Simulation of a Boosted, Dual-Fueled *'Octane-on-Demand'* PFI/DI Engine for the Purpose of Knock Prediction

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in conjunction with

Ethanol Boosting Systems LLC (EBS)
Ford Motor Company
AVL North America

partially under auspices of

DOE Program: “Optimized E85 Engine Application”

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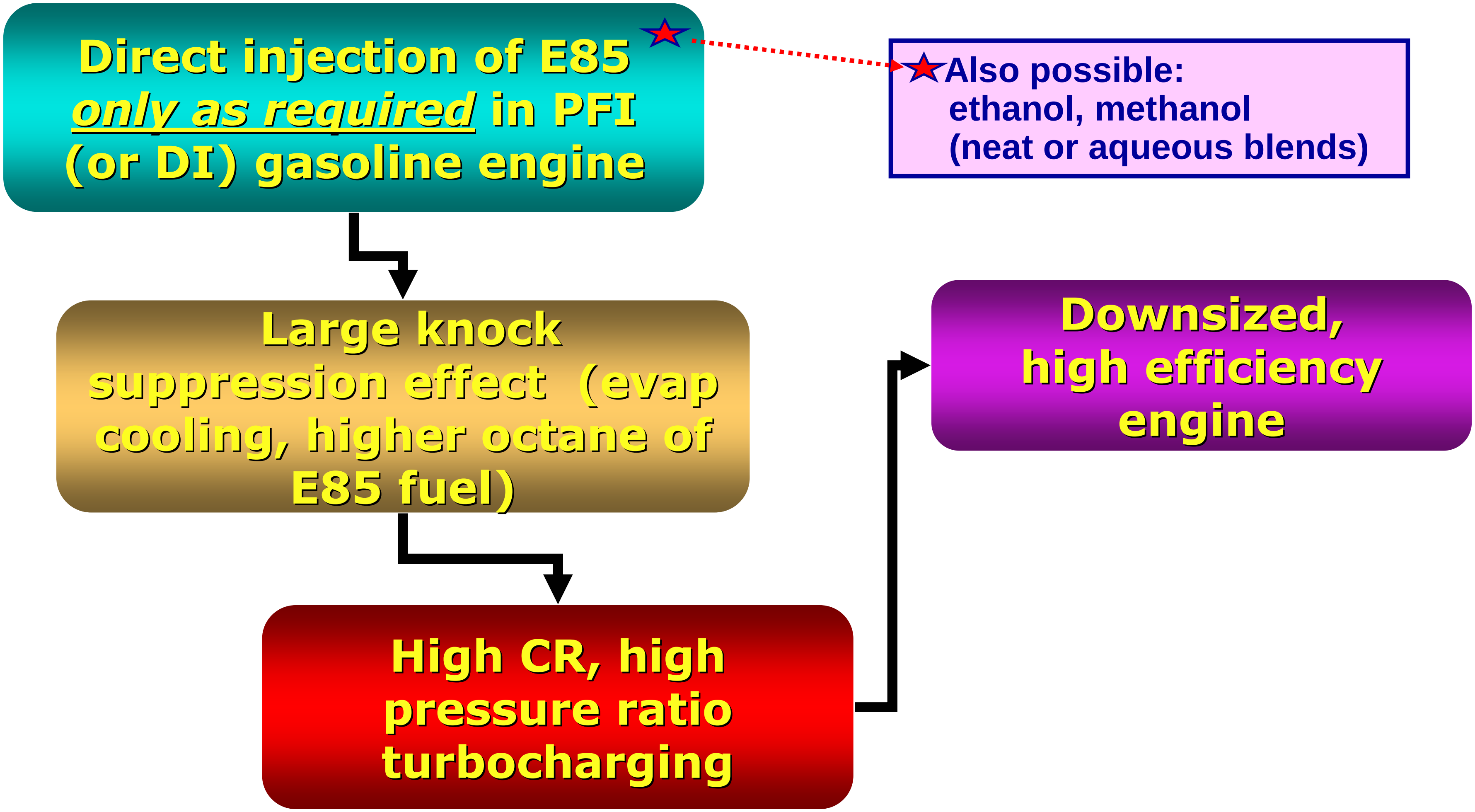
Outline

- Dual-Fueled Engine Concept
- Performance Simulation
  - Calibration
  - Predicted vs. Test Results
- Knock Prediction/Issues
- Conclusions

Ethanol Boosting Systems (EBS) Dual-Fueled “Octane on Demand” Engine Concept

EBS Path to High Efficiency Dual-Fueled Engine



Direct injection of E85 ★
only as required **in PFI**
(or DI) gasoline engine

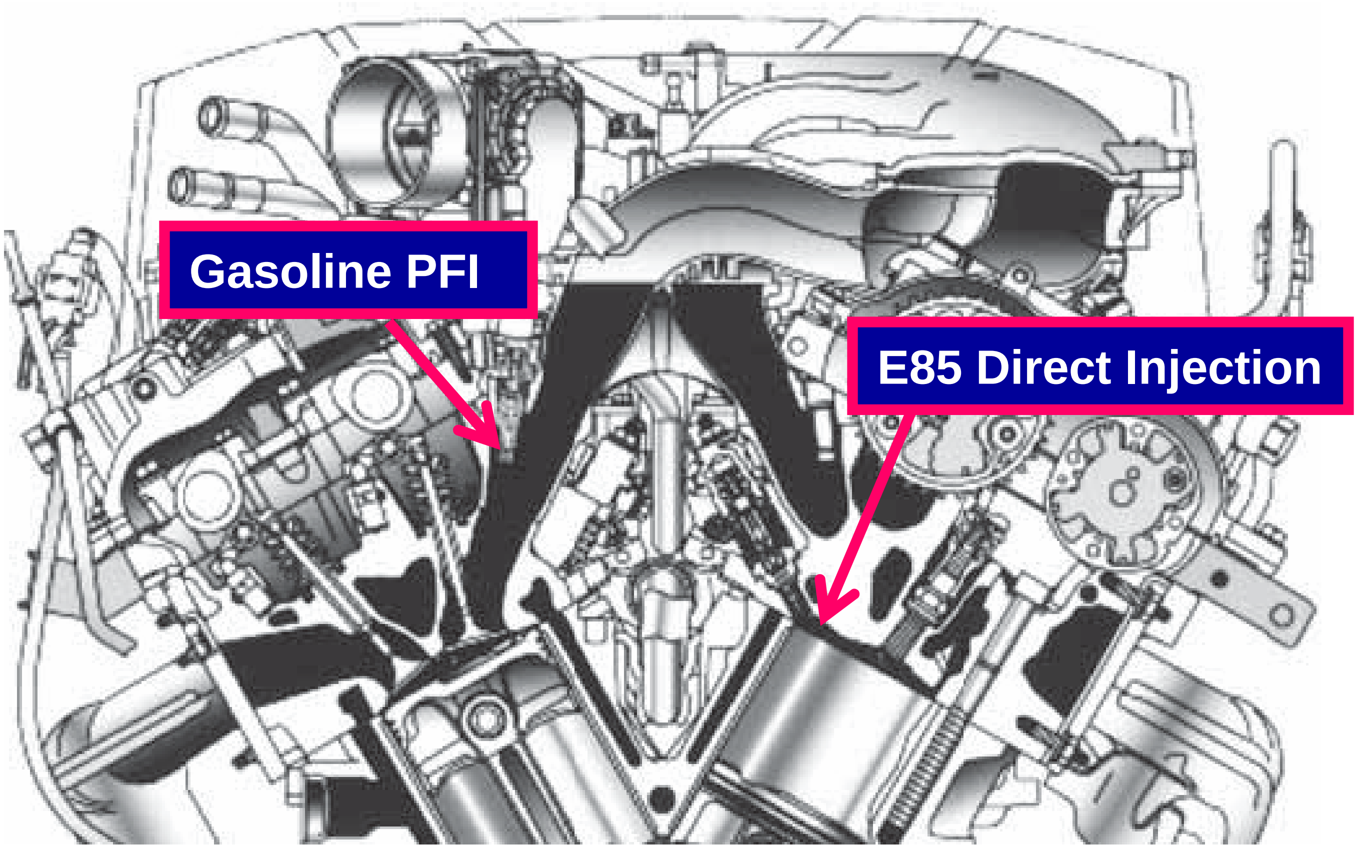
★Also possible:
ethanol, methanol
(neat or aqueous blends)

Large knock suppression effect (evap cooling, higher octane of E85 fuel)

