



Reciprocating Internal Combustion Engines

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Summer Program on Combustion
Course Length: 9 hrs
(Wed., Thur., Fri., June 27-29)

Hour 1

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Short course outline:

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





Motivation

Society relies on IC engines for transportation, commerce and power generation: utility devices (e.g., pumps, mowers, chain-saws, portable generators, etc.), earth-moving equipment, tractors, propeller aircraft, ocean liners and ships, personal watercraft and motorcycles

ICEs power the 600 million passenger cars and other vehicles on our roads today. 250 million vehicles (cars, buses, and trucks) were registered in 2008 in US alone.

50 million cars were made world-wide in 2009, compared to 40 million in 2000.

China became the world's largest car market in 2011.

A third of all cars are produced in the European Union, 50% are powered diesels.

→ IC engine research spans both gasoline and diesel powerplants.

Fuel Consumption

70% of the roughly 86 million barrels of crude oil consumed daily world-wide is used in IC engines for transportation.

10 million barrels of oil are used per day in the US in cars and light-duty trucks

4 million barrels per day are used in heavy-duty diesel engines,

- total oil usage of 2.5 gallons per day per person.

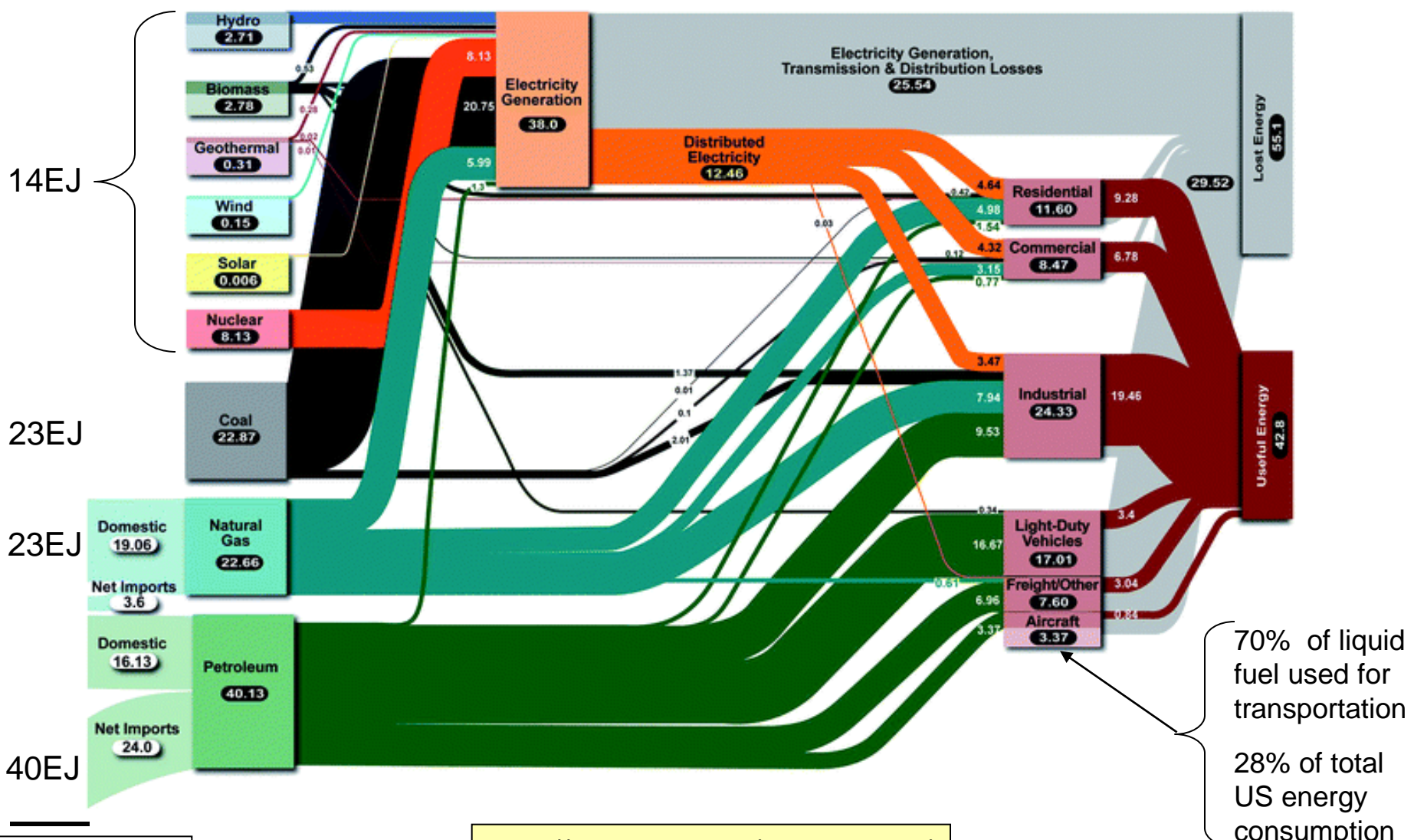
Of this, 62% is imported (at \$80/barrel - costs US economy \$1 billion/day).





US Energy Flow Chart

World energy use = $500 \times 10^{18} \text{ J}$



<http://www.eia.gov/totalenergy/>

70% of liquid fuel used for transportation
28% of total US energy consumption

$100 \times 10^{18} \text{ J}$



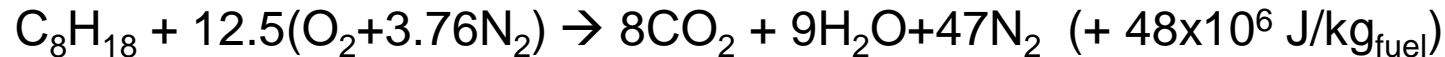
Fuel consumption - CO₂ Emissions

World oil use: 86 million bbl/day = 3.6 billion gal/day (~0.6 gal/person/day)

Why do we use fossil fuels (86% of US energy supply)?

Large amount of energy is tied up in chemical bonds.

Consider stoichiometric balance for gasoline (Octane) in air:



Kinetic energy of 1,000 kg automobile traveling at 60 mph (27 m/s)
 = $1/2 \cdot 1,000 \cdot 27^2$ (m² kg/s² = Nm) $\sim 0.46 \times 10^6$ J
 = energy in 10g gasoline $\sim 1/3$ oz (teaspoon)

Assume:

1 billion vehicles/engines, each burns 2.5 gal/day (1 gal \sim 6.5lb \sim 3kg)

$$\rightarrow 7.5 \times 10^9 \text{ kg}_{\text{fuel}}/\text{day} \cdot 48 \times 10^6 \text{ J/kg} = 360 \times 10^{18} \text{ J/yr}$$

1 kg gasoline makes $8 \cdot 44/114 = 3.1$ kg CO₂

$$\sim 365 \cdot 7.5 \times 10^9 \text{ kg}_{\text{fuel}}/\text{yr} \sim 8,486 \times 10^9 \text{ kg-CO}_2/\text{year} \sim 8.5 \times 10^9 \text{ tonne-CO}_2/\text{year}$$

(Humans exhale \sim 1 kg-CO₂/day \sim 2×10^9 tonnes-CO₂/yr)

Total mass of air in the earth's atmosphere $\sim 5 \times 10^{18}$ kg

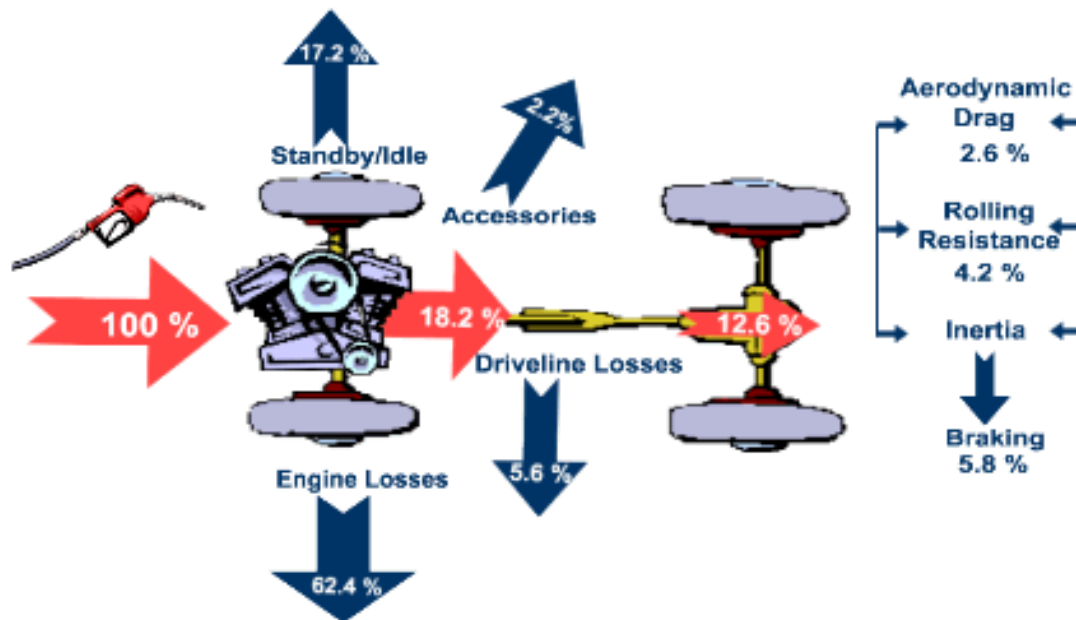
So, CO₂ mass from engines/year added to earth's atmosphere

$$8.5 \times 10^{12} / 5 \times 10^{18} \sim 1.7 \text{ ppm}$$





Where does the energy go?



1%

(Prof. John Heywood, MIT)

Modern gasoline IC engine vehicle converts about 16% of the chemical energy in gasoline to useful work.

The average light-duty vehicle weighs 4,100 lbs.

The average occupancy of a light-duty vehicle is 1.6 persons.

If the average occupant weighs 160 lbs,
 $0.16 \times ((1.6 \times 160) / 4100) = 0.01$

Engine Losses – 62.4%

In gasoline-powered vehicles, over 62% of the fuel's energy is lost in the internal combustion engine (ICE). ICE engines are very inefficient at converting the fuel's chemical energy to mechanical energy, losing energy to engine friction, pumping air into and out of the engine, and wasted heat.

Advanced engine technologies such as variable valve timing and lift, turbocharging, direct fuel injection, and cylinder deactivation can be used to reduce these losses.

In addition, diesels are about 30-35% more efficient than gasoline engines.



Pollutant Emissions

37 billion tons of CO₂ (6 tons each for each person in the world) from fossil fuels/yr, plus other emissions, including nitric oxides (NO_x) and particulates (soot).

CO₂ contributes to Green House Gases (GHG), implicated in climate change

- drastic reductions in fuel usage required to make appreciable changes in GHG

CO₂ emissions linked to fuel efficiency:

- automotive diesel engine is 20 to 40% more efficient than SI engine.

But, diesels have higher NO_x and soot.

- serious environmental and health implications,
- governments are imposing stringent vehicle emissions regulations.
- diesel manufacturers use Selective Catalytic Reduction (SCR) after-treatment for NO_x reduction: requires reducing agent (urea - carbamide) at rate (and cost) of about 1% of fuel flow rate for every 1 g/kWh of NO_x reduction.

