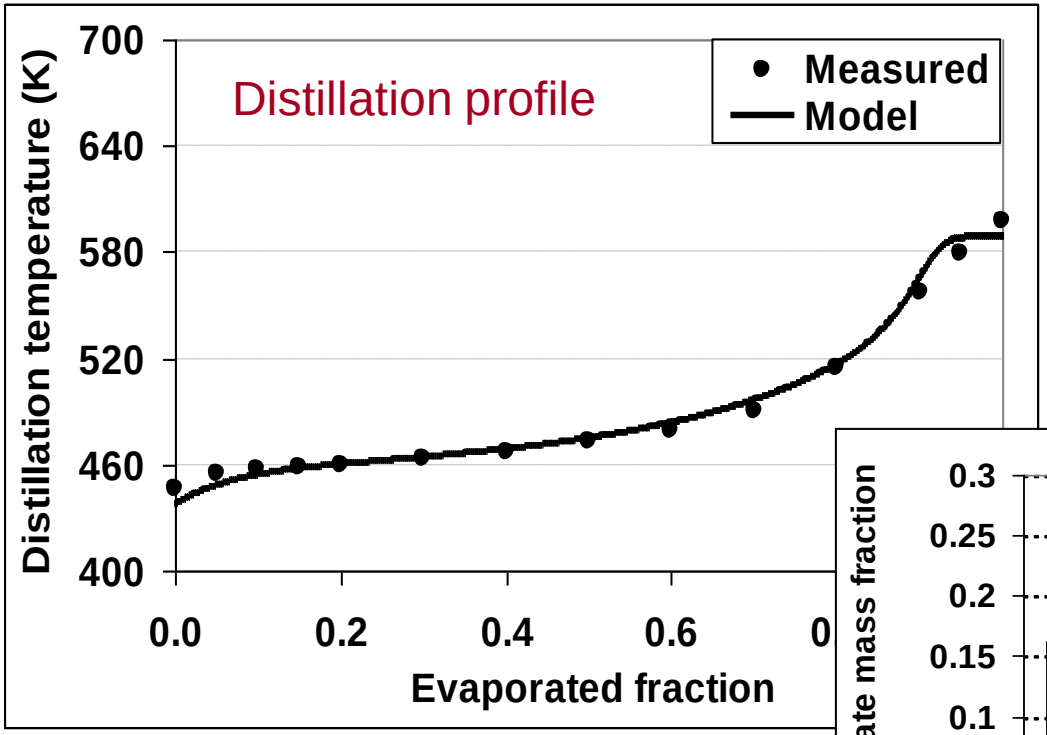
component	chemical structure	activity coefficient γ at 373 K
n-Tetradecane ($C_{14}H_{30}$)		1.01
Cyclohexane (C_6H_{12})		0.88
Decalin ($C_{10}H_{18}$)		1.03
n-Decane ($C_{10}H_{22}$)		1.06
n-Hexadecane ($C_{16}H_{34}$)		0.95
n-Eicosane ($C_{20}H_{42}$)		0.81
Phenanthrene ($C_{14}H_{10}$)		2.22
m-Xylene (C_8H_{10})		1.06
m-Cymene ($C_{10}H_{14}$)		1.07
Pentylbenzene ($C_{11}H_{16}$)		1.08
Tetralin ($C_{10}H_{12}$)		1.17
Heptylbenzene ($C_{13}H_{20}$)		1.10

Departure from Raoult's law - Non-ideal vaporization influences heavy-end of distillation curve *

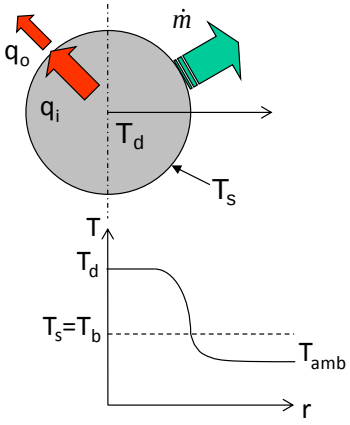
$$p_{i,v} = x_{i,v}P$$
$$= x_{i,l}\gamma_i P_{sat,i}$$