High CR, high pressure ratio turbocharging

Downsized, high efficiency engine

Cross-section of Dual-Fueled DI/PFI Engine

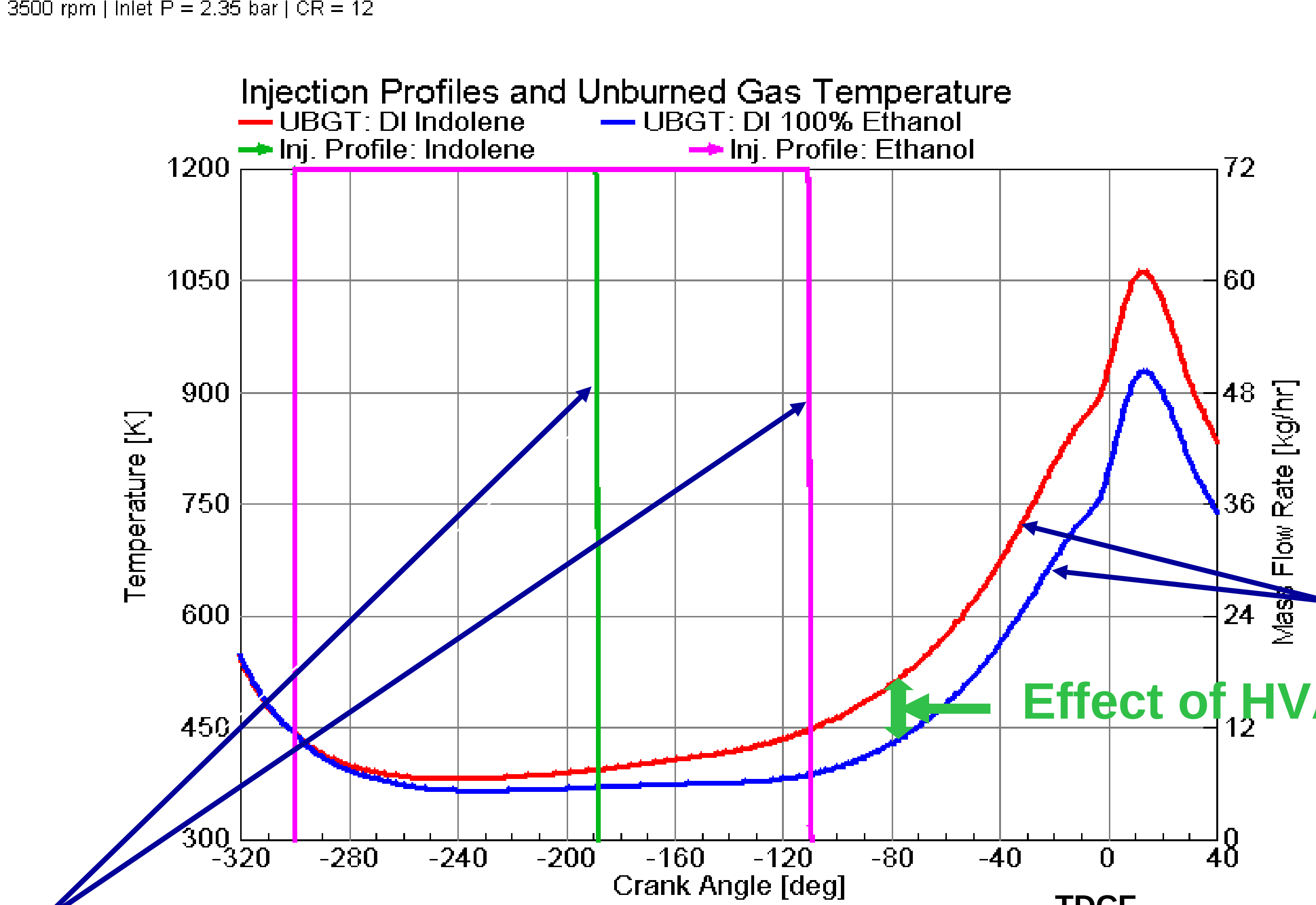


courtesy: Toyota

Ultimately, all fuel could be delivered through a dual-fuel DI injector

Simulated Unburned Gas Temperature vs. CA for DI Indolene and DI Ethanol

(3500 rpm; Stoich. A/F; 2.35 bar inlet P; CR – 12)



TDCF

Injection profiles

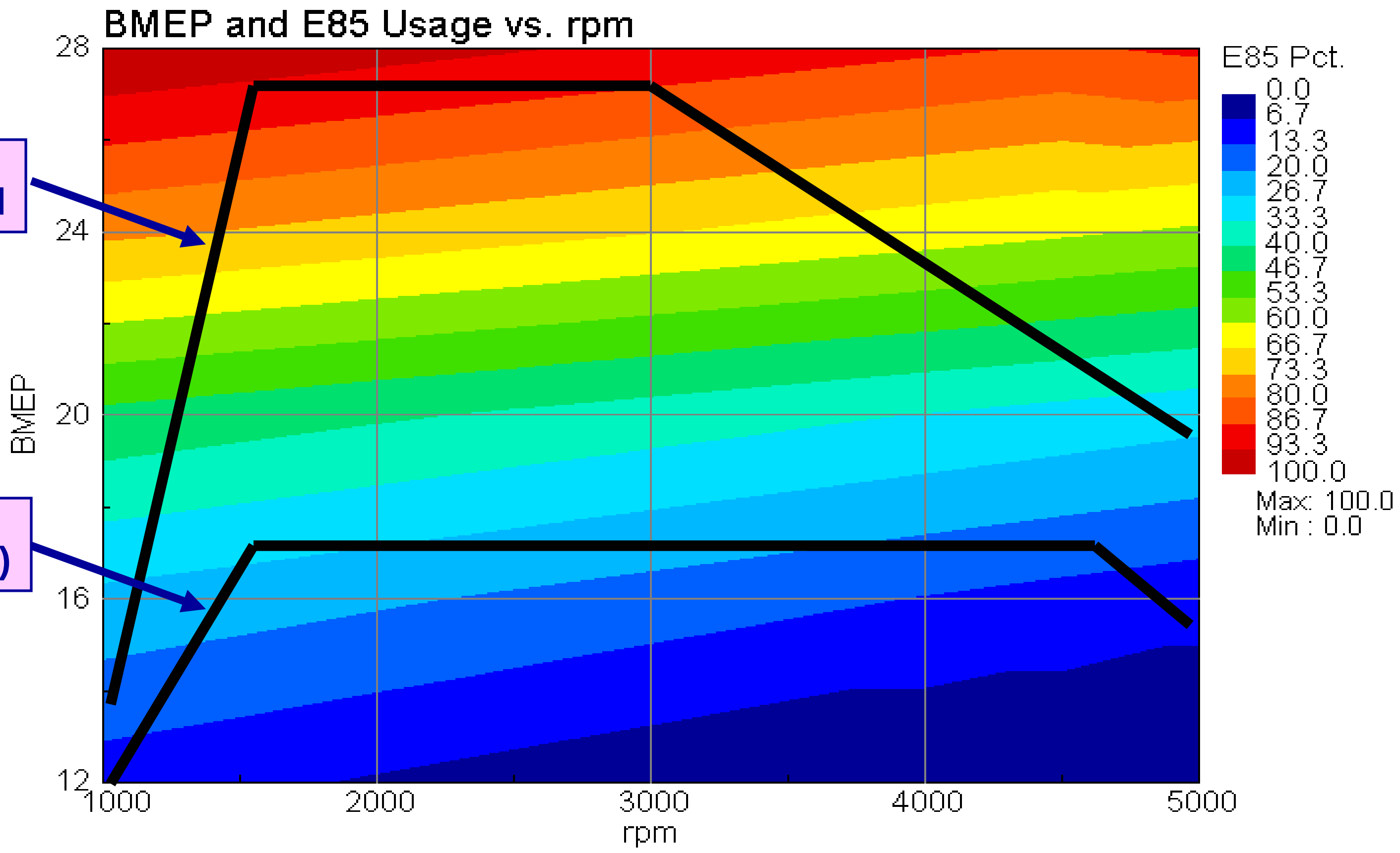
Unburned gas temp. vs. CA

Effect of HVAP

BMEP and E85 Usage vs. rpm (conceptual)

Dual-Fueled EBS DI/PFI vs. GTDI

E85 Usage and BMEP vs. rpm



BMEP EBS Dual-Fuel

BMEP GTDI (91 RON)

Major Features of EBS ‘Octane-on-Demand’ Concept

- E85 (or neat/aqueous ethanol, methanol etc.) provides significant octane benefit when directly injected due to high latent heat of vaporization and high intrinsic octane rating.
- Allows knock-free operation at high CR (11 – 12) and high BMEP (27–30 bar) with very high thermal efficiency (10% – 15% better than GTDI).
- Dual fuel strategy uses DI E85 only as required to eliminate knock in a high CR gasoline engine (typically at lower rpm and/or high BMEP).
- Over typical city and highway drive cycles, the ratio of E85 to gasoline usage is low (~5 – 10%).
- Combines octane benefit of E85 at high load with high gasoline volumetric energy density advantage at part load.
- Provides “smartest” and most leveraged use of available ethanol to achieve high efficiency conversion of a much larger amount of gasoline.

Performance Simulation for Knock Prediction

Overall Objective

To determine mass fraction of DI E85 required to suppress knock at a given speed/load operating point

Parametric Design Optimization

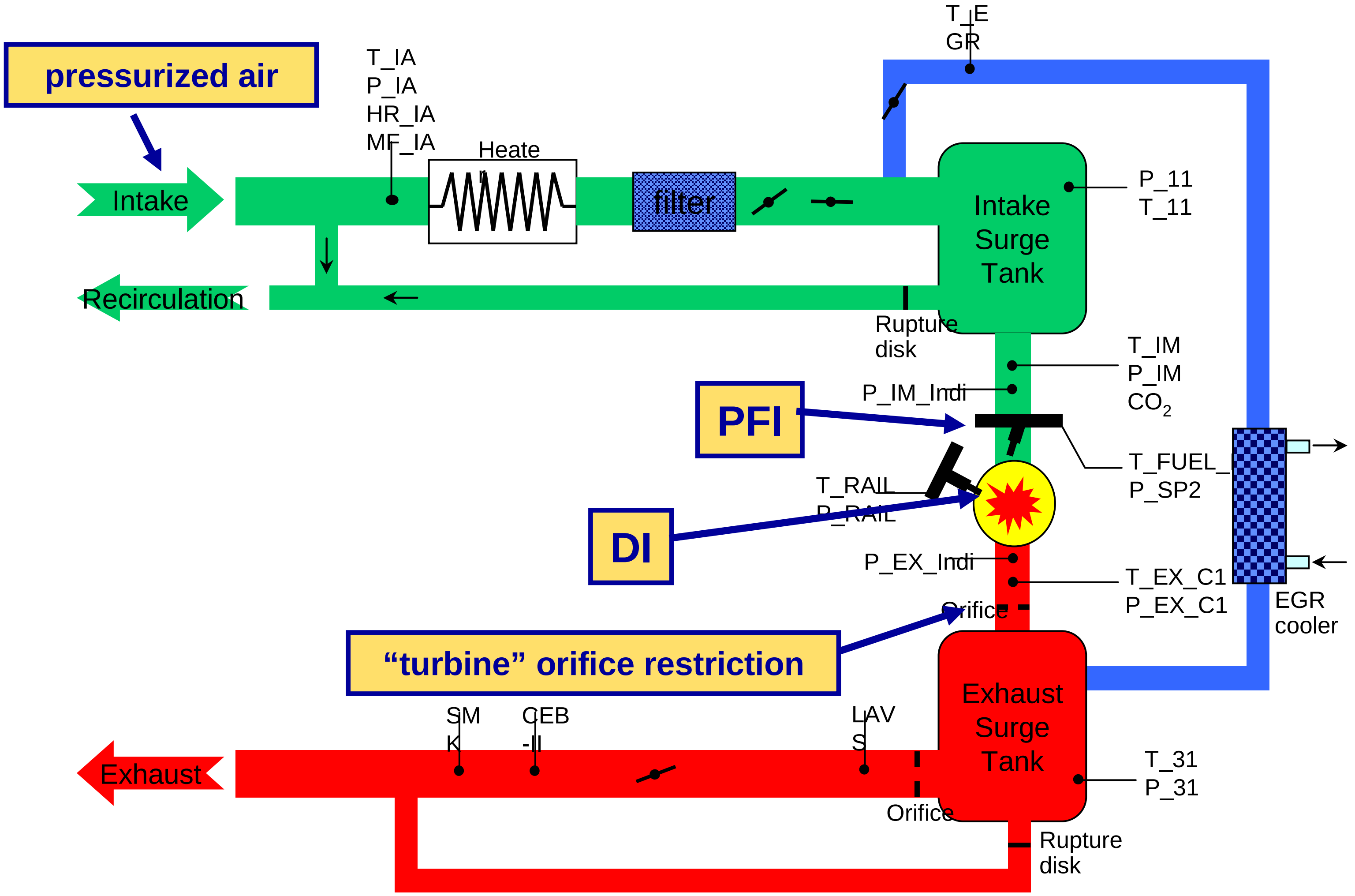
e.g., compression ratio; maximum boost; valve timing, EGR usage etc.