Soot controlled with Diesel Particulate Filters (DPF),

- requires periodic regeneration by richening fuel-air mixture to increase exhaust temperature to burn off the accumulated soot
- imposes about 3% additional fuel penalty.

Need for emissions control removes some of advantages of the diesel engine





New directions

New technologies urgently needed to improve efficiency of gasoline and diesels. Engines need to be optimized to balance emissions, fuel cost, and market competitiveness.

Advanced CFD models and optimization methods increasingly used by the industry.

- made possible by dramatic increases in computer speeds ($\times 10^4$ in last 15 years)
- significantly reduces requirements for expensive experimental testing

Development of predictive models for engine physical processes has been an additional enabling factor for engine design

- CFD tools are mature enough to guide the development of more efficient and cleaner internal combustion engines.

New low temperature combustion (LTC) concepts, such as:

Homogeneous Charge Compression Ignition (HCCI),
Premixed Charge Compression Ignition (PCCI) and
Reactivity Controlled Compression Ignition (RCCI)

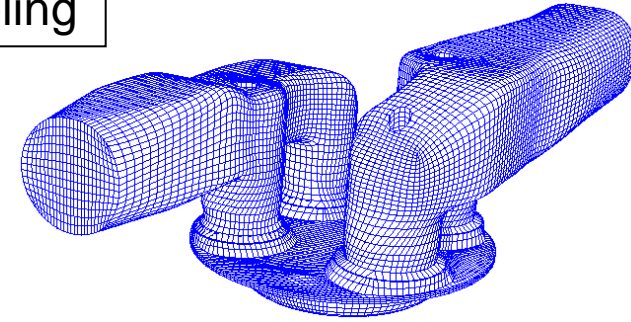
offer promise of dramatically improved engine efficiencies

- can be explored/optimized with CFD tools.



Brief history of engine CFD

Arab oil crisis ~ 1973: US DOE



- Open source codes
 - Los Alamos National Lab, Princeton Univ., UW-ERC
 - 1970's – RICE → REC → APACHE → CONCHAS
 - 1980's – CONCHAS-SPRAY → KIVA family
 - 1985 – KIVA ;1989 – KIVA-II; 1993 – KIVA-3;
 - 1997 – KIVA-3V; 1999 – KIVA-3V Release 2; 2006 - KIVA-4
 - 2004 – OpenFOAM (2011 SGI)
- Commercial codes
 - 1980's Imperial College & others
 - Computational Dynamics, Ltd. → commercialize: STAR-CD
 - 1990's—other commercial codes: AVL FIRE, Ricardo VECTIS
 - 2005– FLUENT (with moving piston and in-cylinder models)
 - 2010 – CONVERGE (CSI), FORTE (Reaction Design).....
- 22nd Annual IMEM-User group meeting: Cray/UW-ERC 2012
- ILASS, SAE Congress Multidimensional Modeling Session



Goal of IC Engine:

Convert energy contained in a fuel into useful work, as efficiently and cost-effectively as possible.

Identify energy conversion thermodynamics that governs reciprocating engines.

Describe hardware and operating cycles used in practical IC engines.

Discuss approaches used in developing combustion and fuel/air handling systems.

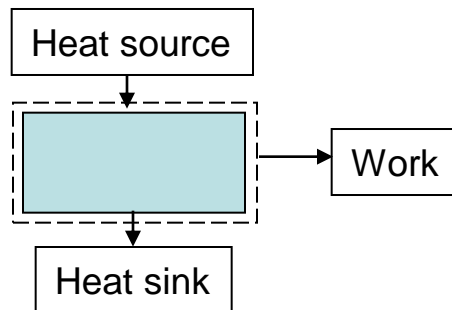
Internal Combustion Engine development

Requires control to:

introduce fuel and oxygen, initiate and control combustion, exhaust products

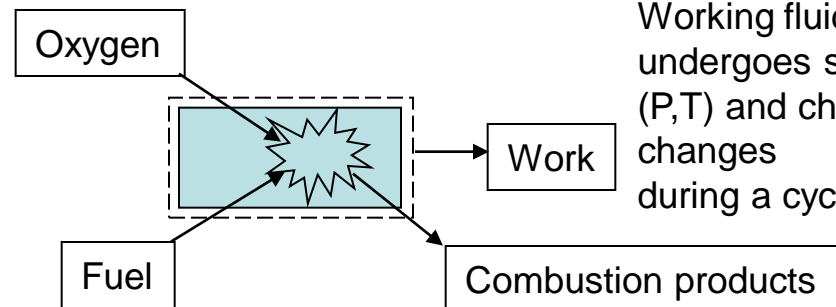
Heat (EC) engine (Carnot cycle)

Energy release occurs external to the system. Working fluid undergoes reversible state changes (P,T) during a cycle (e.g., Rankine cycle)



IC engine (Not constrained by Carnot cycle)

Energy release occurs internal to the system. Working fluid undergoes state (P,T) and chemical changes during a cycle





Components of piston engine

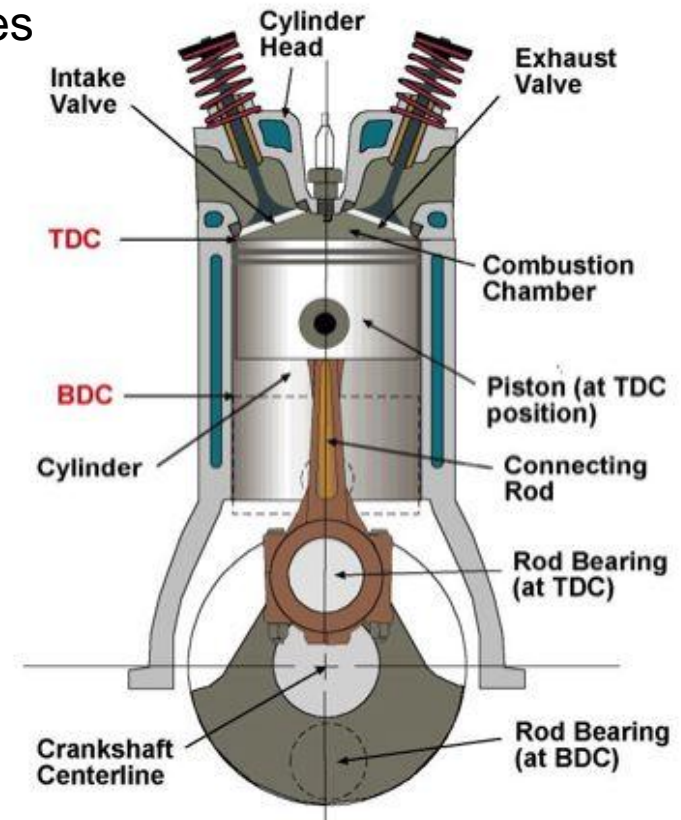
Piston moves between Top Dead Center (TDC) and Bottom Dead Center (BDC).

Compression Ratio = CR = ratio of BDC/TDC volumes

Stroke = S = travel distance from BDC to TDC

Bore = B = cylinder diameter

D = Displacement = (BDC-TDC) volume.# cylinders
 $= \pi B^2 S/4 \cdot \# \text{ cylinders}$



Basic Equations

$$P = W.N = T.N$$

$$P \text{ [kW]} = T \text{ [Nm]}.N \text{ [rpm]}.1.047 \text{ E-04}$$

$$\text{BMEP} = P.(\text{rev/cyc}) / D.N$$

$$\text{BMEP [kPa]} = P \text{ [kW]}.(2 \text{ for 4-stroke}) \text{ E03} \\ / D \text{ [l]}. N \text{ [rev/s]}$$

$$\text{BSFC} = \dot{m}_{\text{fuel}} / P$$

$$\text{BSFC} = \dot{m}_{\text{fuel}} \text{ [g/hr]} / P \text{ [kW]}$$

**Brake = gross indicated + pumping + friction
 = net indicated + friction**

P = (Brake) Power [kW]
 T = (Brake) Torque [Nm] = Work = W
 BMEP = Brake mean effective pressure
 \dot{m}_{fuel} = fuel mass flow rate [g/hr]
 BSFC = Brake specific fuel consumption





Engine Power

Heywood, 1988

Indicated power of IC engine at a given speed is proportional to the air mass flow rate, \dot{m}_{air}

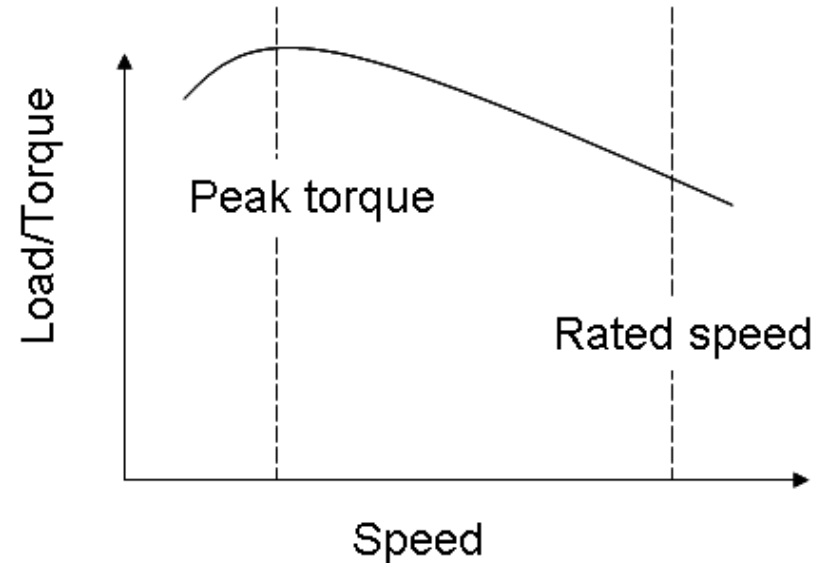
$$P = \eta_f \cdot \dot{m}_{air} N \cdot LHV \cdot (F/A) / n_r$$

η_f = fuel conversion efficiency

LHV = fuel lower heating value

F/A fuel-air ratio m_f/m_{air}

n_r = number of power strokes / crank rotation
= 2 for 4-stroke



Efficiency estimates:

SI: $270 < bsfc < 450$ g/kW-hr

Diesel: $200 < bsfc < 359$ g/kW-hr

$$\eta_f = 1/46 \text{ MJ/kg} / 200 \text{ g/kW-hr} = 40\text{-}50\%$$

→ 500 MW GE/Siemens combined cycle gas turbine natural gas power plant ~ 60% efficient





4-stroke (Otto) cycle

1. Intake:

piston moves from TDC to BDC with the intake valve open, drawing in fresh reactants

2. Compression:

valves are closed and piston moves from BDC to TDC, Combustion is initiated near TDC