* Anand, 2011

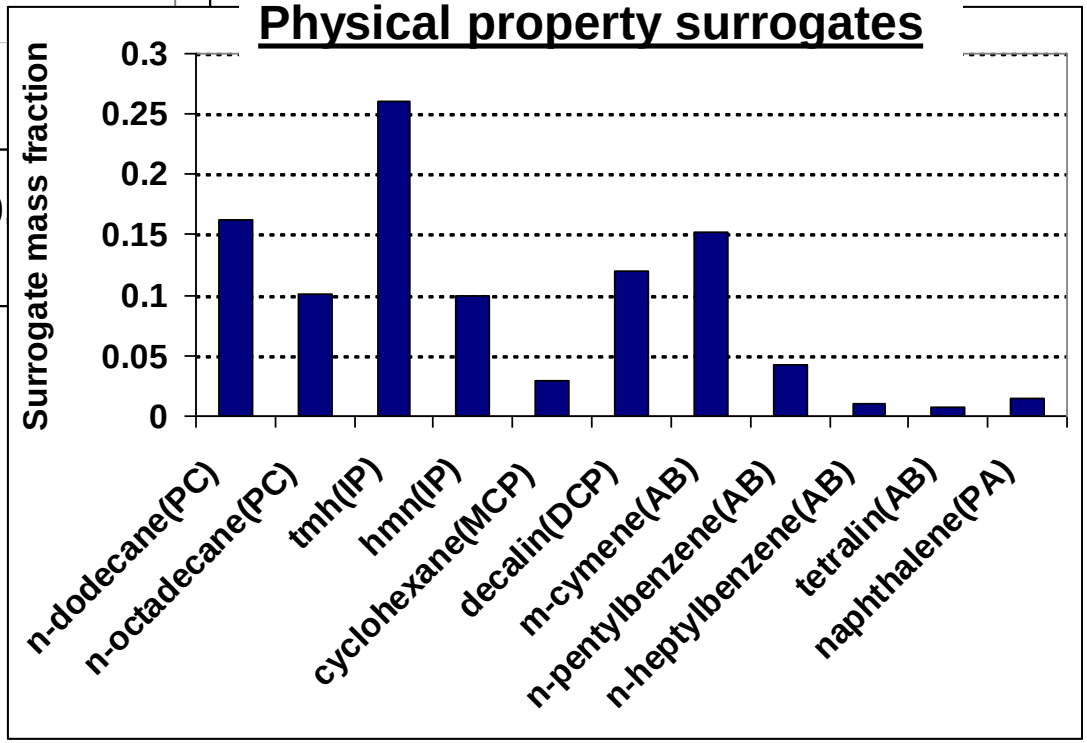
Example - Face Fuel #1 Surrogate Composition



Batch distillation modeled as flash boiling droplet



Physical property surrogates

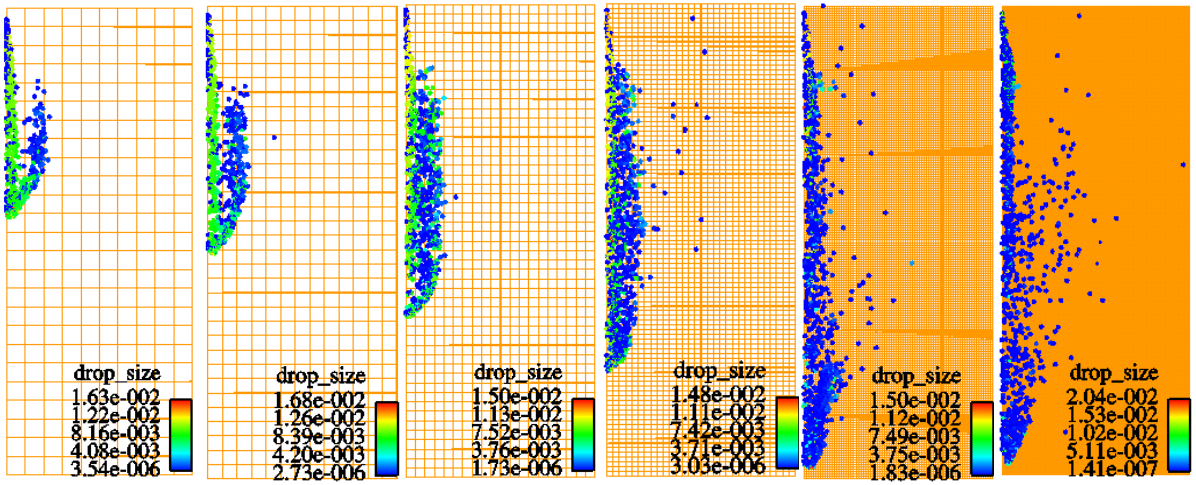


Chemical classes

PC – normal paraffins
IP – iso-paraffins
MCP – mono cyclo paraffins
DCP – di-cycloparaffins
AB – Alkyl benzenes
PA – poly aromatics

