Statistical Overview of 5 Years of HCCI Fuel and Engine Data from ORNL

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U.S. DEPARTMENT OF ENERGY

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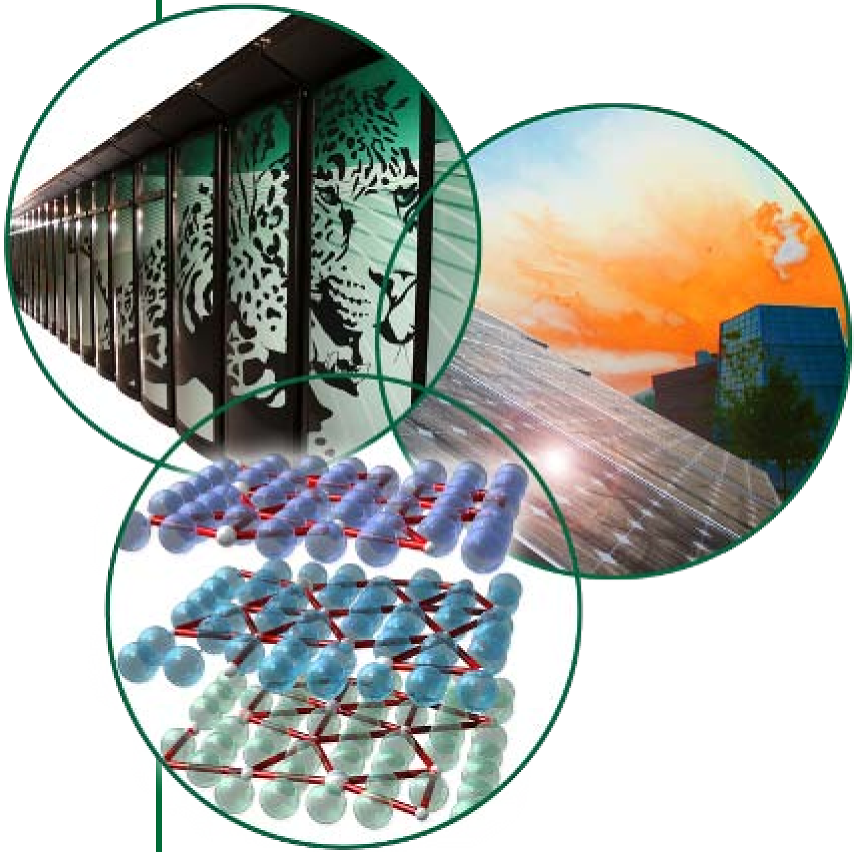
DETROIT

DIRECTIONS IN ENGINE-EFFICIENCY AND EMISSIONS RESEARCH CONFERENCE



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Goal of analysis

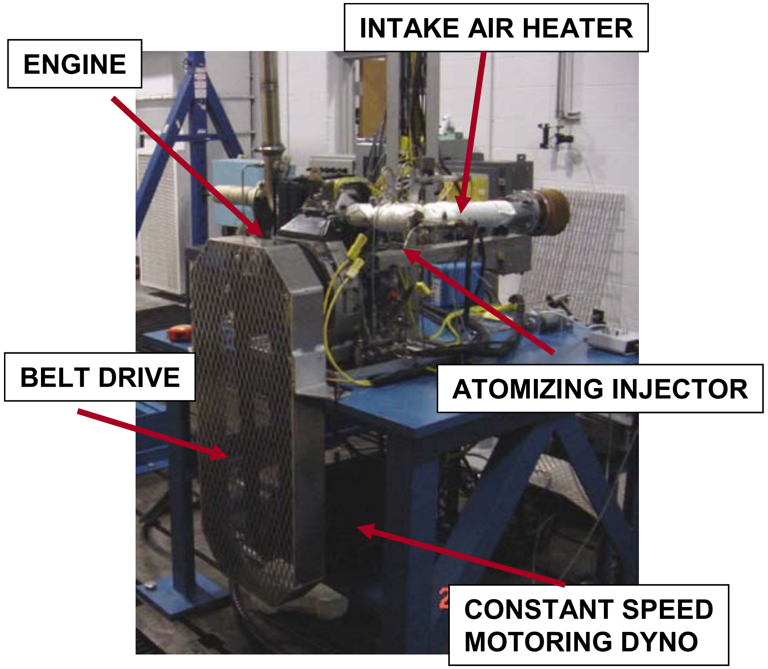
- Demonstrate power of statistical methods for understanding engine response to fuels
  - Show how cetane relates to fuel variables
    - Cetane appears to be the most important diesel range fuel variable for predicting for engine response
  - Show how engine response relates to fuel variables
    - Determine most important fuel variables for future experiments
    - Optimize fuel characteristics for this engine
- Look for future opportunities to apply techniques and knowledge base

- We can only present a small sampling of outputs here
    - Will follow with a full technical paper