3. Expansion:

high pressure forces piston from TDC to BDC, transferring work to crankshaft

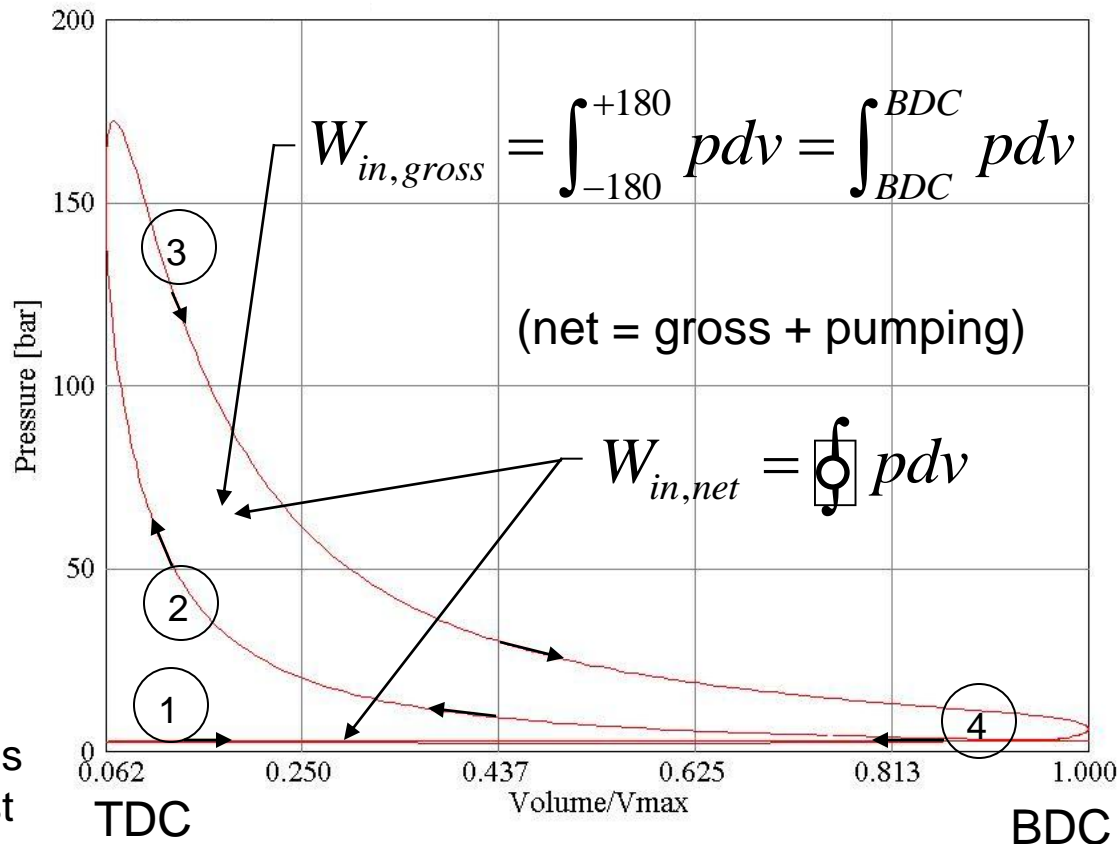
4. Exhaust:

exhaust valve opens and piston moves from BDC to TDC pushing out exhaust

1,4 Pumping loop – An additional rotation of the crankshaft used to:

- exhaust combustion products
- induct fresh charge

“Suck, squeeze, bang, blow”



Four-stroke diesel pressure-volume diagram at full load





Combustion process - initiated near end of compression stroke.

Instantaneous combustion has high theoretical efficiency, but is impractical due to need to manage peak pressures and due to high heat transfer.

Spark-ignition engine:

mixture of air (oxygen carrier) and fuel enters chamber during intake process. Mixture is compressed - combustion initiated using a high-energy electrical spark.

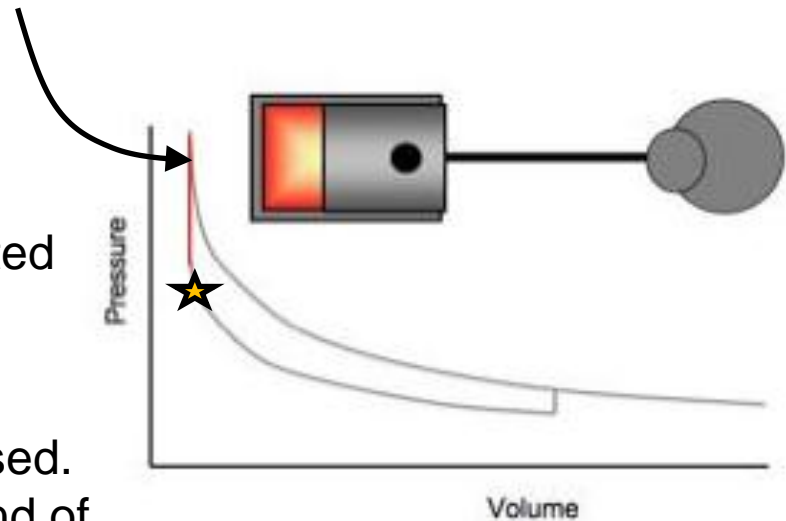
Compression-ignition (Diesel) engine:

air alone is drawn into chamber, compressed. Fuel injected directly into chamber near end of compression process.

(Fuel used in compression-ignition engine must easily spontaneously ignite when exposed to high temperature and pressure compressed air.)

Diesel is often portrayed as having a slower combustion process (constant pressure instead of constant volume)

Goal of rapid combustion near TDC for maximum efficiency is true for both Diesel and spark-ignition engines.

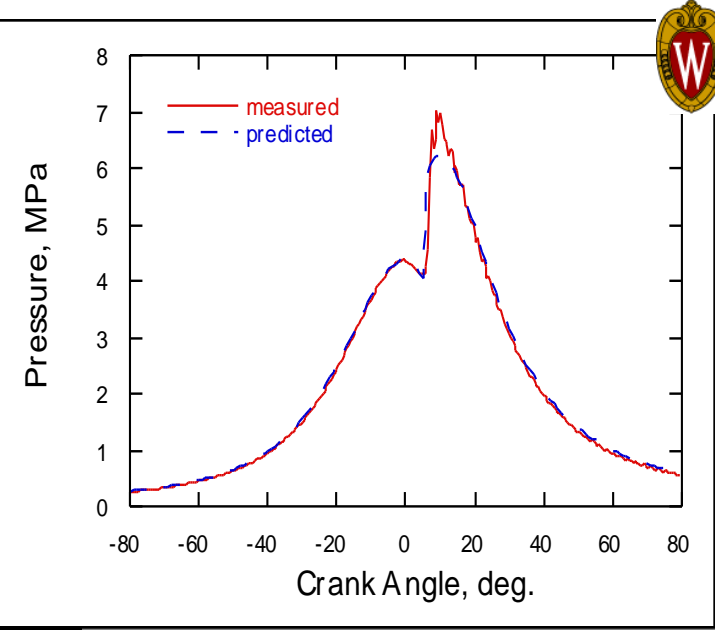
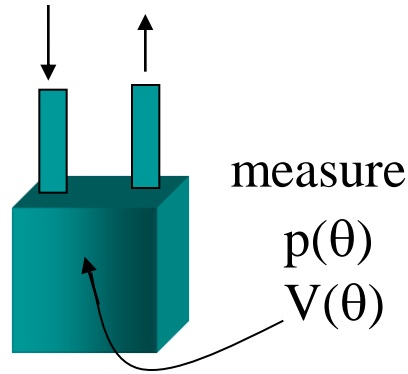


f. Combustion process

Zero-Dimensional Models

Heywood, 1988

Single zone model



$$mc_v \frac{dT}{dt} + p \frac{dV}{dt} + \sum_j \dot{m}_j h_j = q_{Comb} - q_{Loss} = q_{Net}$$

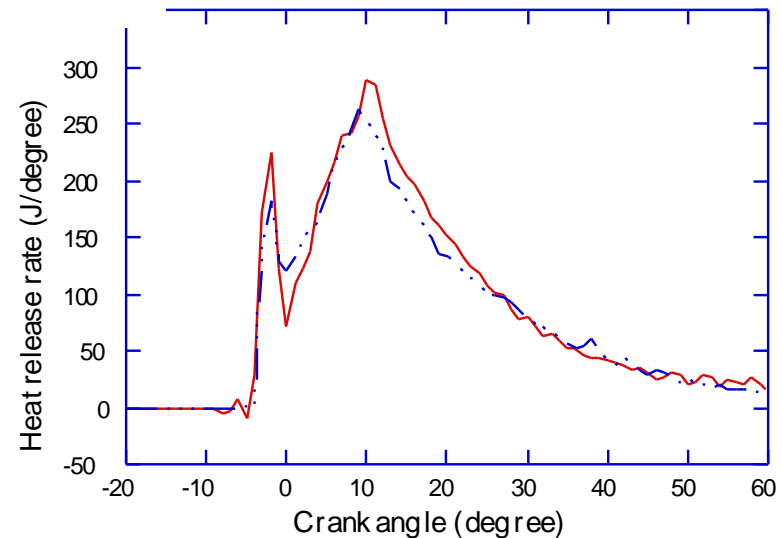
Use the ideal gas equation to relate p & V to T

$$q_{Net} = p \frac{dV}{dt} + \frac{1}{\gamma - 1} \frac{dpV}{dt}$$

where

$$q_{Loss} = hA(T - T_{wall})$$

Assume h and T_{wall}





3-Dimensional Models

Solve conservation equations on (moving) numerical mesh

Mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \dot{\rho}^s$$

Spray source terms

Species

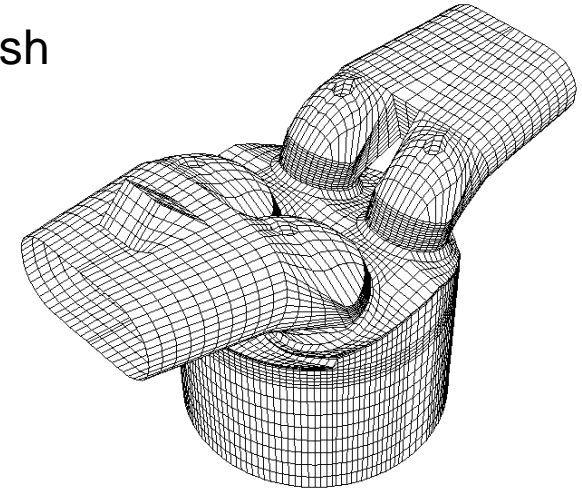
$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}) = \nabla \cdot \left[\rho D \nabla \left(\frac{\rho_m}{\rho} \right) \right] + \dot{\rho}_m^c + \dot{\rho}_m^s$$

Momentum

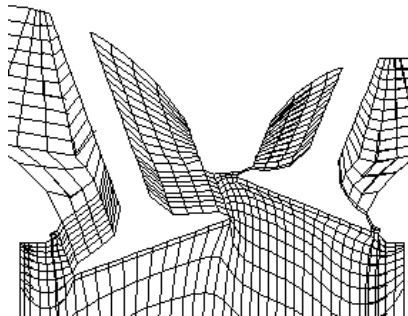
$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \rho \mathbf{g} + \mathbf{F}^s - \nabla p + \nabla \cdot \bar{\sigma}$$