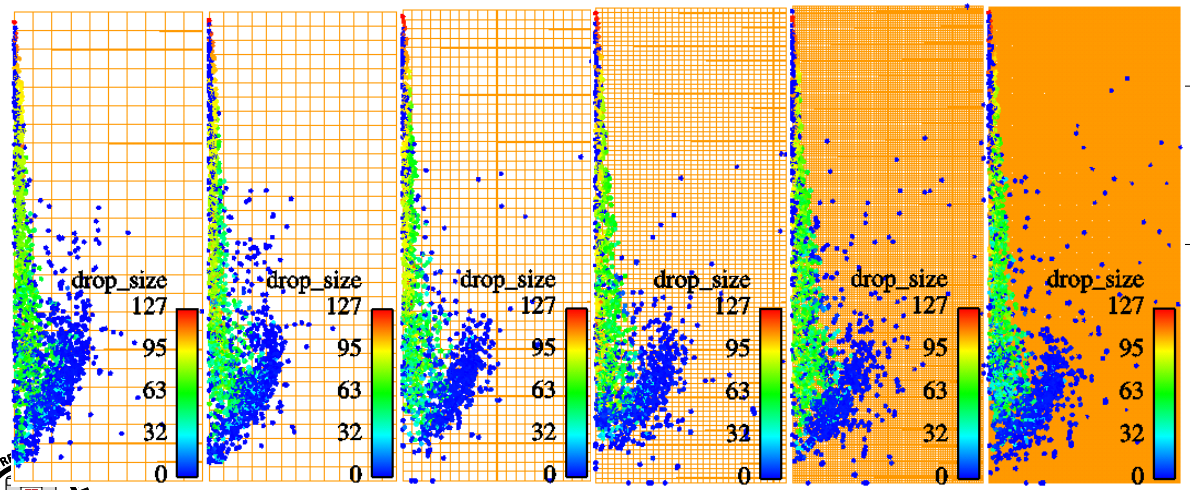
Putting them all together - Grid independent spray model