Performance Simulation – Procedure

- ☐ Create GT-Power model which faithfully reproduces AVL Single Cylinder Engine (SCE) test setup, with extensive diagnostics (e.g., fuel liquid/vapor, max. unburned gas temperature, spatial gas-side surface temperatures etc).
- ☐ Choose expt’l operating point for calibration – 3500/27; DI E85 = 0.604 fuel mass fraction; light knock.
- ☐ Use experimental combustion parameters (CA50; CA1090), accounting for crevice fuel (~ 1.5%) in MFB vs. CA (‘EngCylCombMultWiebe’).
- ☐ Use experimental mass fraction of DI E85 (gives A/F at stoich.), inlet and exhaust boundary conditions.
- ☐ Calibrate ‘half-life’ in-cylinder fuel evaporation model ‘EngCylEvaporation’ using a more fundamental offline droplet evaporation calculation.
- ☐ Employ ‘built-in’ FEA wall temperature solver ‘EngCylTWallSoln’.
- ☐ Calibrate Woschni heat transfer correlation multiplier to give best fit of data (airflow, IMEP720, PMEP, ISFC, P vs. CA/Vol and dynamic exhaust pressure).

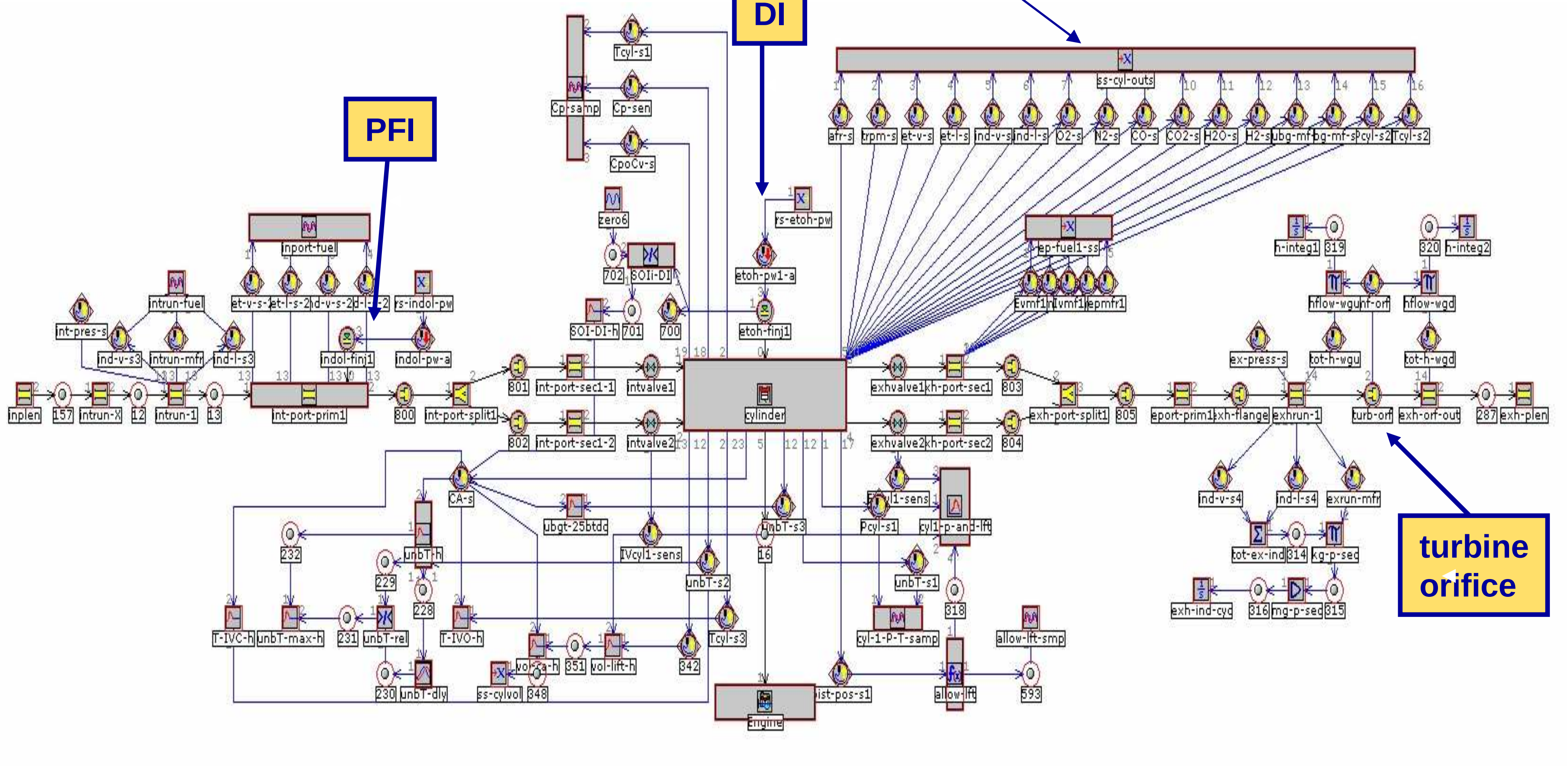
Single Cylinder Engine (SCE) Test Setup

[Compression Ratio = 9.3]



courtesy: AVL NA

Main SCE Section of Project Map (gtm)



Fuel vap/liq and species diagnostic signals

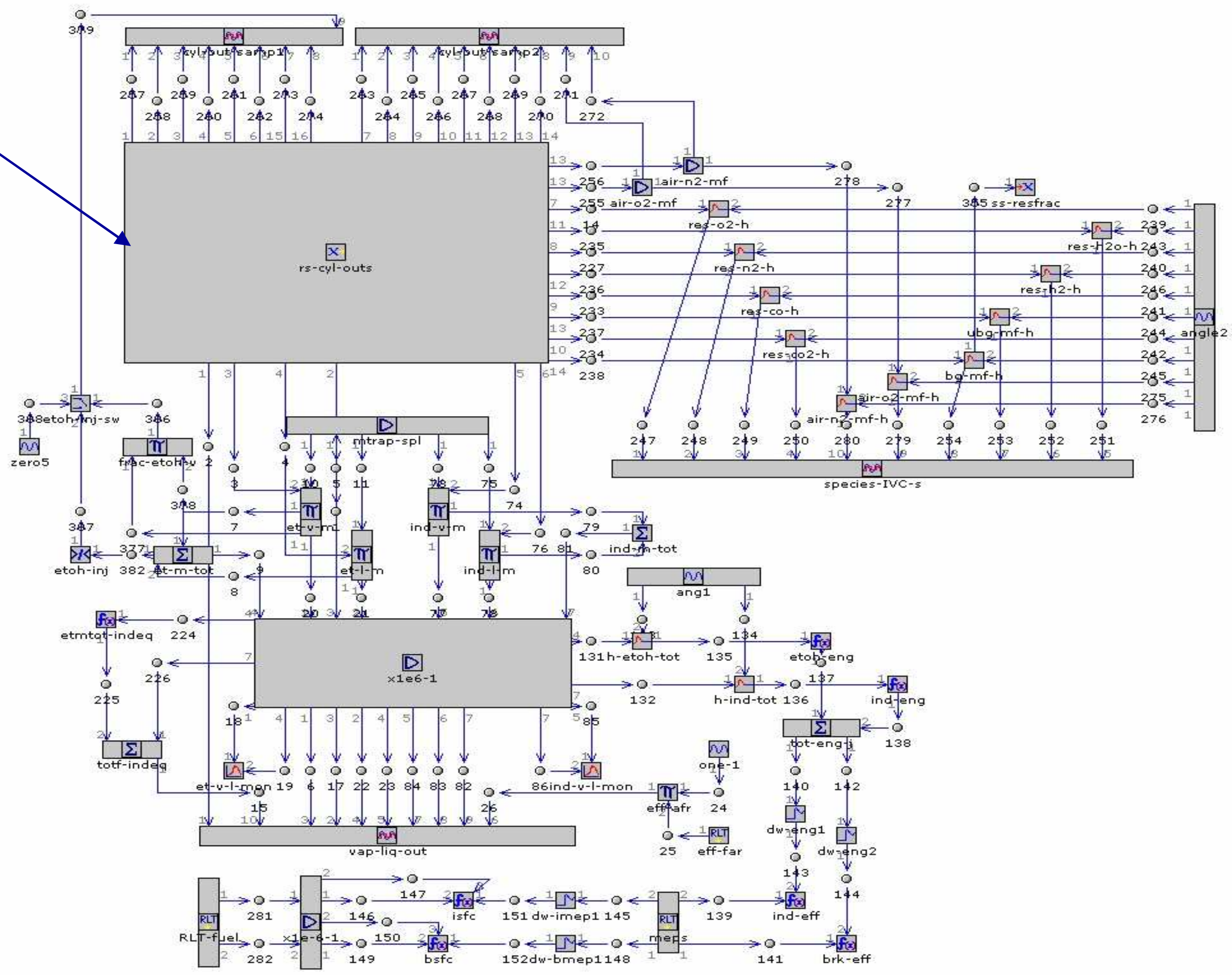
DI

PFI

turbine orifice

Fuel Liquid/Vapor and Species Diagnostic Section of Project Map (gtm)