Energy

$$\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = -\nabla \cdot \mathbf{J} + \dot{Q}^c + \dot{Q}^s - p \nabla \cdot \mathbf{u} + \bar{\sigma} : \nabla \mathbf{u}$$



combustion source terms

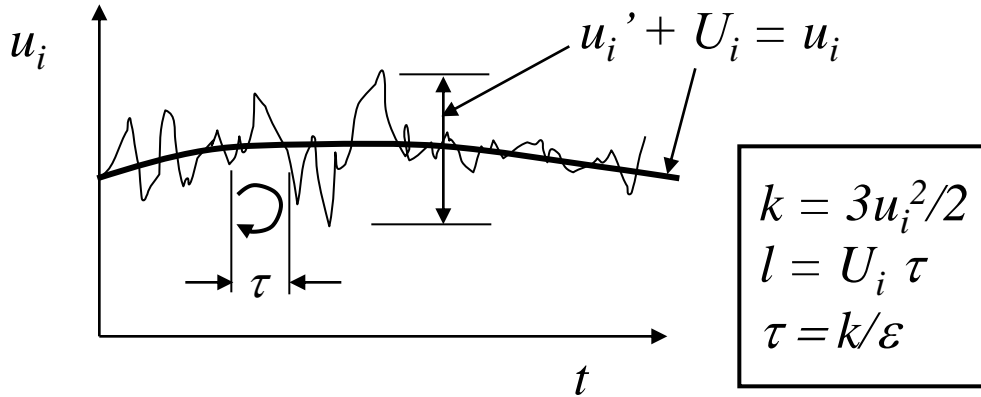


Amsden, 1989





Turbulence models (RANS - RNG k-ε)



$$\rho \frac{Dk}{Dt} = P - \rho\epsilon + \text{Diffusion}$$

$$\rho \frac{D\epsilon}{Dt} = C_1 \frac{P\epsilon}{k} - C_2 \rho \frac{\epsilon^2}{k} + \text{Diffusion} - R + C_3 \rho \epsilon (\nabla \cdot \mathbf{u})$$

$$R = \frac{C_\mu \rho \eta^3 (1 - \eta/\eta_0) \epsilon^2}{1 + \beta \eta^3 k}$$

$$\eta = \frac{k}{\epsilon} \sqrt{2S_{ij}S_{ij}} \sim \text{turbulent/mean flow time scale}$$

Production

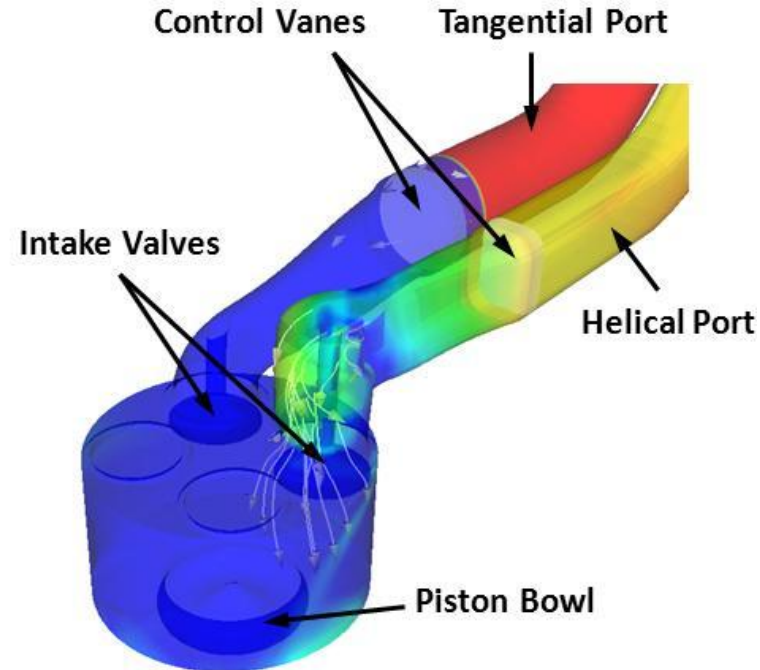
$$P = -\rho u_i u_j S_{ij}$$

Mean flow strain rate

$$S_{ij} = \frac{1}{2} (\partial u_i / \partial x_j + \partial u_j / \partial x_i)$$

Reynolds stresses

$$u_i u_j - \frac{2}{3} k \delta_{ij} = -2v_t (S_{ij} - \frac{1}{3} (\nabla \cdot \mathbf{u}) \delta_{ij})$$



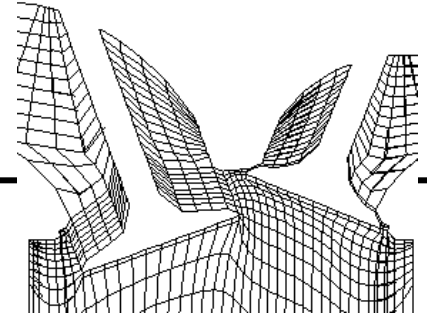
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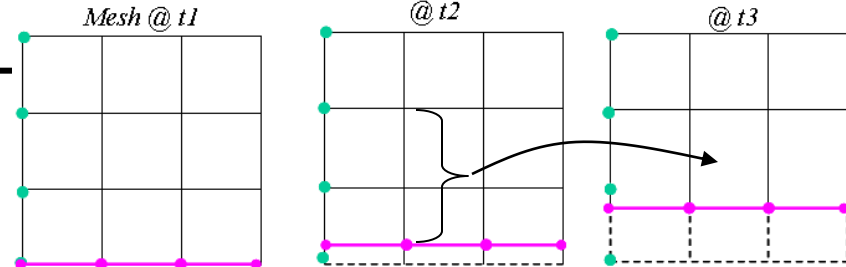


KIVA-3V CFD code: Flow solver

Main program and approximately 50 subroutines



<p>Initialization</p>	<p>Read input data Calculate gas viscosity Initialize time step, piston velocity</p>	
<p>Phase A</p> <div style="border: 1px solid red; padding: 2px; display: inline-block; color: red; font-weight: bold;">Big Iteration</div>	<p>Spray modeling (injection, drop breakup, collision, evaporation...) Combustion chemistry Emission modeling Mass and energy contribution due to spray and combustion</p>	
<p>Phase B</p>	<p>Fluid phase calculation Mass, momentum, velocity, temperature, pressure, turbulence properties (Implicit solver, iterations) Update droplet velocity</p>	
<p>Phase C</p>	<p>Snapping/Rezoning grids Remapping fluid properties to new grids Update cell properties</p>	<div style="border: 1px solid black; padding: 5px; text-align: center;"> <p>“Snapper” add/delete grid cells</p> </div>



Amsden, 1997



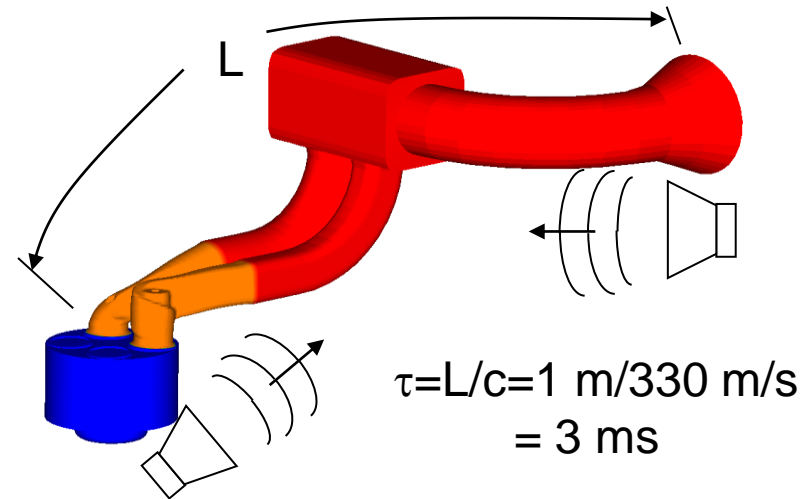
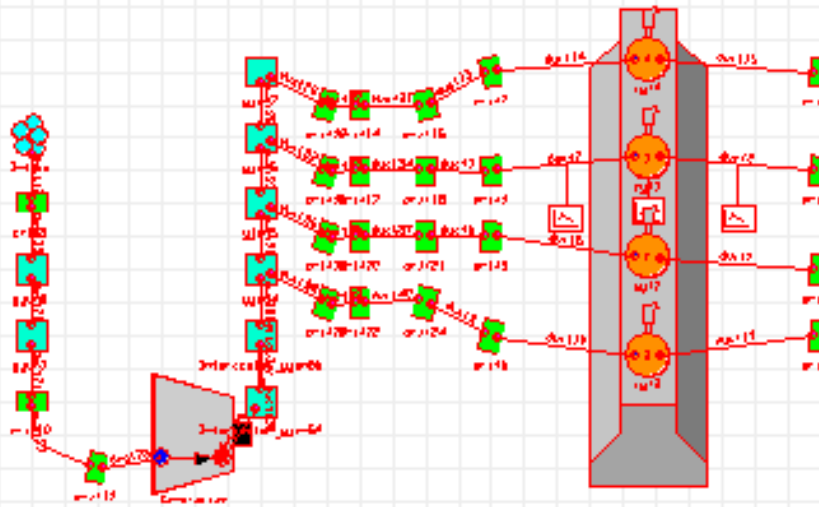


1-D Models

1-D codes (e.g., GT-Power, AVL-Boost, Ricardo WAVE) predict wave action in manifolds
 At high engine speed valve overlap can improve engine breathing
 → inertia of flowing gases can cause inflow even during compression stroke.

Variable Valve Actuation (VVA) technologies, control valve timing to change effective compression ratio (early or late intake valve closure), or exhaust gas re-induction (re-breathing) to control in-cylinder temperatures.

Residual gas left from the previous cycle affects engine combustion processes through its influence on charge mass, temperature and dilution.



1 ca deg = 0.1 ms @ 1800 rev/min

AVL Boost, Ricardo WAVE, GT-Power





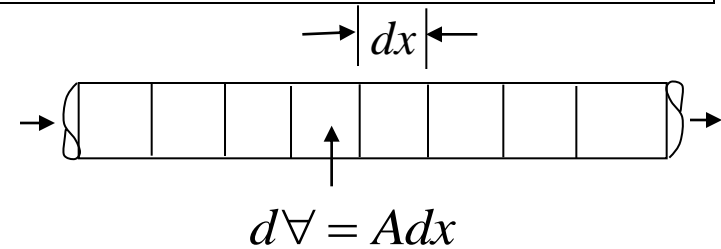
1D Models

Mass conservation:

$$g = 1 \quad dMg / dt)_{System} = 0$$

Reynolds Transport Equation

$$\left. \frac{dMg}{dt} \right)_{system} = \frac{d}{dt} \int_{system} \rho g d\forall = \frac{d}{dt} \int_{cv} \rho g d\forall + \int_{cs} \rho g \mathbf{V}_{rel} \cdot \mathbf{n} dA$$



cv fixed Divergence theorem

$$0 = \int_{cv} \left\{ \frac{\partial(\rho A)}{\partial t} + \nabla \cdot (\rho A \mathbf{V}) \right\} dx$$

$$1. \quad \frac{\partial(\rho A)}{\partial t} + \frac{\partial(\rho AV)}{\partial x} = 0$$

Momentum conservation:

$$2. \quad \frac{\partial V}{\partial t} + V \frac{\partial V}{\partial x} + \frac{1}{\rho} \frac{\partial P}{\partial x} + 2fV^2 / D = 0$$

Energy conservation:

$$3. \quad \frac{\partial e}{\partial t} + V \frac{\partial e}{\partial x} = \dot{q} + 2fV^3 / D - \frac{P}{\rho A} \frac{\partial(VA)}{\partial x}$$

Supplementary:

$$\left. \begin{aligned} 4. \quad P &= \rho RT \\ 5. \quad e &= c_v T \end{aligned} \right\} \text{State}$$

$$f = \tau_w / \rho V^2 / 2$$

$$\dot{Q} = \dot{q} \rho A dx$$

5 unknowns U: $\rho, V, e, P,$ and T

5 equations for variation of flow variables in space and time

Need to evaluate derivatives $\partial / \partial x, \partial / \partial t$

Anderson, 1990





Gas Exchange Process

Gasoline engine intake system:

air filter, carburetor and throttle plate or port fuel injector, intake manifold, intake port, intake valves.