Data set analyzed for this presentation

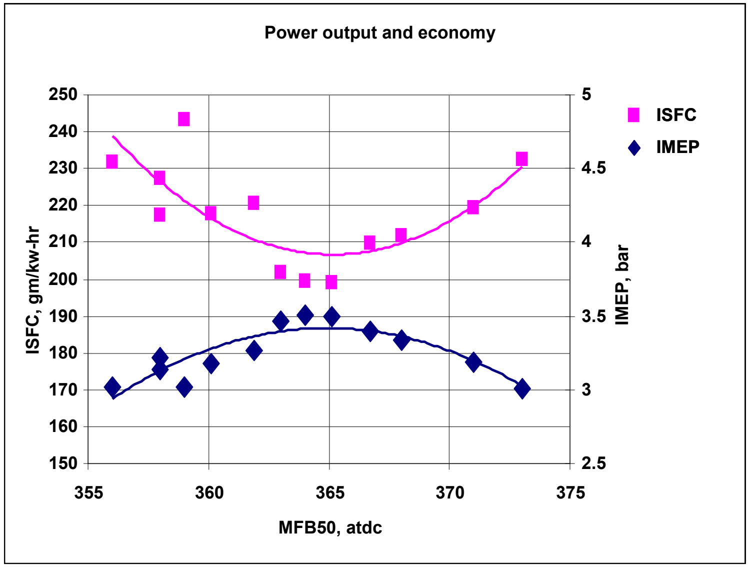
- All diesel range fuel data from ORNL HCCI single cylinder engine
- 9 experimental series of fuels, covering 2005 to 2009
  - Conventional, biodiesel, oil sands, oil shale, surrogate, primary and secondary reference, FACE
  - 95 fuels total, 18 fuel related variables selected
- 1879 engine data points, 24 engine related variables selected
  - All at 1800 rpm, 10.5 C/R
  - Varying fuel rate and combustion phasing
  - Engine is simple and correspondingly easy to model
    - 3 variable model: fuel rate, airflow, intake temperature
    - 2 variable model: IMEP and MFB50 (must remove points where boosting or throttling was used (6% of data)
- Data set is 82% ‘full’, i.e., 18% of data is missing
  - Dilemma between including more data points or more variables

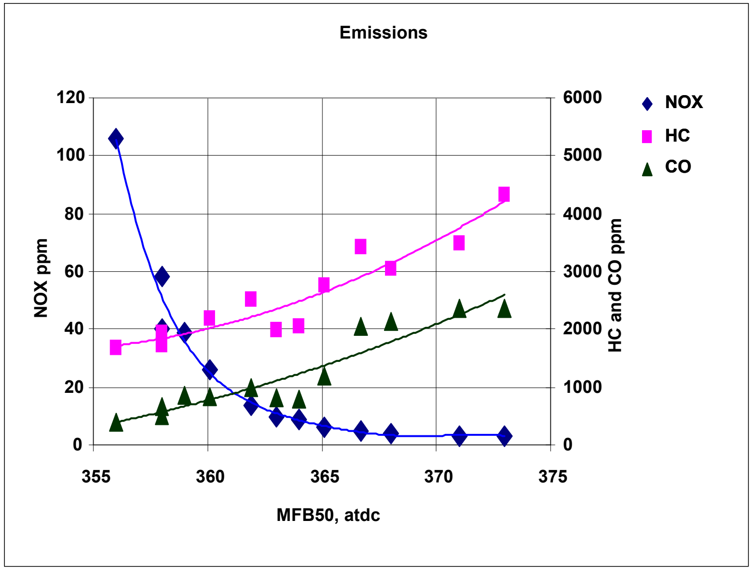
ORNL HCCI engine



- Modified from Hatz single cylinder diesel
- Fully premixed, dilute, with ignition controlled by intake heating
- Simple platform for fuels research
  - Performance dominated by fuel effects
  - Uses minimal fuel
  - Can run almost anything
  - Easy to model
- Some experiments included boosting and throttling