Receive fuel vap/liq and species diagnostic signals

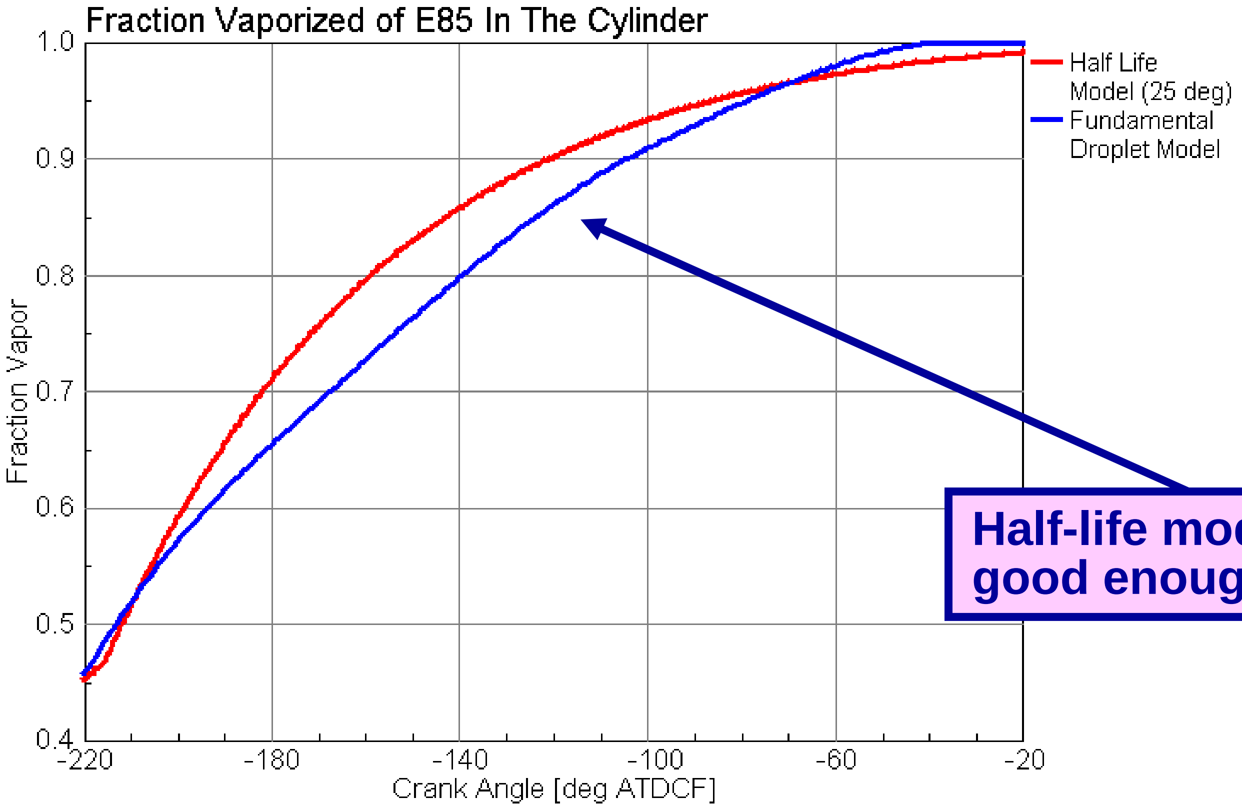


Calibration at 3500 rpm – 27 bar IMEP720

- ☐ DI E85 = 0.604 mass fraction of total fuel
- ☐ Stoichiometric A/F = 11.76
- ☐ Retarded timing – peak pressure constraint
- ☐ Light knock