Supercharging – increases inducted air mass (in both gasoline and diesel engines).

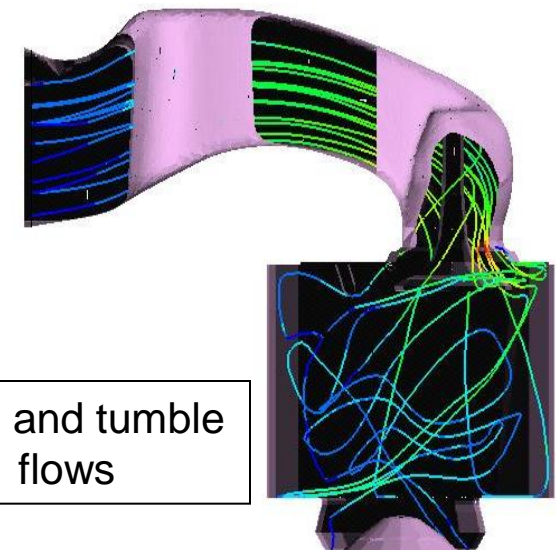
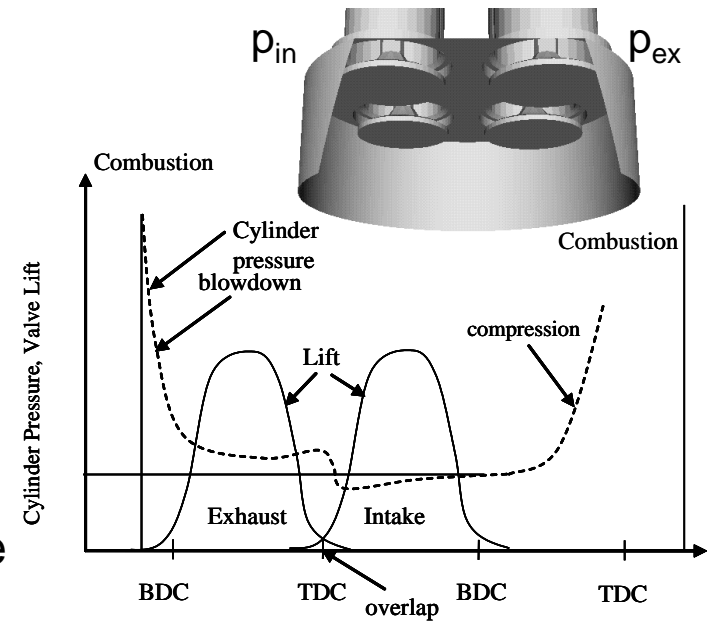
Intake and exhaust manifold designed to maximize cylinder filling and scavenging.

Intake system pressure drops (losses) occur due to quasi-steady effects (e.g., flow resistance), and unsteady effects (e.g., wave action in runners).

Engine breathing affected by intake/exhaust valve lifts and open areas (most of the losses).

Valve overlap can cause exhaust gases to flow back into intake system, or intake gases can enter the exhaust (depending on p_{in}/p_{ex})

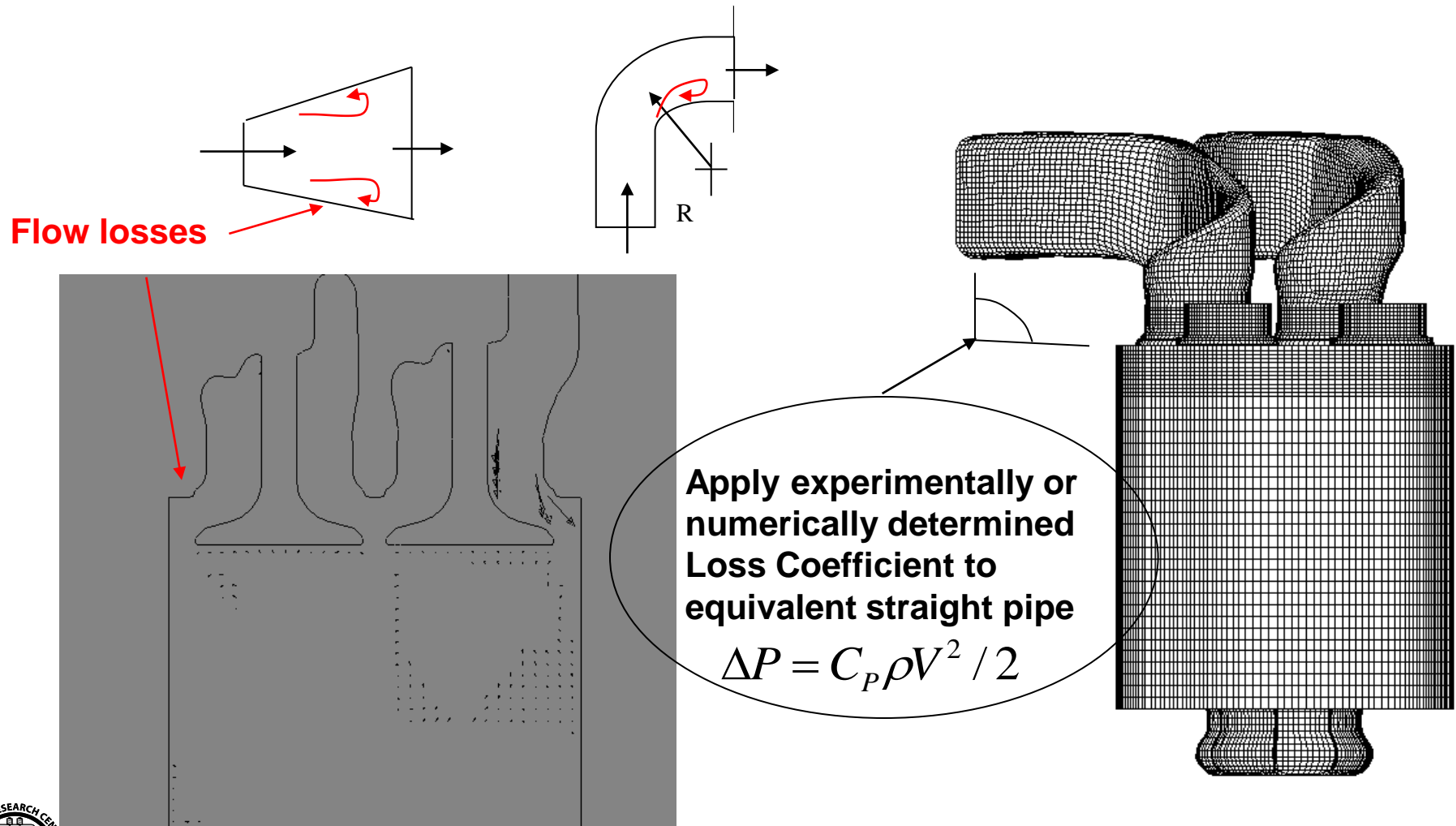
Intake also generates large scale flow structures that can be used to promote turbulent mixing



Swirl and tumble flows



In 1-D models friction factors used to account for losses at area change or bends by applying a friction factor to an “equivalent” length of straight pipe





WAVE Knowledge Center v5.2

Ricardo WAVE friction models

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ports where C_p should be set to 0.0 because wall friction is already included in the valve flow coefficients.

2.3.5 Duct Bend Losses

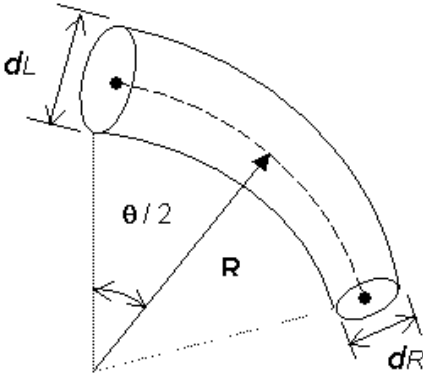
Pressure loss coefficients due to bends can usually be taken from handbook values. However, the handbook loss measurements must be adjusted to subtract friction losses due to bend length, which WAVE calculates separately. This is especially true for large-radius bends, which are long and thus can have a large friction loss¹.

Experience seems to indicate that bends in intake runners for engines require higher C_p values than those given by handbooks. This may be due to the highly pulsing nature of the flow. Tables of loss coefficients always give steady flow values. There are not many authoritative sources for losses in pulsing flow.

A distributed pressure loss can be imposed in a duct via the C_p parameter in the DUC:DUCT block where

$$C_p = \Delta p / \left(\frac{1}{2} \right) \rho v^2$$

To simplify the setup of a model, the C_p value for a curved duct can be calculated by specifying the bend angle in the DUC:BENDS block. The bend loss coefficient is calculated as follows:



First C_p is found: <http://www.ricardo.com/en-GB/What-we-do/Software/Products/WAVE/>

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CEFRC1 June 27, 2012



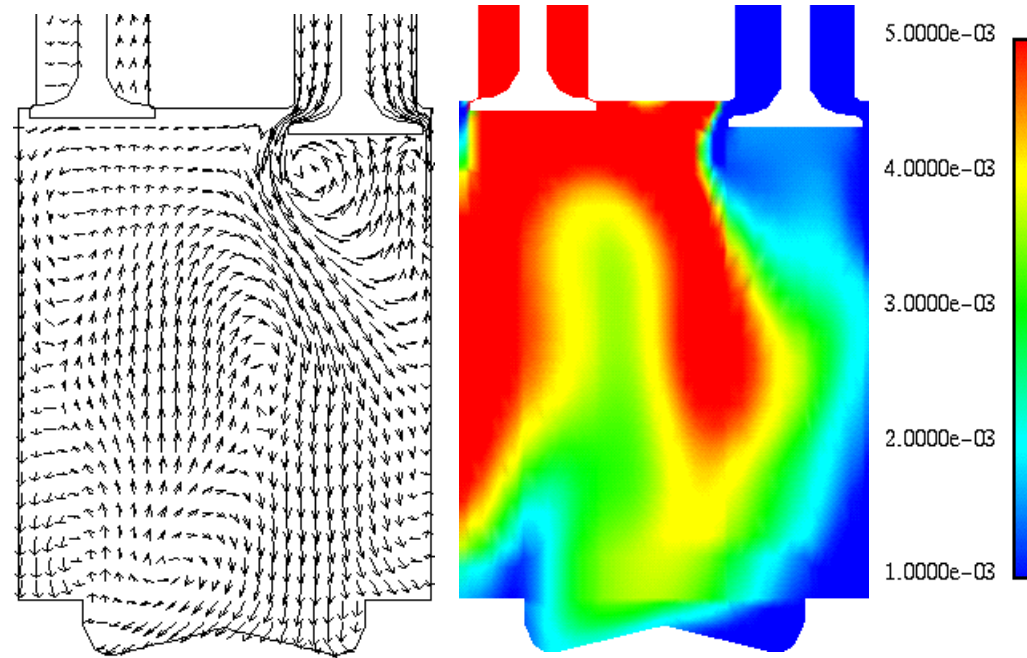
$$\eta_v = \frac{m_{air}}{\rho_{a,i} V_d} \cdot \text{Volumetric efficiency}$$

m_{air} is the mass of air trapped in the cylinder at intake valve closure (IVC),
 $\rho_{a,i}$ is the intake air density, and

V_d is the volume displaced by the piston.