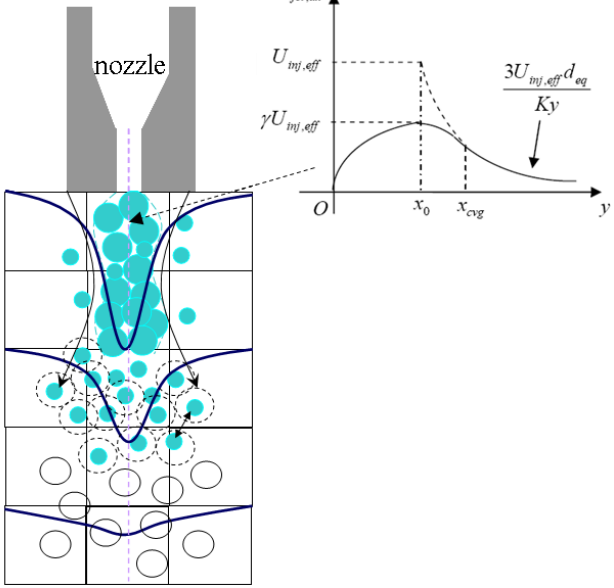
Abani SAE 2008-01-0970



4 mm 3mm 2 mm 1 mm 0.5 mm 0.25m

Gas-jet sub-grid momentum exchange near nozzle



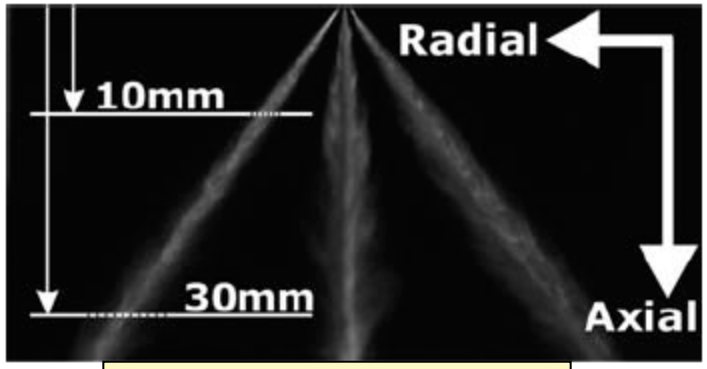


Coarse mesh:
Drop drag over-predicted

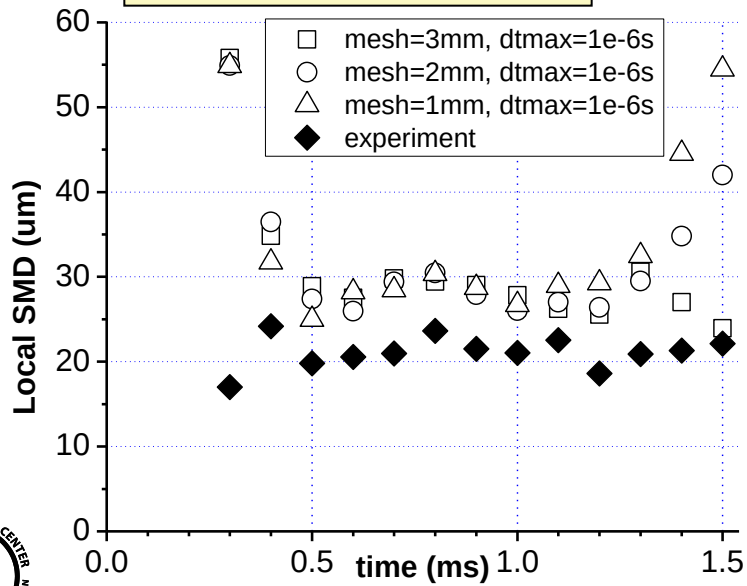
Fine mesh:
Drop coalescence under-predicted

Spray model validation

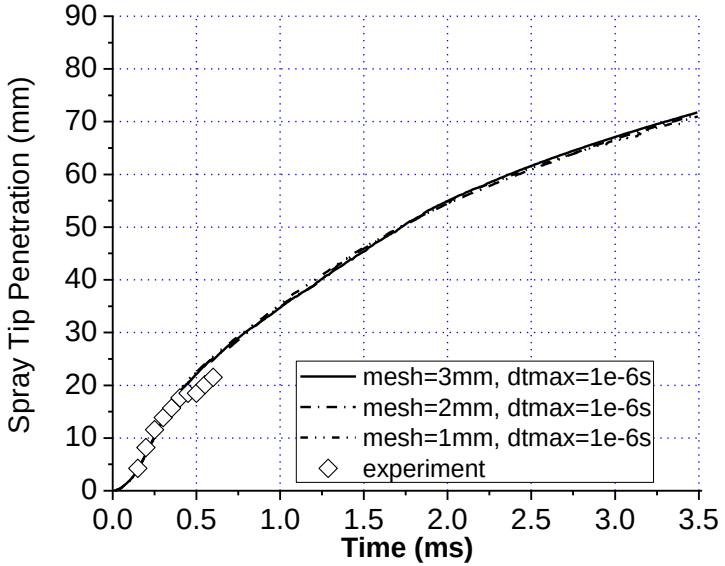
6-hole injector; Iso-octane; constant volume chamber, cold ambient; Injection pressure: 120, 200bar; chamber pressure: 12bar;