Comparison of Half-Life Evaporation Model with ‘Fundamental’ Droplet Model

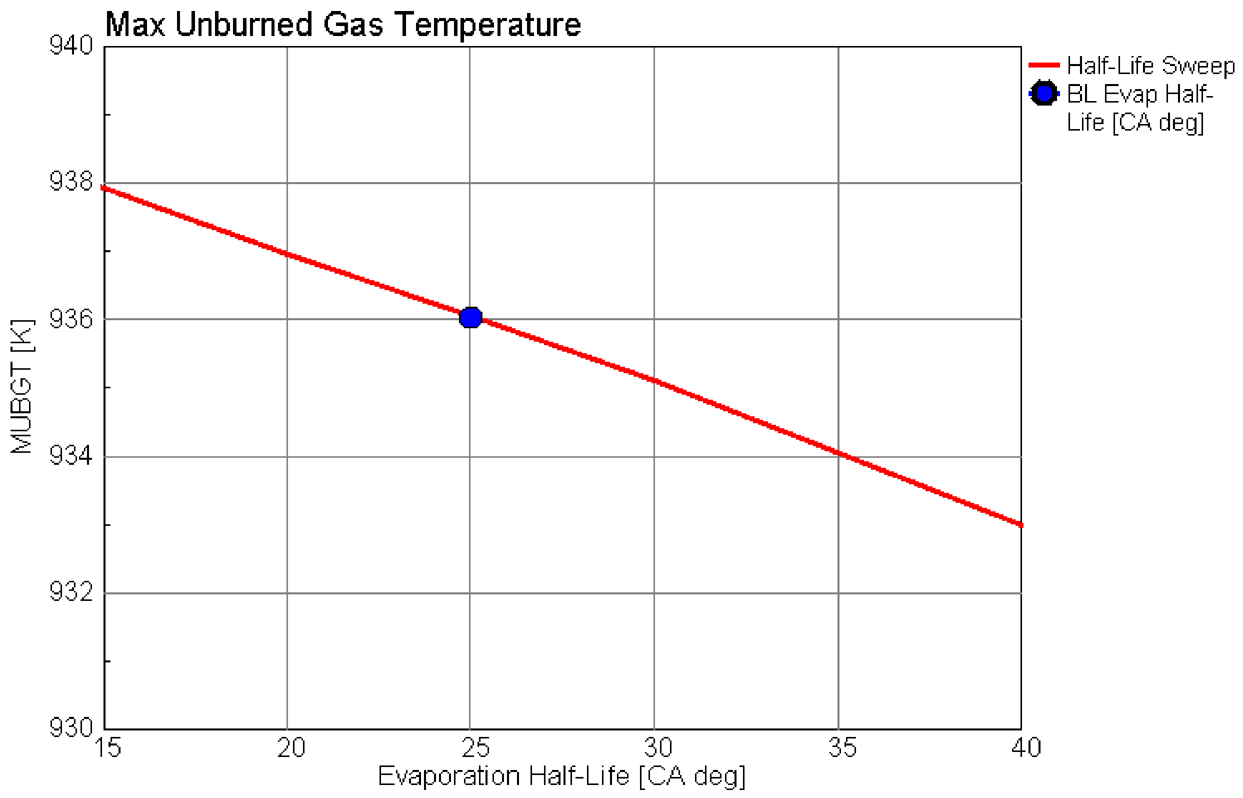
3500/27 -- Mean Cycle



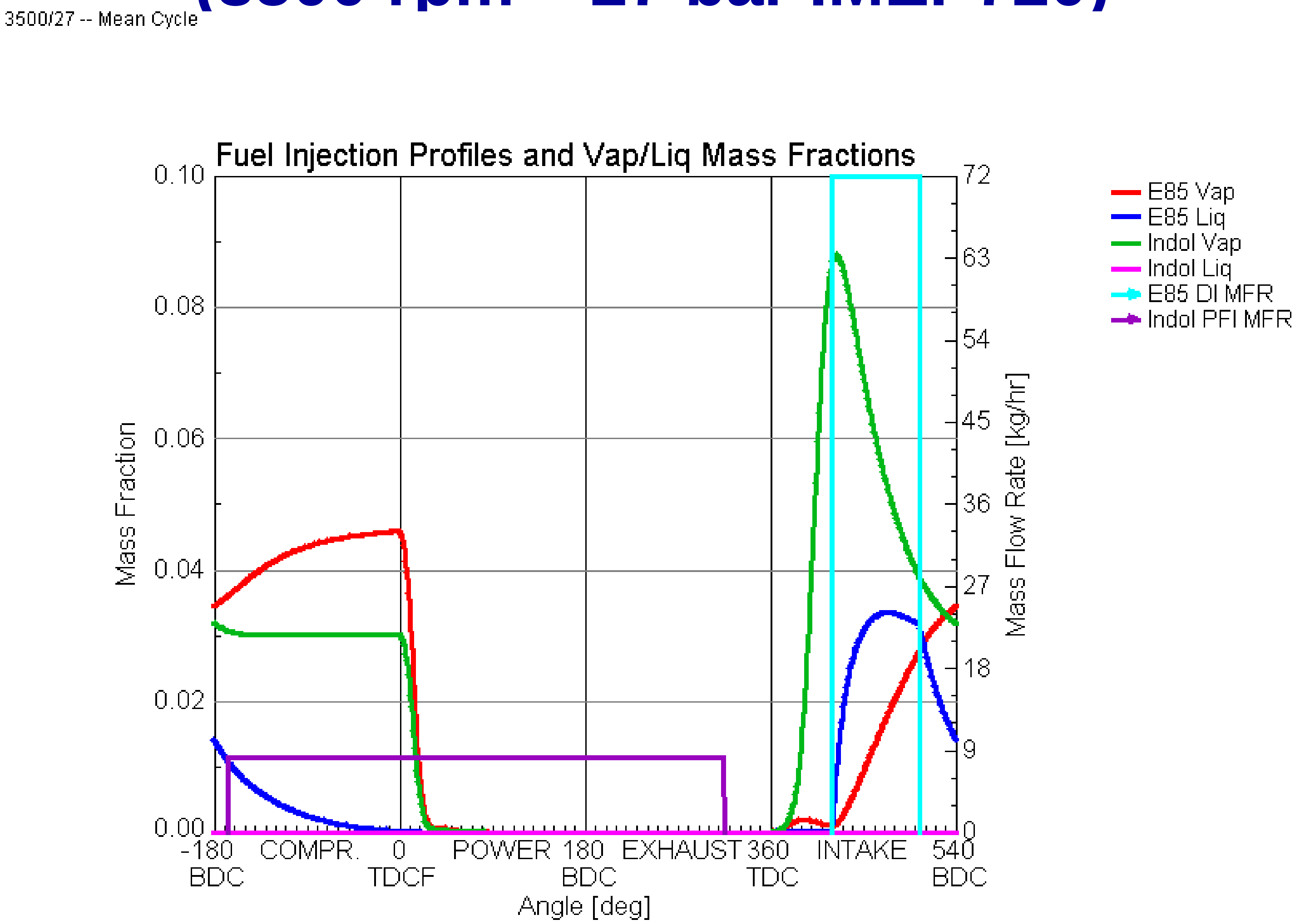
Half-life model is good enough

Effect of Evaporation Half-Life on Maximum Unburned Gas Temperature

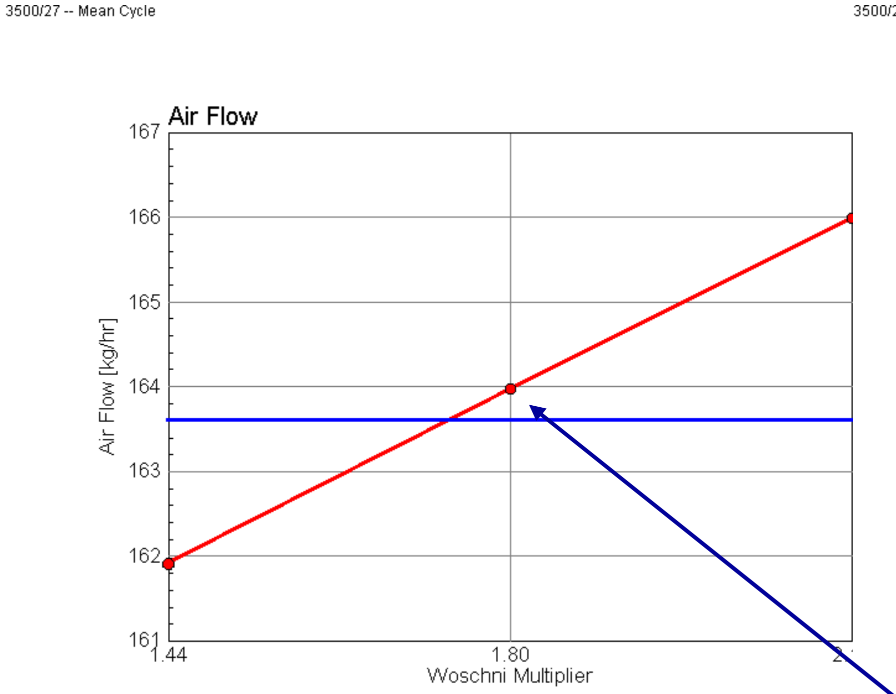
3500/27 -- Evap Half-Life Sweep

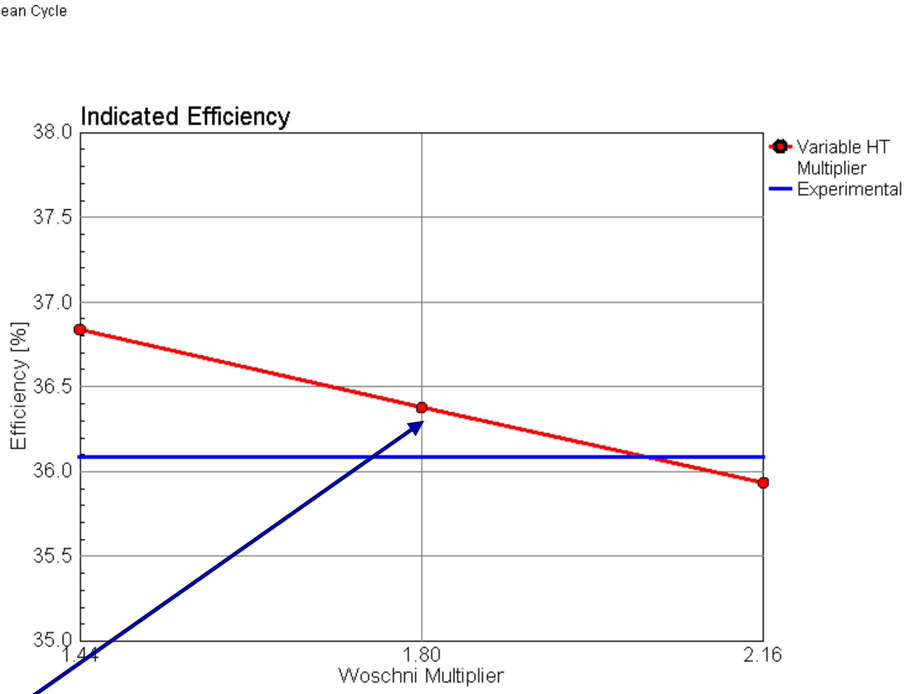


In-Cylinder Fuel Vapor/Liquid Mass Fractions (3500 rpm – 27 bar IMEP720)



Calibration of Woschni Heat Transfer Multiplier (3500 rpm – 27 bar IMEP720)





Best overall fit:
Woschni multiplier = 1.8
(high turbulence – fast burn combustion)

Comparison of Simulated and Experimental ‘Macro’ Data

3500 rpm – 27 bar IMEP720: Mean Cycle

Parameter	SCE Data (AVL)	GT-Power Simulation	% Diff
RPM	3500.00	3500.00	0.000
IMEP720 (bar)	27.16	27.07	-0.331
PMEP (bar)	2.48	2.43	-1.858
Air flow (kg/hr)	163.6[a]	164.00	0.244
E85 Fuel Flow (kg/hr)	8.40	8.42	0.238
Gasoline Fuel Flow (kg/hr)	5.50	5.52	0.364
Total Fuel Flow (kg/hr)	13.90	13.94	0.288
ISFC (gm/kW-hr)	283.40	285.70	0.812
Avg. Pre-Turbine Orifice Pres. (bar)	b	2.40	b
Avg. Pre-Turbine Orifice Temp (K)	1184.00	1187.00	0.253
Exhaust Plenum Pressure (bar)	2.15	2.16	0.279
Exhaust Plenum Temp. (K)	975.00	980.90	0.605

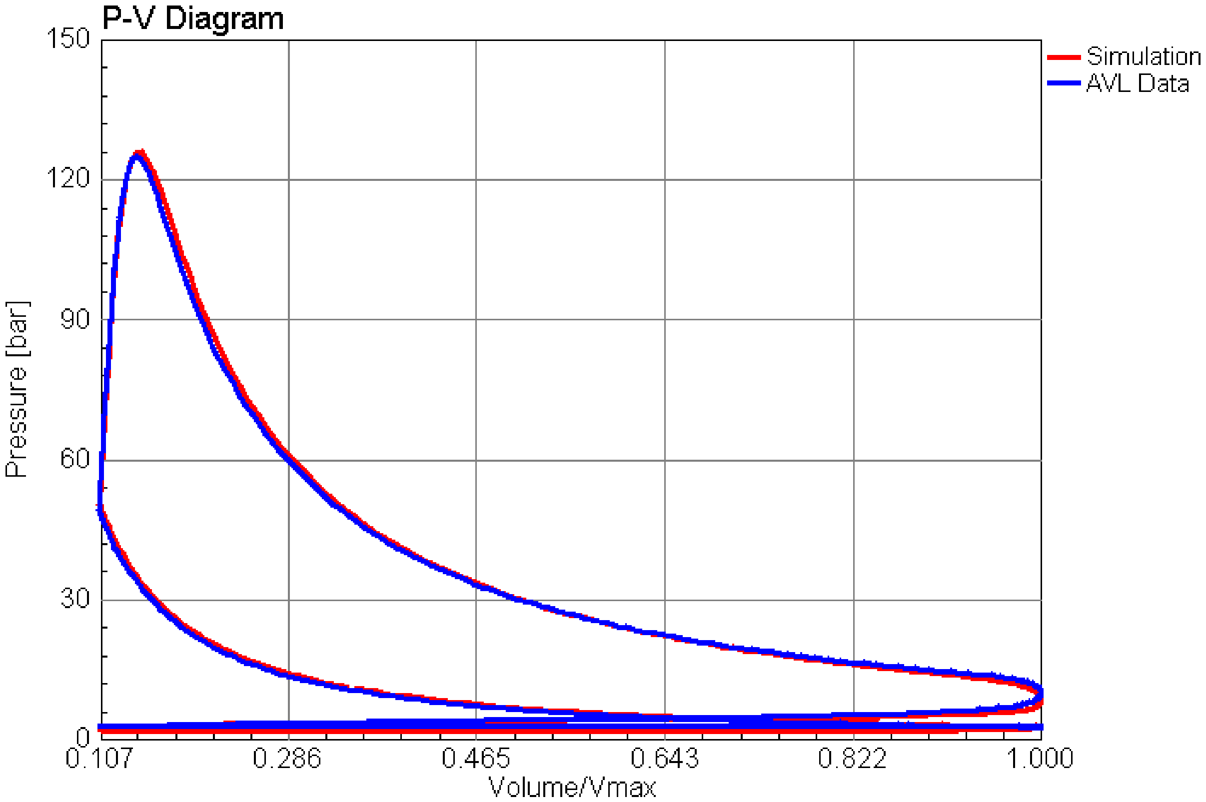
a. Corrected for stoich. A/F properties

b. Experimental value not reliable –
slow response thermocouple.