Accurate descriptions of valve flow losses require consideration of multi-dimensional flow separation phenomena and their effect initial conditions at intake valve closure (IVC).

Highest mixing of incoming fresh charge and combustion products occurs when intake flow velocities are largest due to high flow turbulence (half-way through stroke).



CFD flow velocity and residual gas distribution during gas exchange in plane of valves (intake valves about to close 144 degrees ATDC - 1600 rev/min)



Hour 1: IC Engine Review, 0, 1 and 3-D modeling



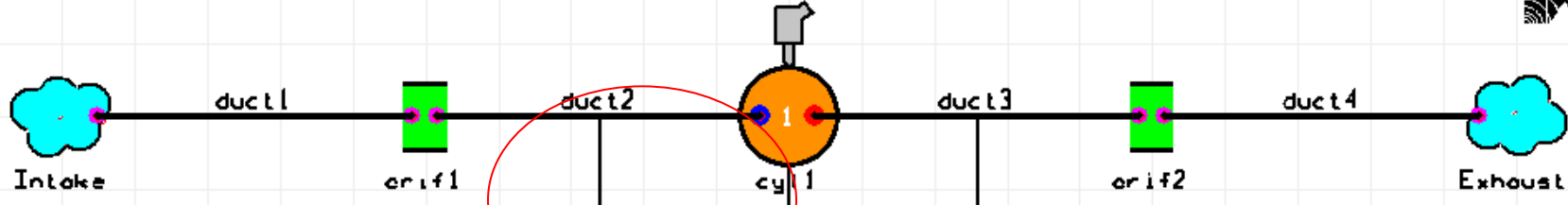
WaveBuild V5.2 Build 25: Tut_C11.wvm

File Edit Simulation Model Tools Run Help

Ricardo WAVE valve model

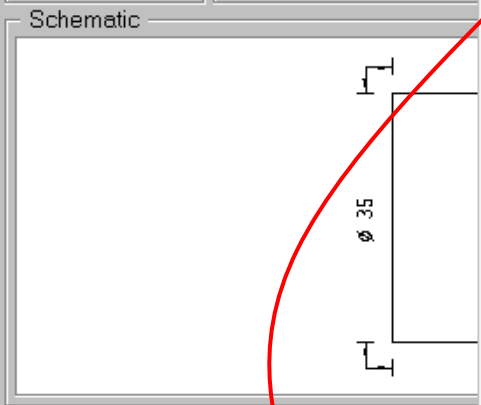


CI (tutorial) 1.4L 4-cyl HSDI at 4500



Case #1: Duct Panel

ID: duct2
Connectivity: LeftID: orif1



Dimensions Coefficients Initial Conditions

Coefficients

Friction: 0

Heat Transfer: 1.5

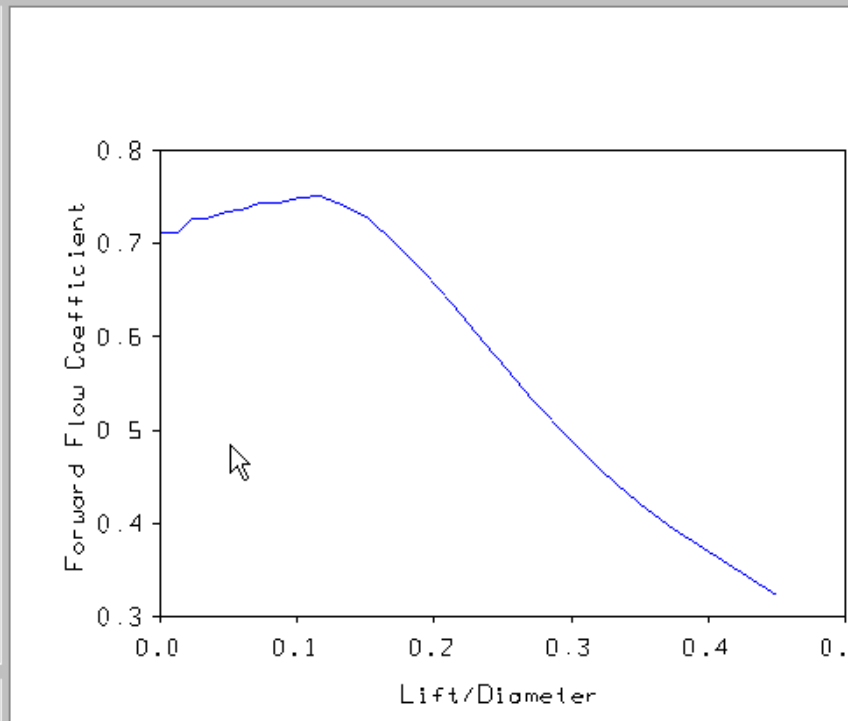
Pressure Loss: 0.0

Profile Editor

Flow Coefficient Profiles

	L/D	CDF	
1	0.0000	0.7116	0.
2	0.0130	0.7116	0.
3	0.0230	0.7279	0.
4	0.0330	0.7270	0.
5	0.0480	0.7344	0.
6	0.0580	0.7370	0.
7	0.0730	0.7433	0.
8	0.0860	0.7442	0.
9	0.1020	0.7501	0.
10	0.1160	0.7521	0.
11	0.1350	0.7407	0.
12	0.1520	0.7270	0.
13	0.1700	0.7029	0.
14	0.1920	0.6706	0.
15	0.2140	0.6343	0.
16	0.2370	0.5928	0.
17	0.2530	0.5642	0.

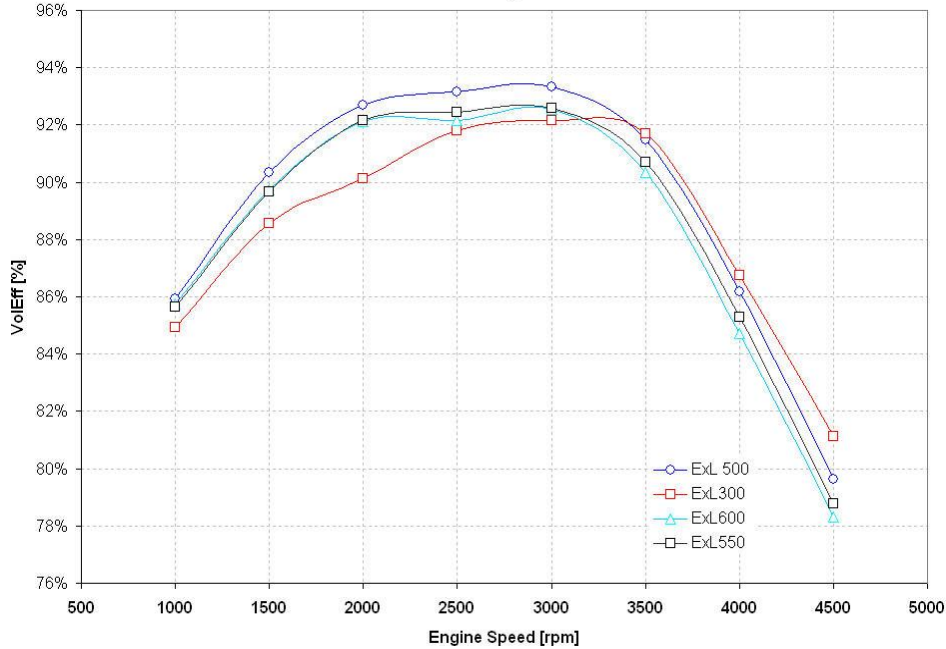
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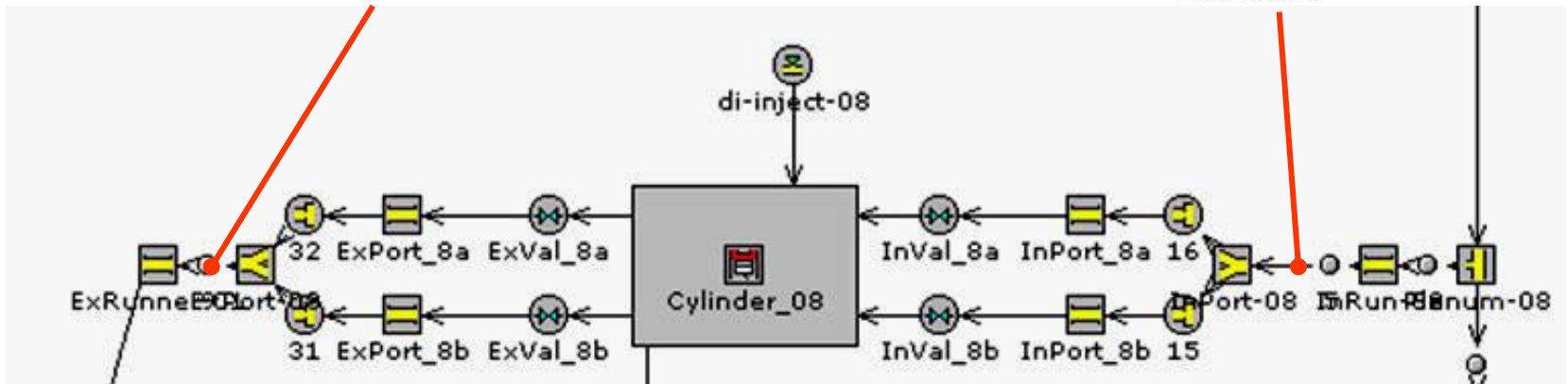
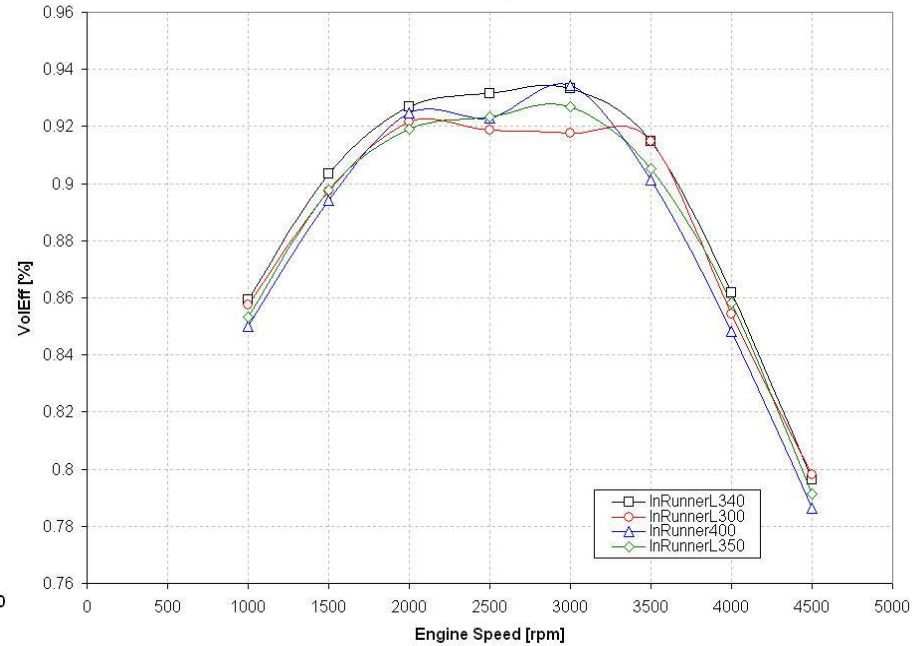