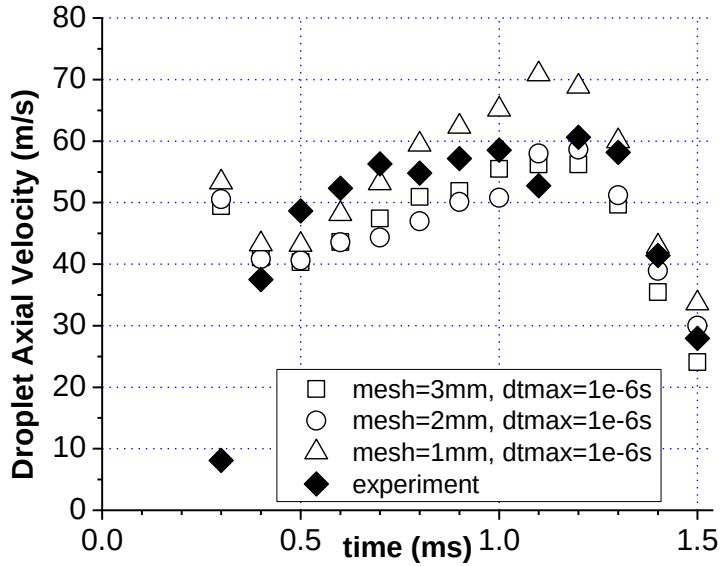


Expts: Mitroglou, 2006

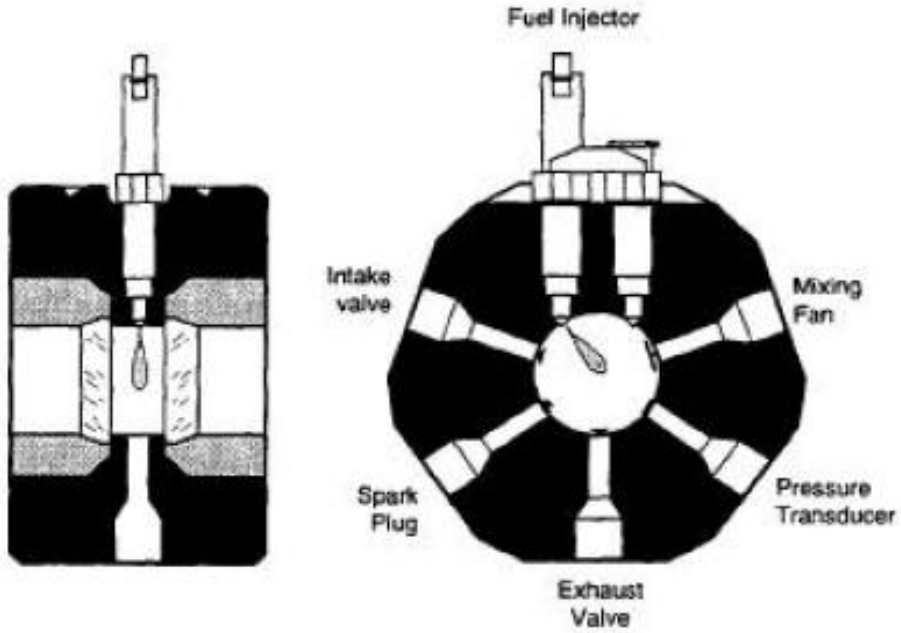


Wang, SAE 2010-01-0626





Validation – Evaporating sprays



Naber & Siebers, SAE 960034

Siebers, SAE 980809,

Diesel and other fuels;

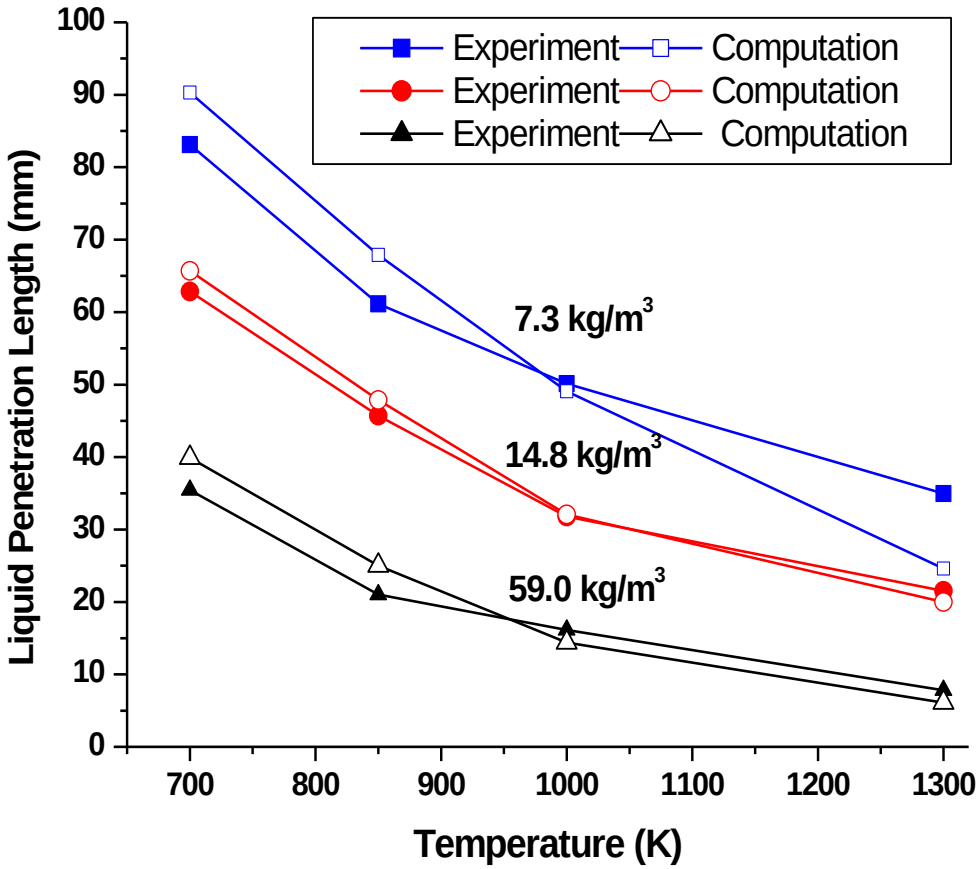
Constant volume chamber; various temperatures;

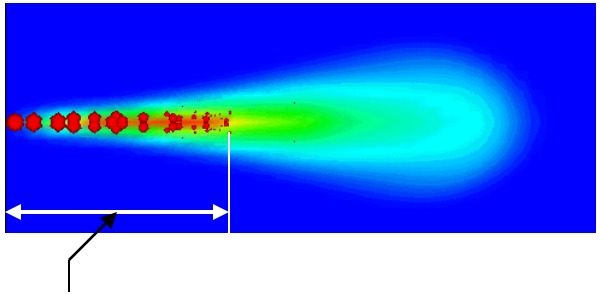
Varying chamber densities: 13.9, 28.6, 58.6kg/m^3.