3500/27 Mean Cycle: P– V

Simulation vs. Experiment

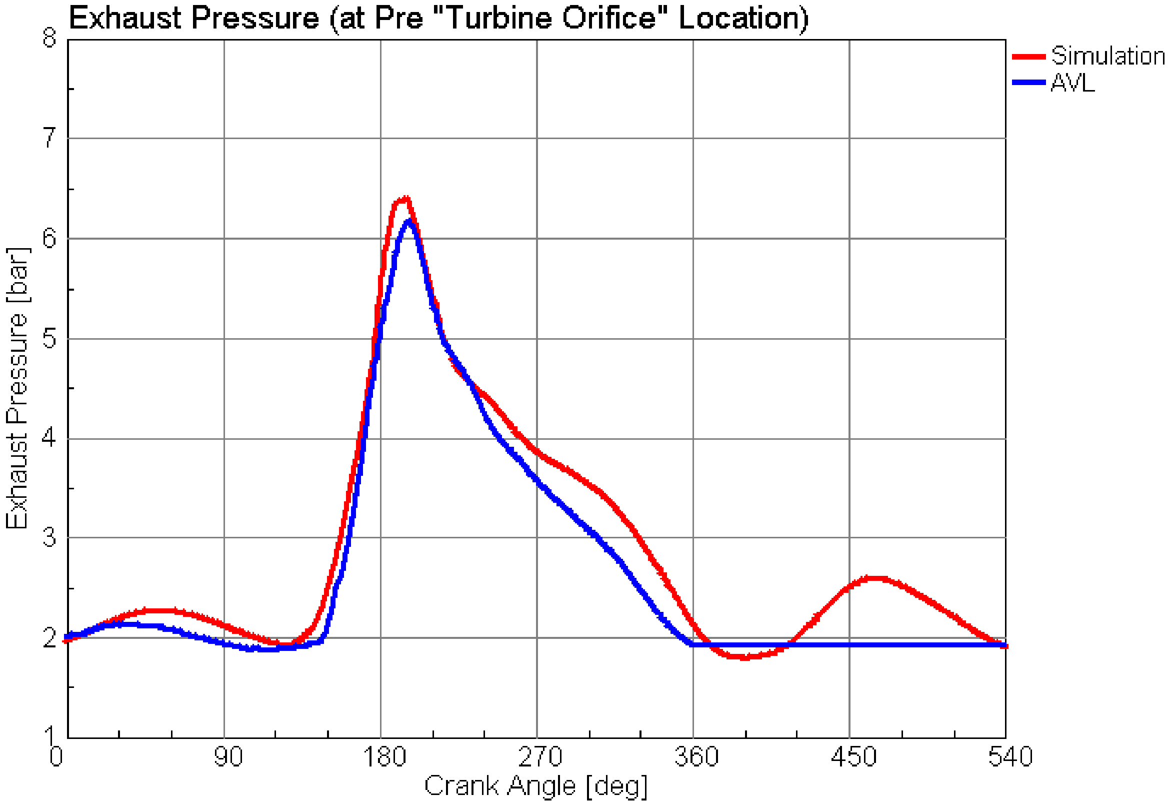
3500/27 Mean Cycle Cyl and Exh Pressure: Simulation & Expt



3500/27 Mean Cycle: “Pre-Turbine” Pressure

Simulation vs. Experiment

3500/27 Mean Cycle Cyl and Exh Pressure: Simulation & Expt



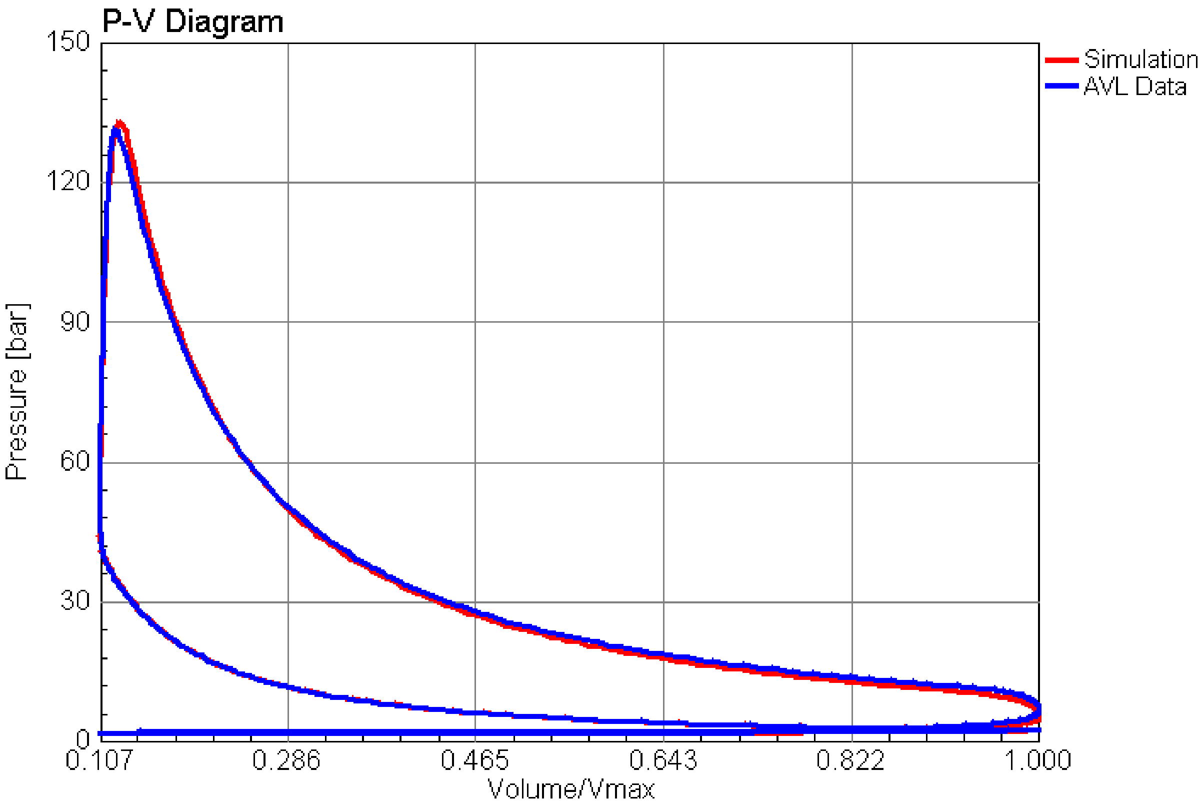
Simulation at 2000 rpm – 25 bar IMEP720

(using 3500/27 model calibration)

- DI E85 = 0.787 mass fraction of total fuel
- Stoichiometric A/F = 10.90
- MBT timing
- Light knock

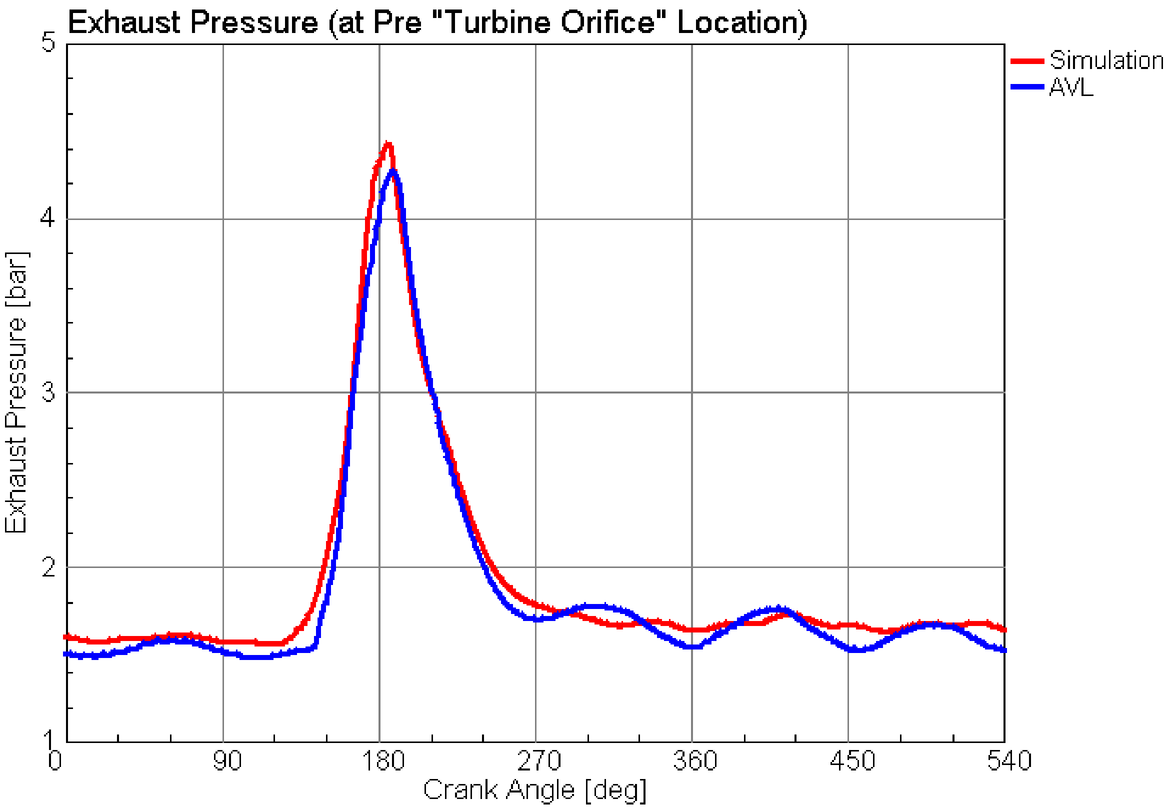
2000/25 Mean Cycle: P– V
Simulation vs. Experiment
(3500/27 model calibration)

2000/25 Mean Cycle Cyl and Exh Pressure: Simulation & Expt



2000/25 Mean Cycle: “Pre-Turbine” Pressure
Simulation vs. Experiment
(3500/27 model calibration)