Model Optimization: Volumetric Efficiency

Exhaust Runner Length Effects: VoIEff



Intake Runner Length Effects: VoIEff



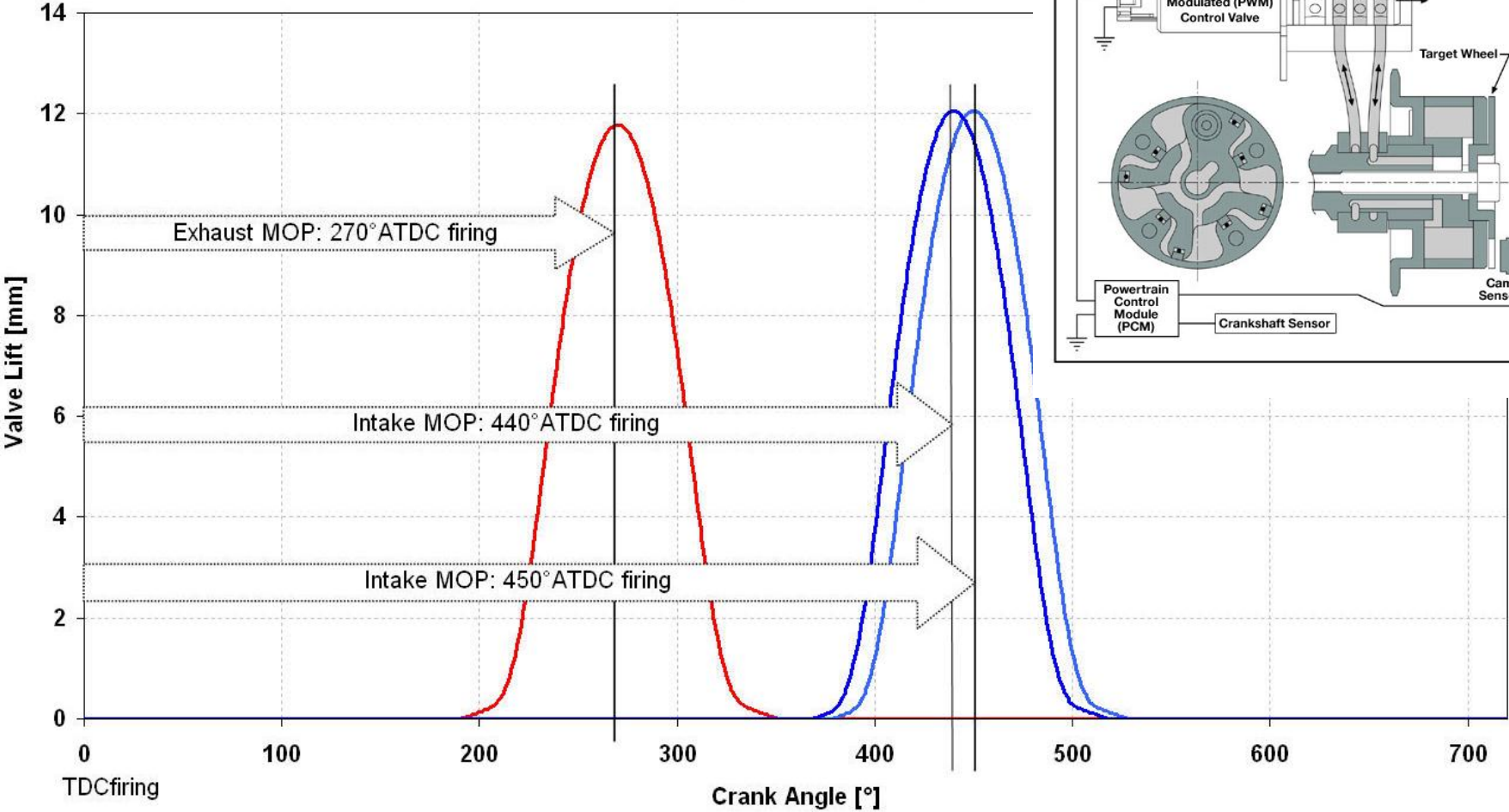
<http://www.gtisoft.com/>



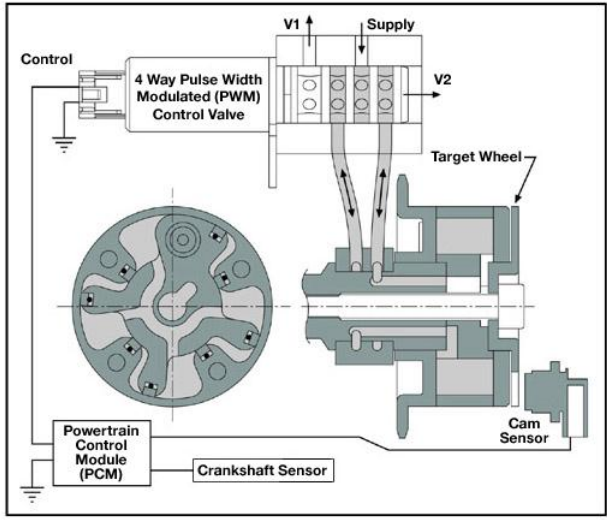


Optimization: Volumetric Efficiency

Variable Valve Timing for VolEff Optimizati



Delphi Cam Phaser



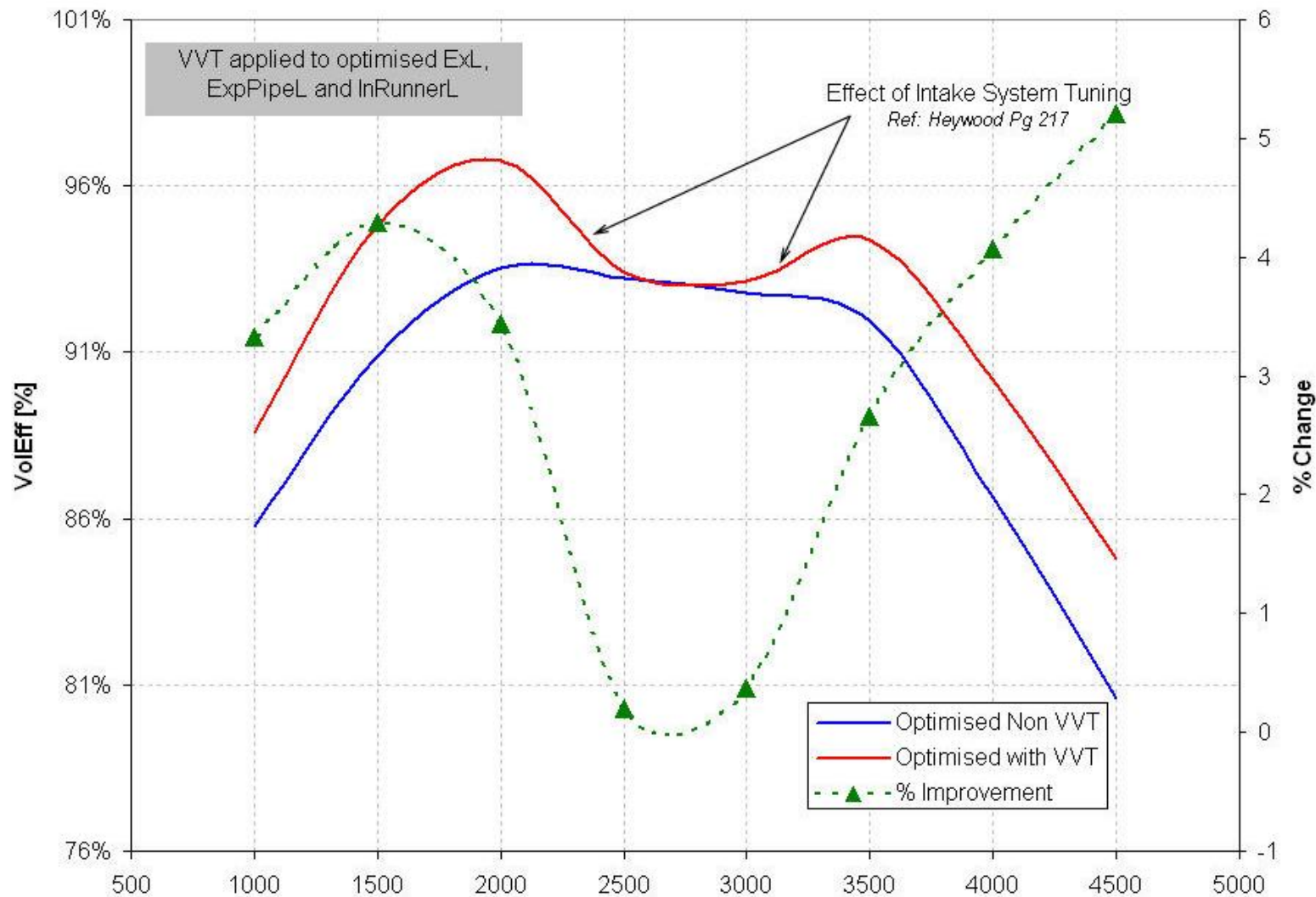
<http://delphi.com/manufacturers/auto/powertrain/gas/valvetrain/vcp/>