Schlieren imaging

Pickett, Sandia National Laboratory, "Engine Combustion Network", https://share.sandia.gov/ecn/, 2007

Evaporating Diesel Spray - Liquid length





Siebers, SAE 980809,

Injection Pressure : 135 MPa

Fuel : DF2

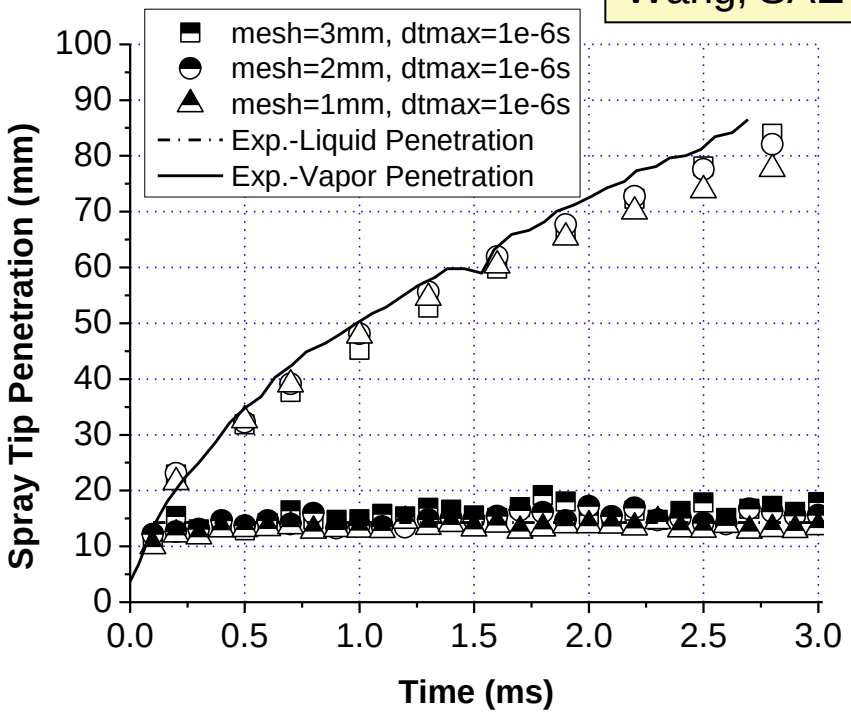
Orifice Diameter : 246 µm

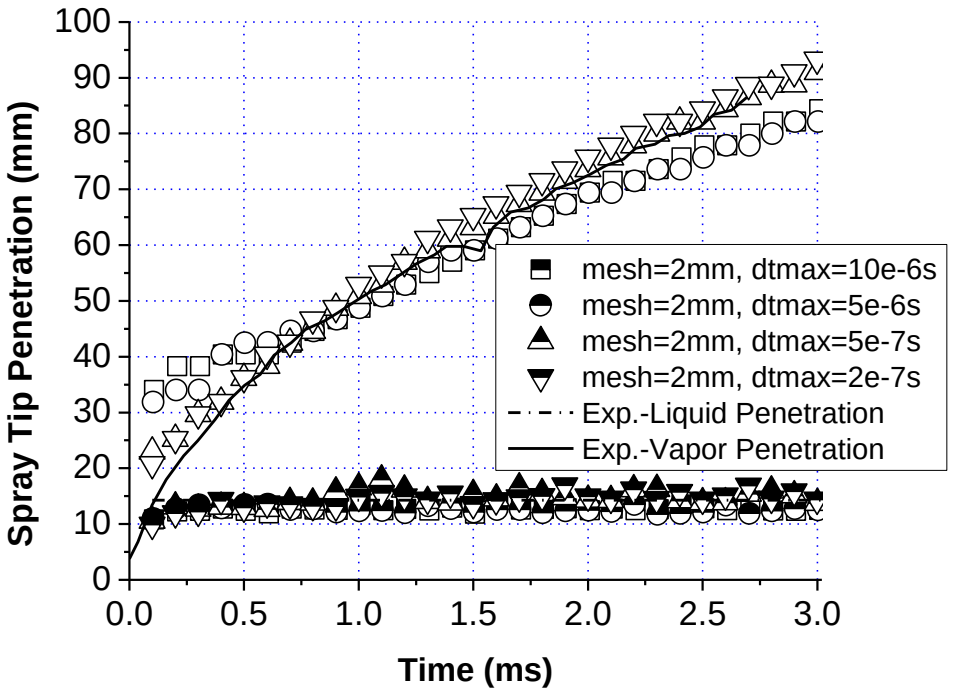
Comparison of model results with experimental liquid penetration length data