2000/25 Mean Cycle Cyl and Exh Pressure: Simulation & Expt



Calculation of Knock at 3500/27

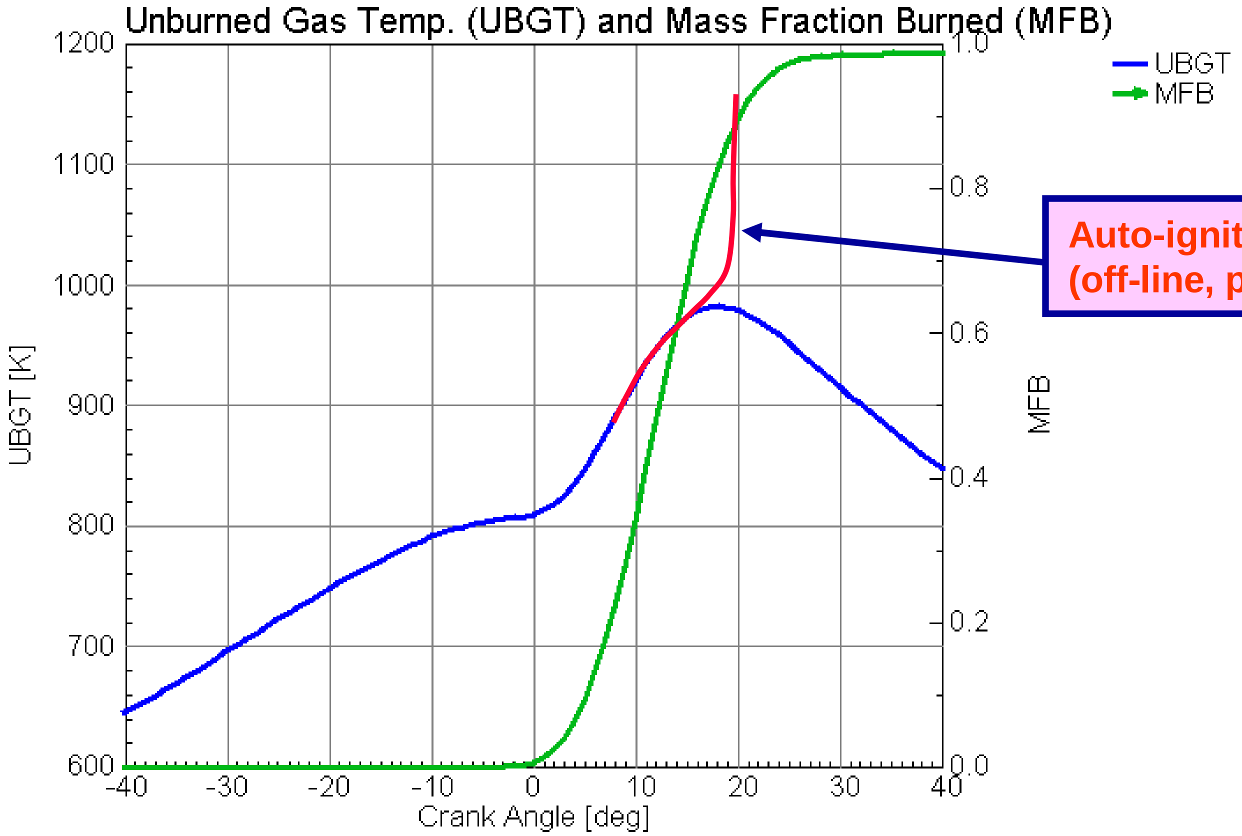
- DI E85 = 0.604 mass fraction of total fuel
- Stoichiometric A/F = 11.76
- Retarded timing – peak pressure constraint
- Light knock

Knock Calculation – Procedure

- Offline calculation using chemical kinetics code, CHEMKIN, with unburned gas temperature, pressure, composition and residual fraction from GT- Power performance simulation.
- Curran mechanism (~ 8000 species; 1000 reactions) for gasoline (represented as combination of Primary Reference Fuels correlated to octane rating); Marinov mechanism for ethanol.
- Use combustion statistical variation of CA50 and CA1090 corresponding to fraction of cycles knocking, i.e. light knock – 10% cycles knocking →1.25 sigma. (This is an assumption – could be other variabilities).
- Integration from approximately 625 deg K, below which precombustion kinetics not active.
- Auto-ignition (temperature spike) must occur with at least 10% of fuel still unburned to constitute “knock”.

Auto-Ignition (Knock) – Conceptual

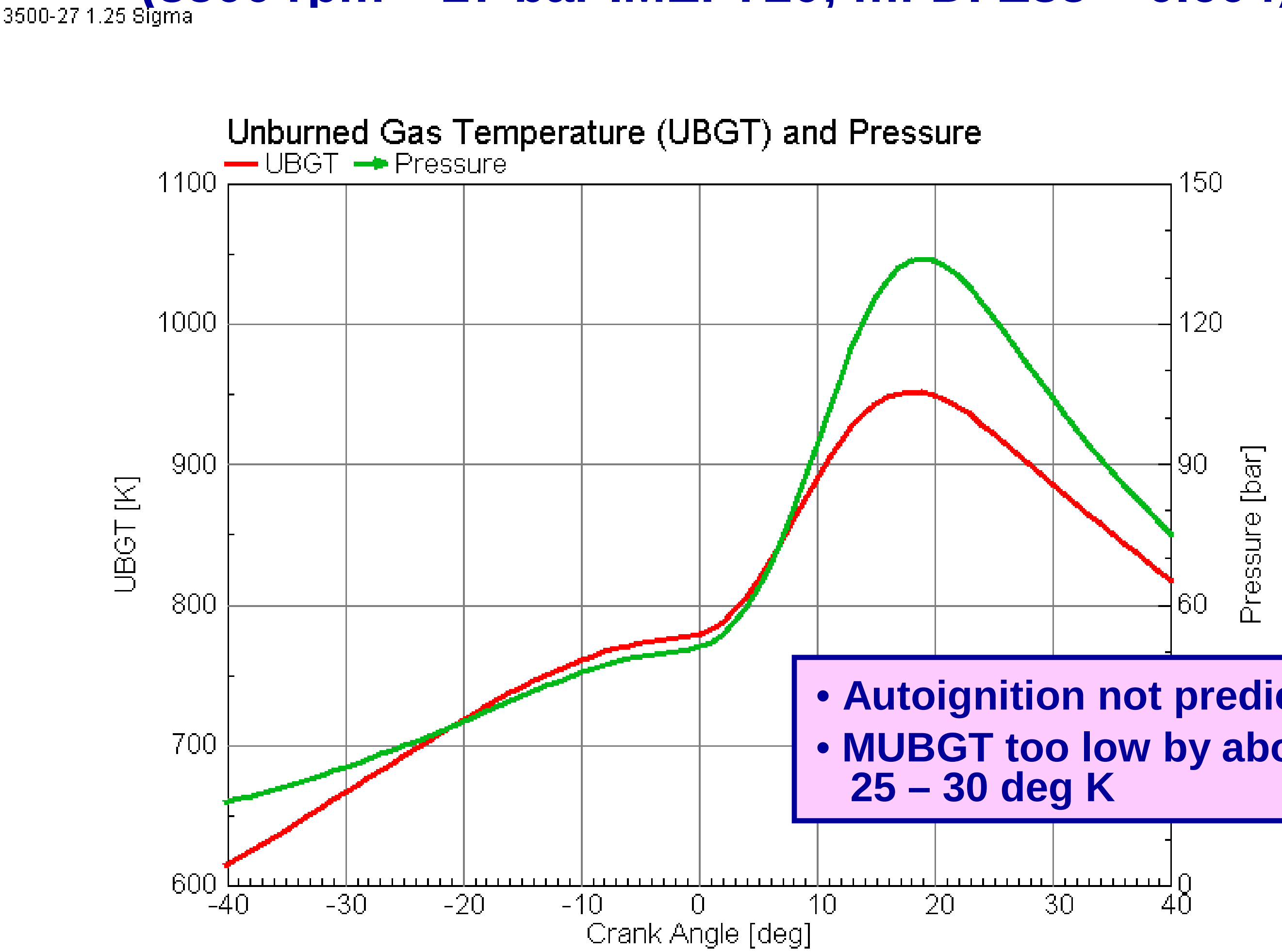
UBGT @ 1.25 Sigma + 30 deg K



Auto-ignition temp rise (off-line, parallel calculation)

Unburned Gas Temp. and Pressure for 1.25 Sigma Cycle

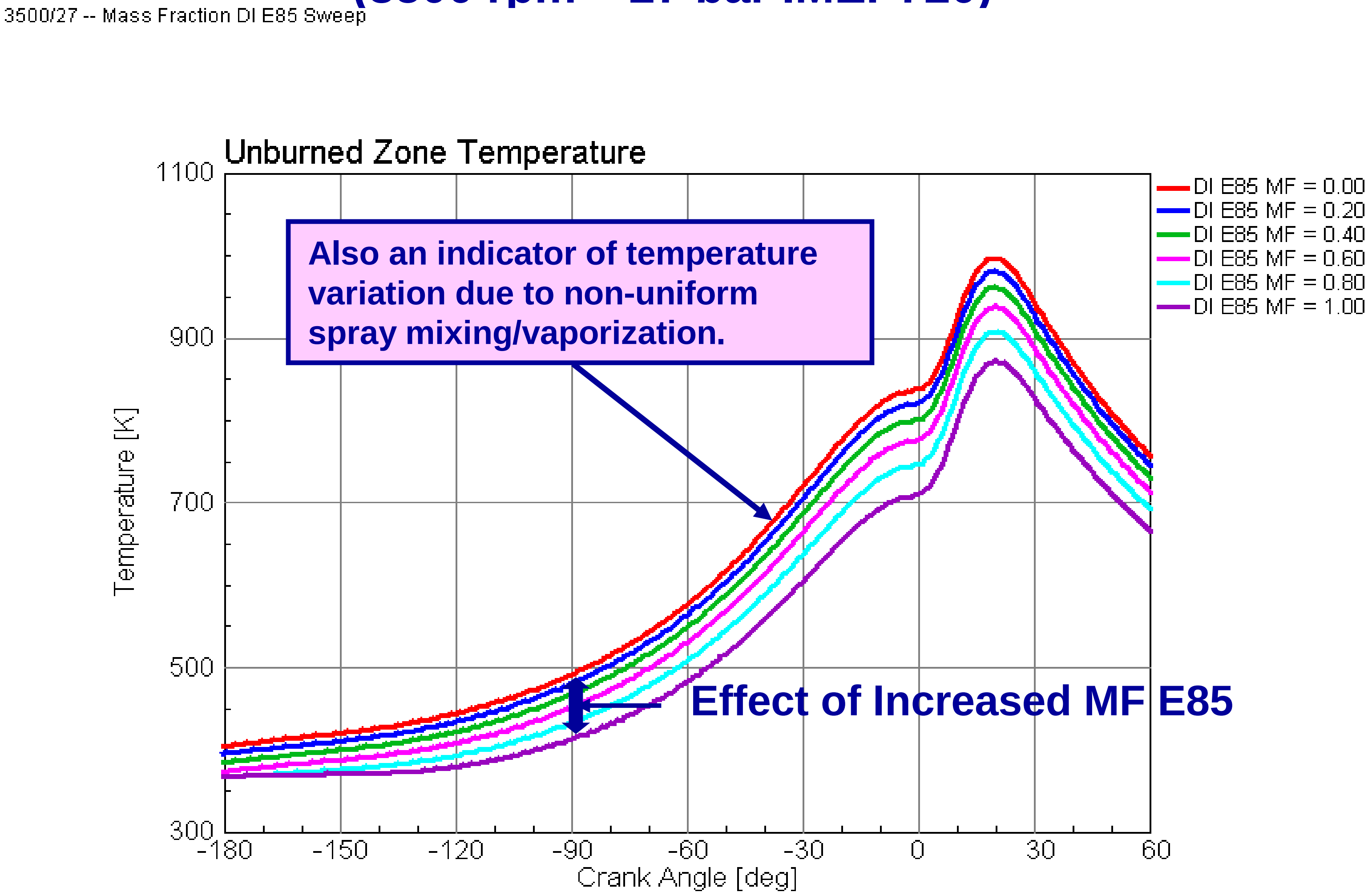
(3500 rpm – 27 bar IMEP720; mf DI E85 = 0.604)