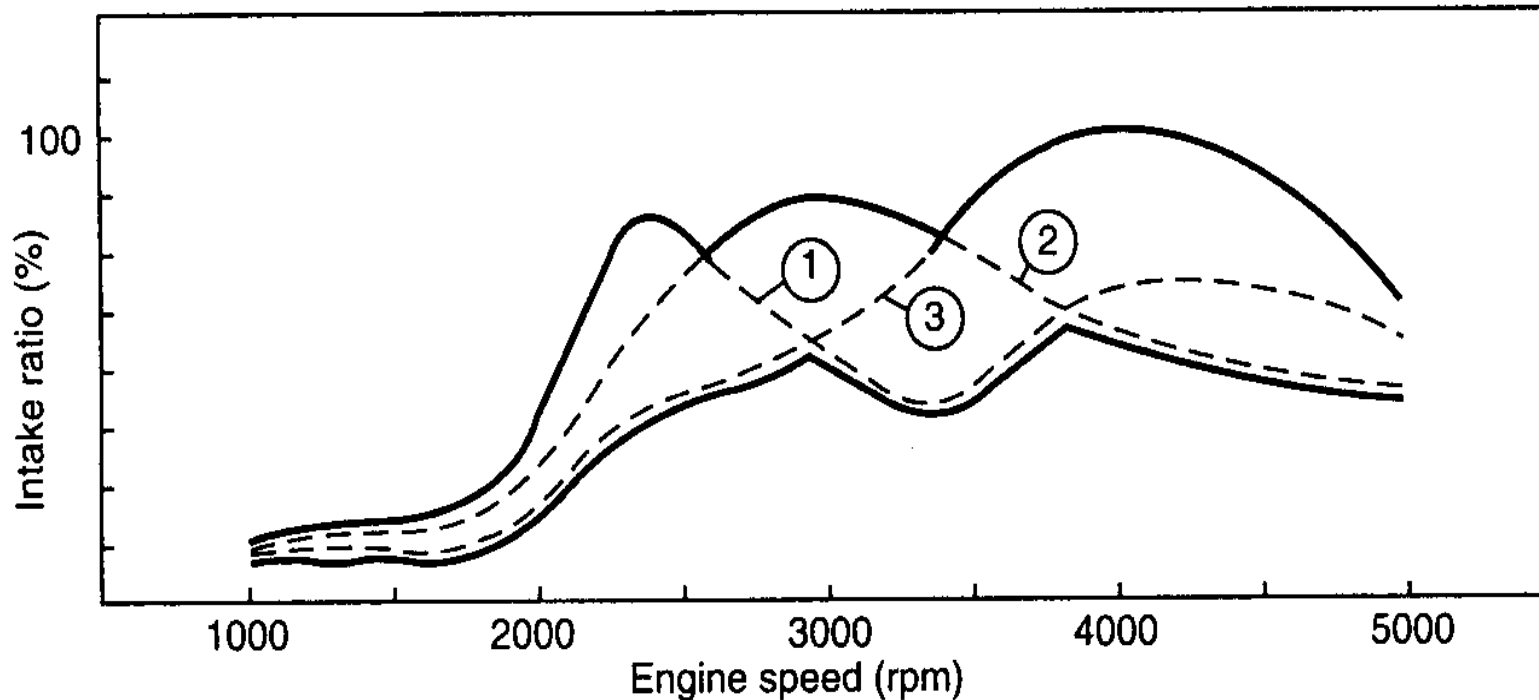
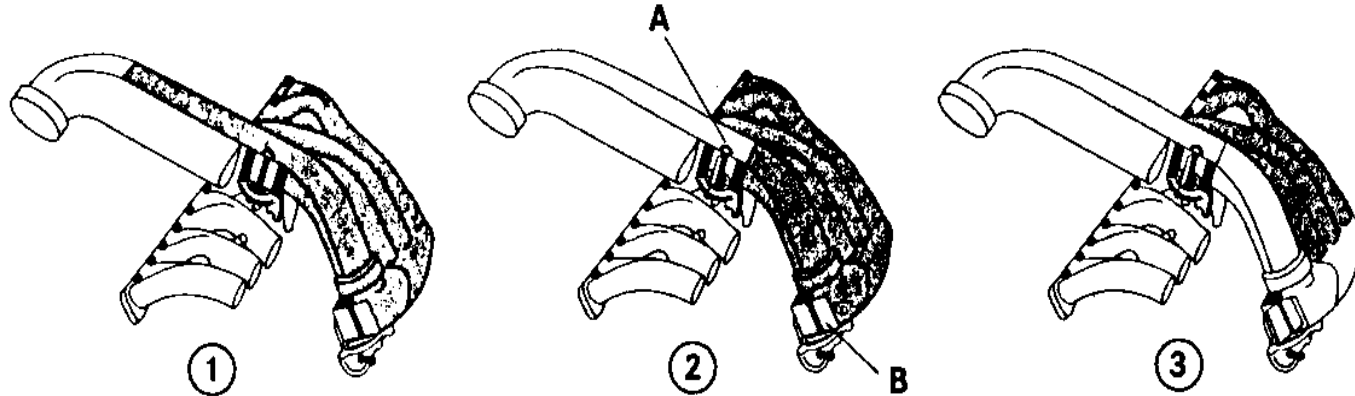
Optimization: Volumetric Efficiency

Optimised Voleff





Optimization: Volumetric Efficiency

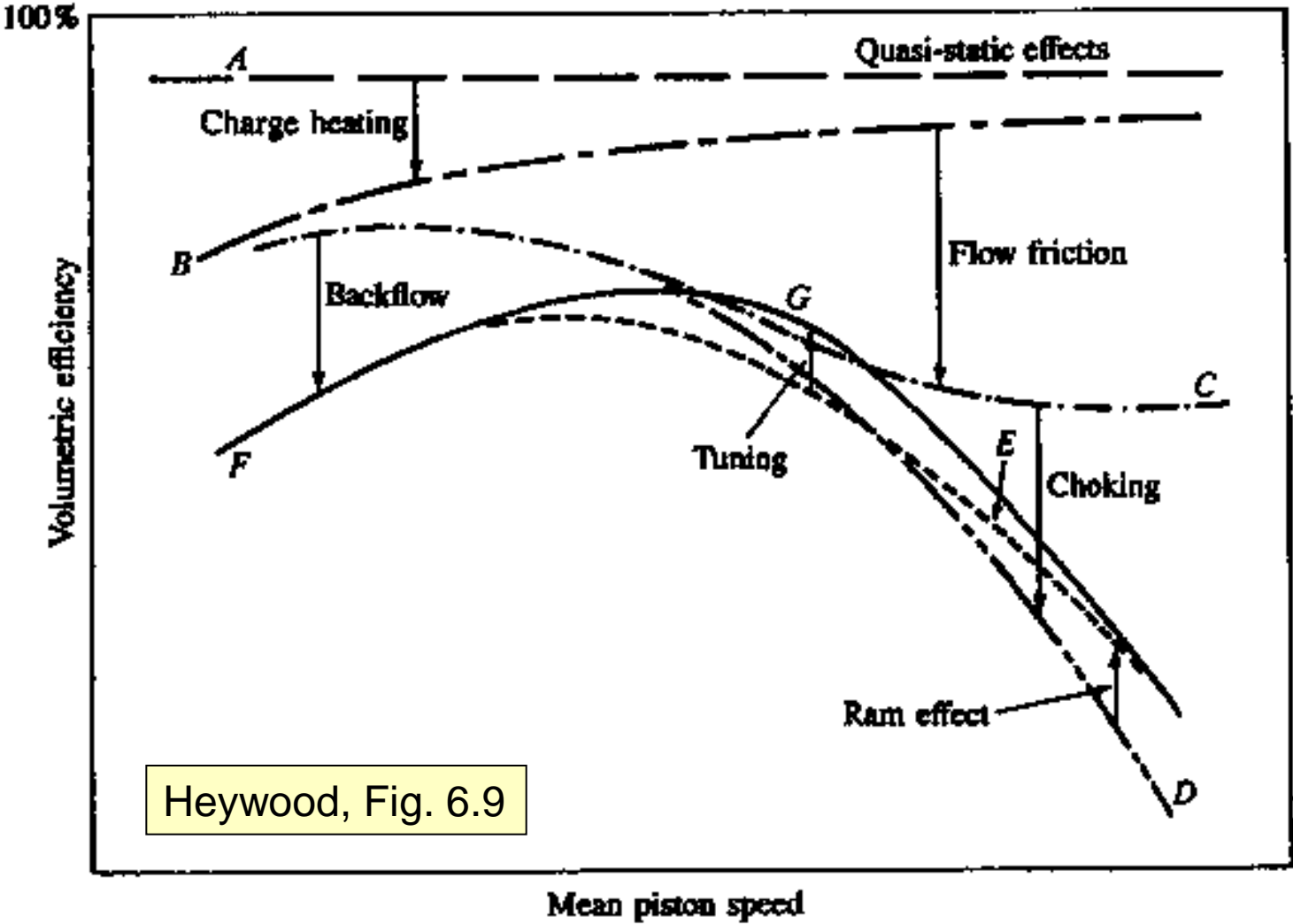


Mercedes-Benz three stage resonance intake system





Volumetric efficiency parameters (SI engine < CI engine)



Heywood, Fig. 6.9

A → B → C
 → D → E
 → F → G

Losses in Carburetor, Intake manifold heating (rho), Fuel vapor displaces air

MAP Pin~Pex in diesel

Lower CR - SI more residual

Diesel - more residual is air



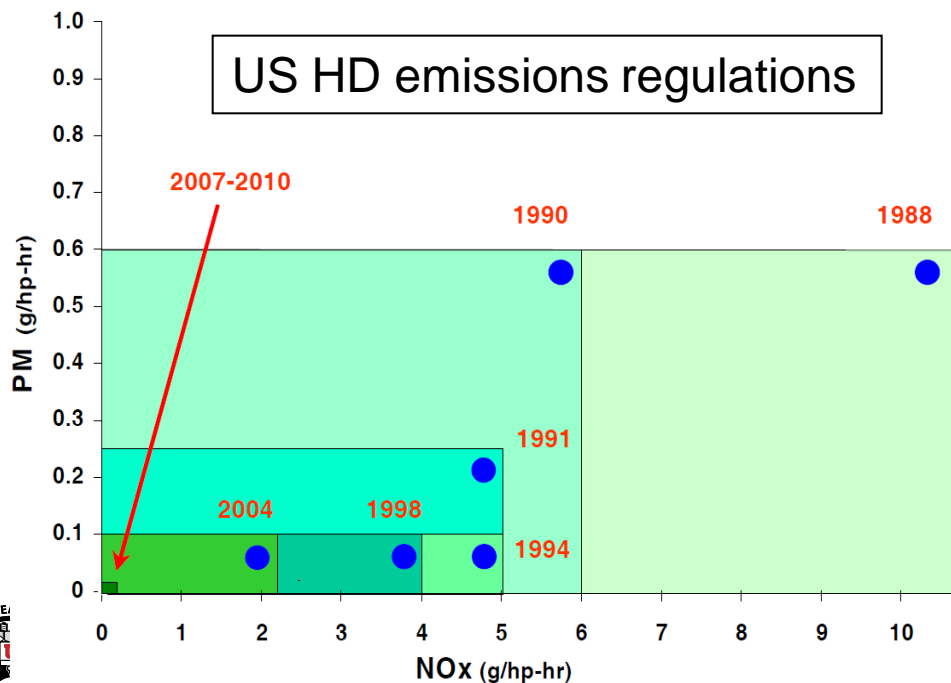
Summary

Transportation uses ~1/3 of the total energy use in the US

Internal combustion engines can be among the most efficient power plants known to man, but research is needed to improve them further

The industry faces significant challenges to meet emissions regulations, but great progress has been made in the last 20 years.

Modeling tools are available to help quantify engine performance and to provide directions for improved efficiency



Oil Consumption, 2010:

US	21.1%
Total Europe & Eurasia	22.9%
China	10.6%

Charmley, SAE 2004-01-2708