Juneja, SAE 2004-01-0530

Evaporating Diesel Spray – grid size and time step independency

Wang, SAE 2010-01-0626



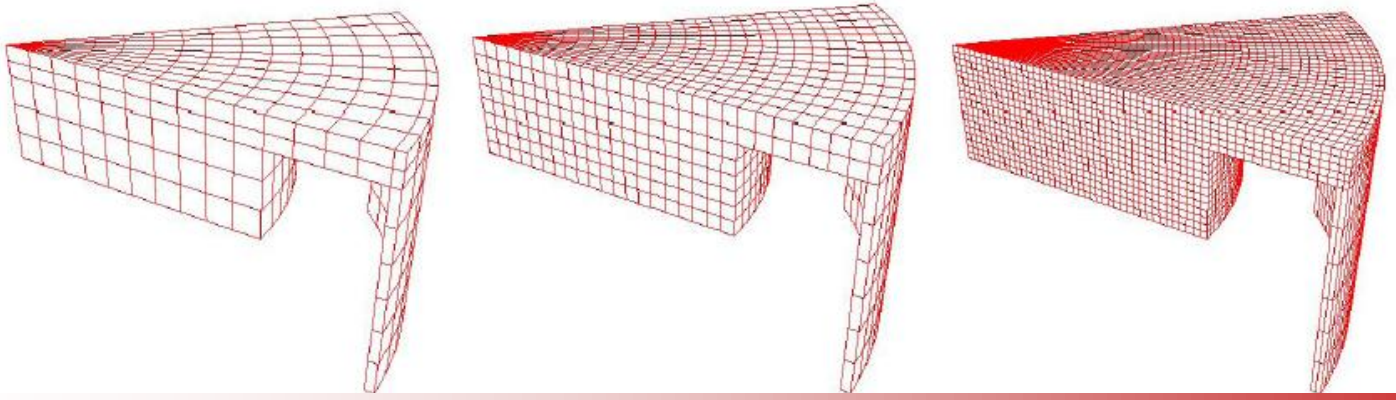


Predicted vapor and liquid penetrations.
Experimental data of Naber and Siebers (1996) and Pickett (2007).
Diesel fuel injection, nozzle diameter 257 mm, injection pressure 1370bar, gas temperature 1,000K, gas density 58.6 kg/m^3 .

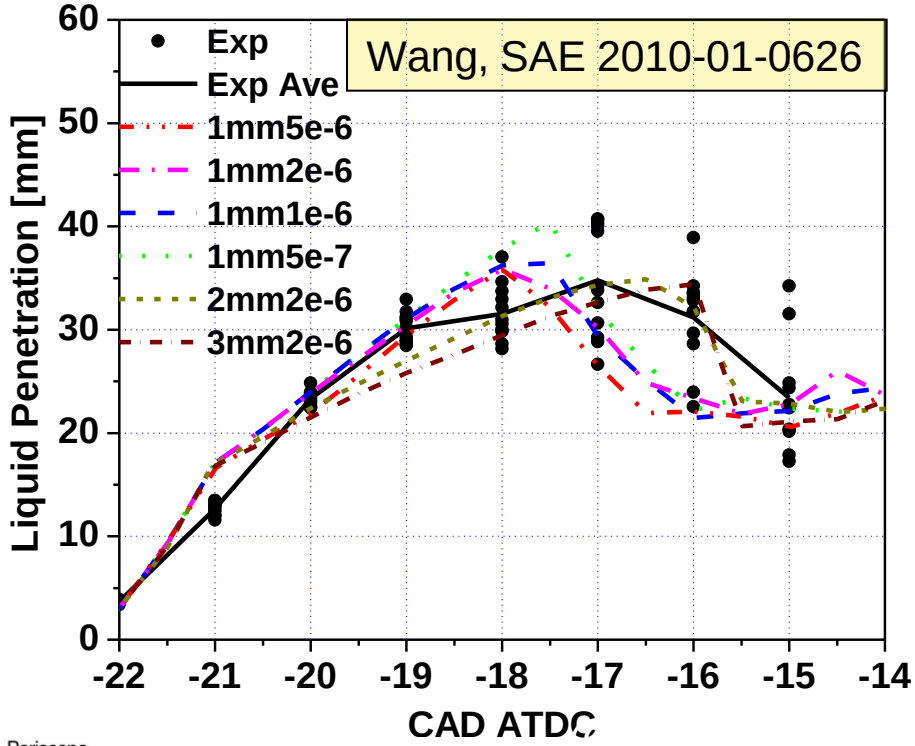
Validation – Cummins-Sandia Optical Engine