- **Autoignition not predicted.**
- **MUBGT too low by about 25 – 30 deg K**

UBGT vs. CA at Various DI E85 Mass Fractions of Total Fuel

(3500 rpm – 27 bar IMEP720)

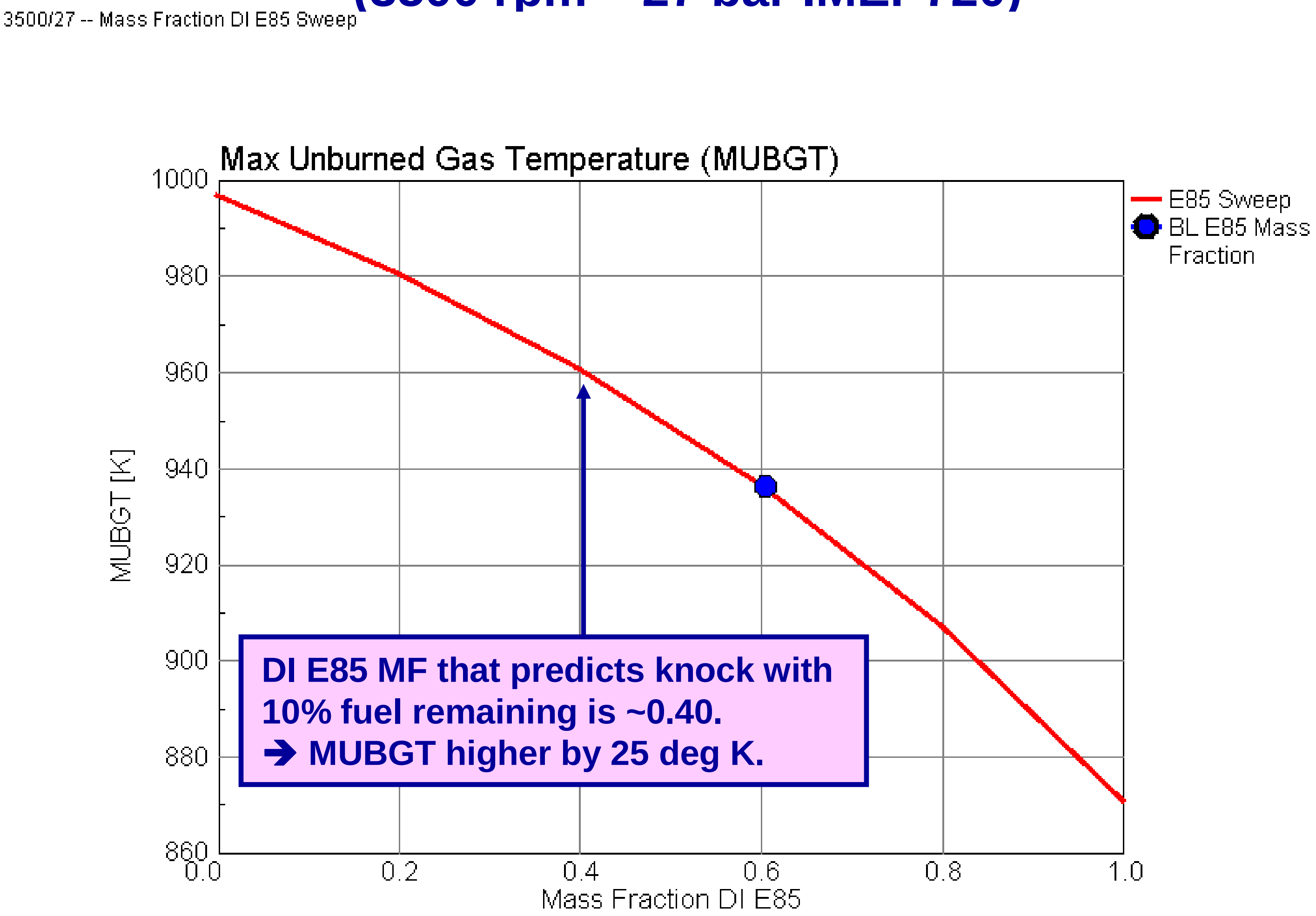


Also an indicator of temperature variation due to non-uniform spray mixing/vaporization.

Effect of Increased MF E85

MUBGT vs DI E85 Mass Fraction of Total Fuel

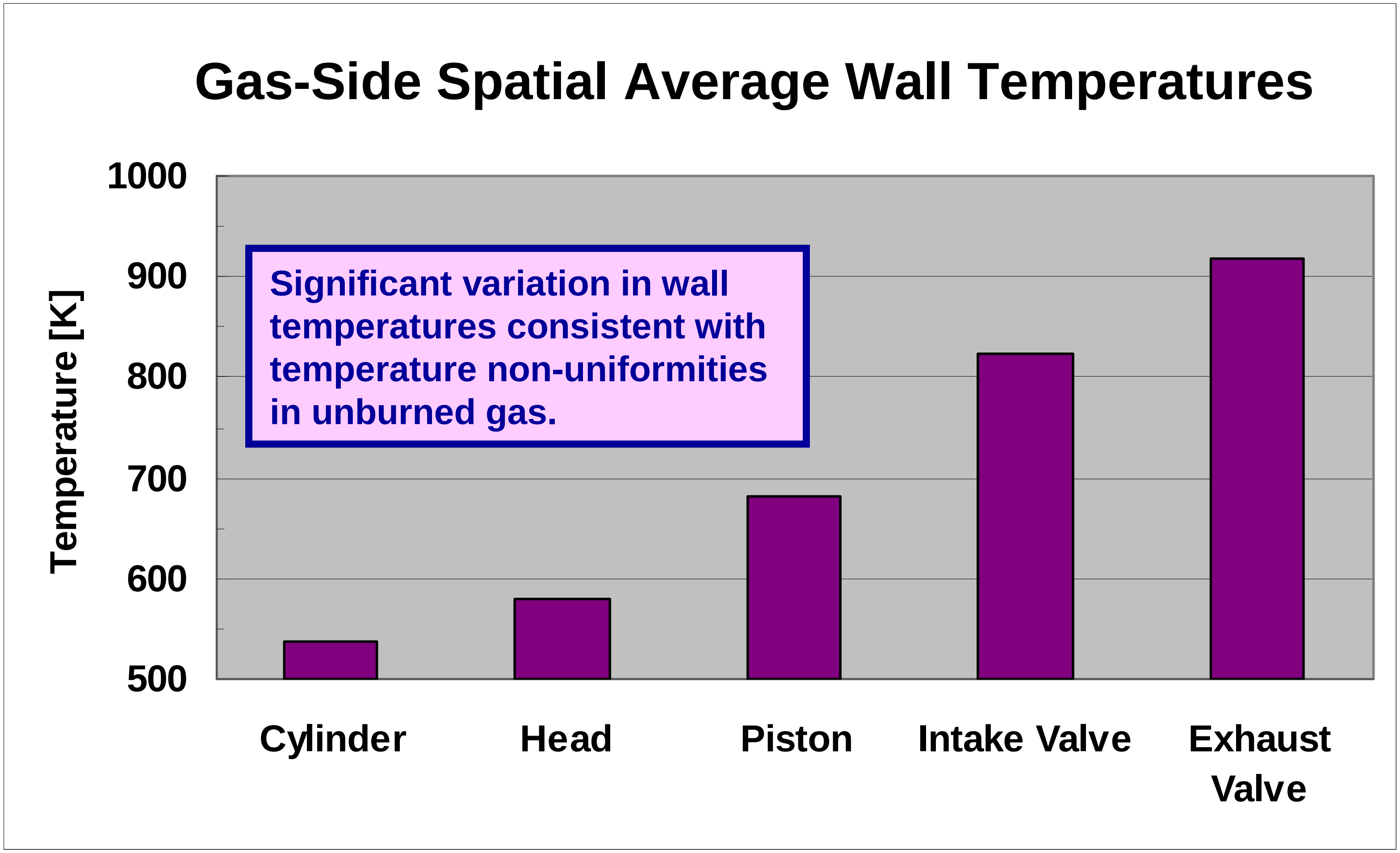
(3500 rpm – 27 bar IMEP720)



DI E85 MF that predicts knock with 10% fuel remaining is ~0.40.
➔ MUBGT higher by 25 deg K.

Spatial Average Wall Temperatures for 1.25 Sigma Cycle

(3500 rpm – 27 bar IMEP720)



Significant variation in wall temperatures consistent with temperature non-uniformities in unburned gas.

General Conclusions - I

- GT-Power can simulate dual-fueled (PFI/DI) engine very adequately.
- As demonstrated by comparison to high quality experimental data, engine performance can be very well predicted using homogeneous unburned and burned gas zones, after appropriate calibration of fuel vaporization rate and heat transfer level.
- A uniform unburned zone temperature underpredicts the occurrence of knock when coupled with a detailed fundamental chemical kinetic mechanism.
- Sources of unburned gas non-uniformity support higher temperatures than the well-mixed single zone value – i.e., contact with hotter surfaces and non-uniform spray mixing and vaporization.

General Conclusions - II

- A 1-D gas dynamic/thermodynamic engine model must take this into account using an ‘overlay’ of gas temperature variation within unburned zone. Ideally, ‘overlay’ could be realted to physical paramters such as variable in-cylinder wall temepratures.
- Otherwise, chemical kinetics must be empirically adjusted/calibrated to higher rates at lower temperatures (whether a fundamental kinetic mechanism or a knock integral method is used).
- Only alternative to an ‘overlay’ or empirical calibration of chemical kinetics would be full, well-calibrated CFD engine simulation coupled with detailed knock kinetics (assuming kinetics were fully validated).