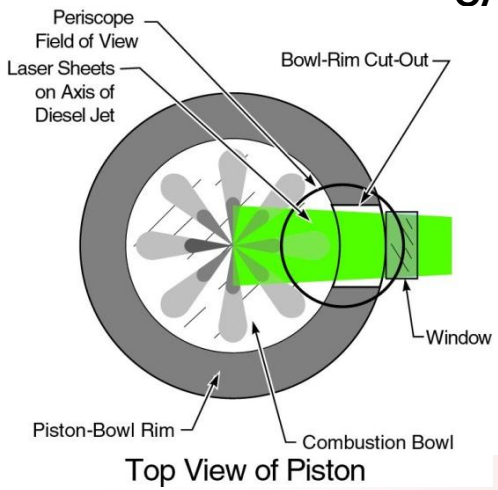
Wang, SAE 2010-01-0626

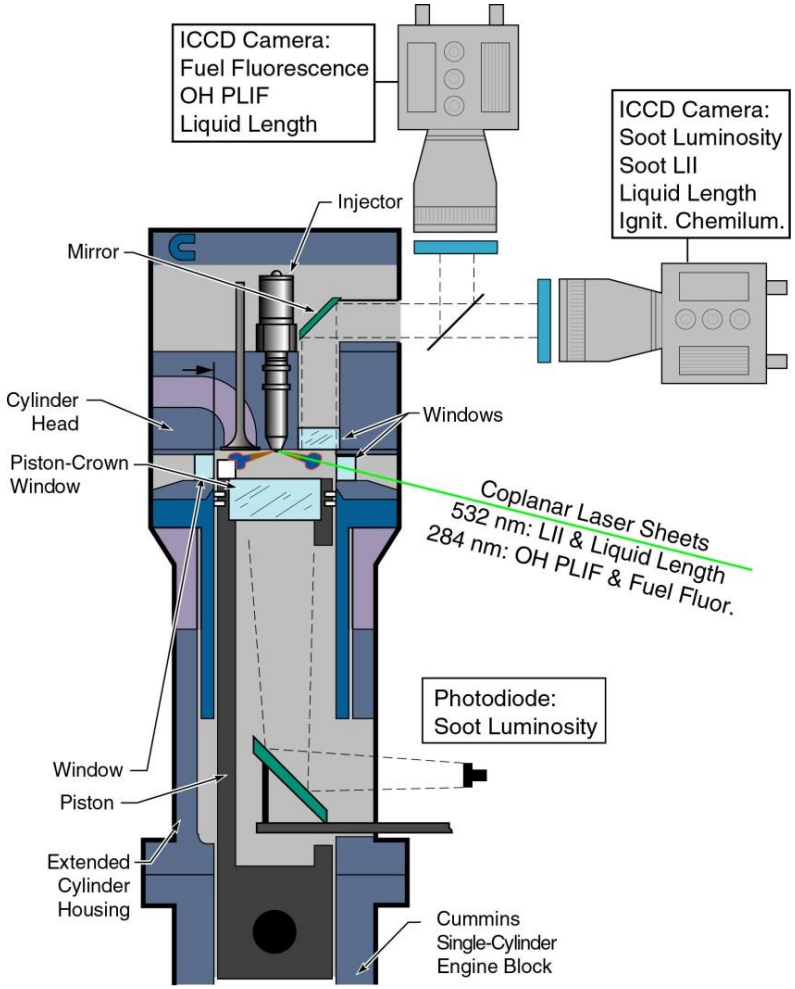
	Case A (Early Injection, Low Temperature)	**Case B** (Late Injection, Low Temperature)	**Case C** (Long Ignition Delay, High Temperature)
IMEP [bar]	3.9	4.1	4.5
Injection Pressure [bar]	1600	1600	1200
SOI [deg ATDC]	-22	0	-5
Injection Quantity [mg]	56	56	61
DOI [deg]	7	7	10
Peak Temperature	2200 K	2200 K	2700 K
O2 Concentration [Vol %]	12.7 (with EGR)	12.7 (with EGR)	21 (without EGR)



Liquid and Vapor Fuel Penetration







Singh, 2007

Summary

Extensively validated spray models accurately capture the physics of vaporizing sprays under engine conditions

Realistic fuels with non-ideal vaporization effects can be represented

Improved spray models provide consistent fuel distribution predictions, which is a prerequisite for combustion modeling and engine optimization.

Spray predictions can be independent of mesh size and time step;

Recent experimental and modeling work can be accessed through the Sandia Engine Combustion Network (ECN) http://www.sandia.gov/ecn/

Singh, 2007

Blue:
Liquid Scatter
Green:
UV Fluorescence