EMISSIONS AND ECONOMY TRADEOFFS VS. COMBUSTION PHASING



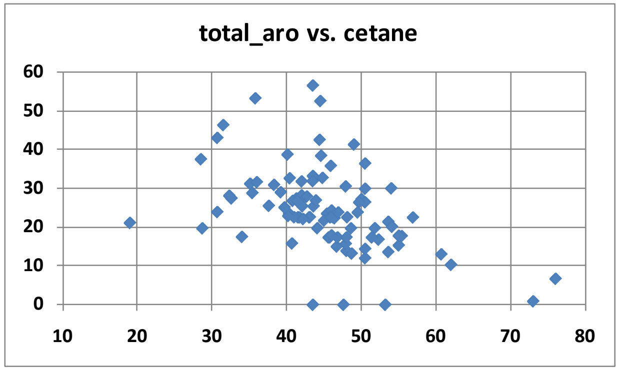


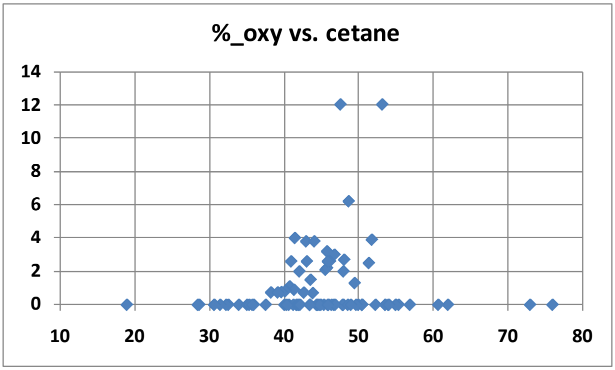
Two approaches used in analysis

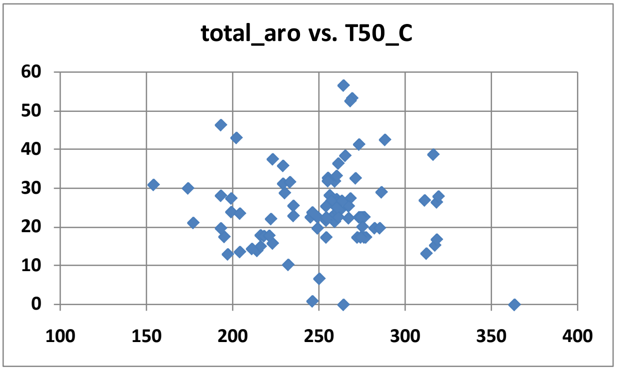
- AVL CAMEO© powertrain calibration software package
  - Very flexible, easy to use, modeling, optimization, mapping, and graphics tools
  - Normally used to map and optimize engine response to control variables
  - Fuel variables can be considered as an addition to engine control variables
  - For this work, we analyzed a subset of fuels for a more detailed study of bio-fuel effects
  - For this work, we used 2nd order models with interactions, auto offset and transformation of DVs, auto selection of significant terms
- Statistical analysis using PCA representation of fuels
  - We have previously showed that principal components to be an efficient way to represent data sets with correlated variables, such as fuels
  - PCA does not eliminate correlations, but allows correlations to be carried through statistical analysis
  - In some cases, principal components represent actual degrees of freedom, such as specific blending streams
  - For this work, we analyzed entire data set
  - For this work, we used 1st order models with interactions, Ln transformation of DVs, manual selection of significant terms

Design space considerations

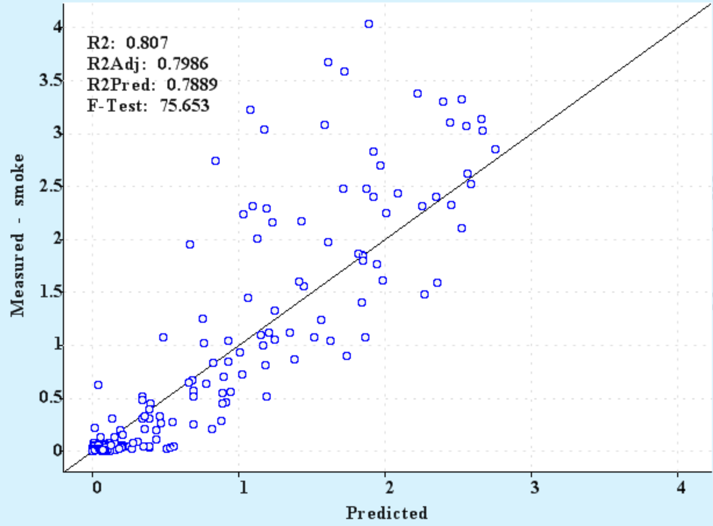
- When multiple studies are combined or one dives deeper that original experimental design, the design space is rarely complete or orthogonal
  - You can picture the design space as a series of rubber bands stretched around experimental data points in multiple dimensions
- Rigorous tracking of design space keeps use of models safely within experimental bounds
  - Cameo allows rigorous tracking of design space for up to 8 model parameters
  - Design space tracking can be computationally intensive

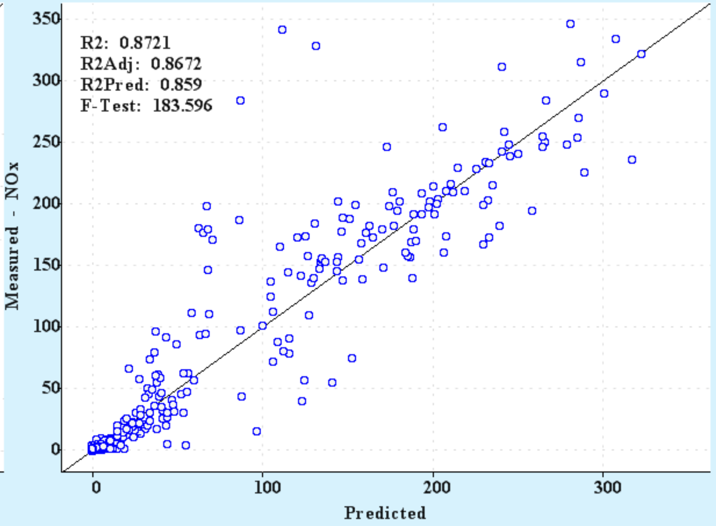

total_aro vs. cetane

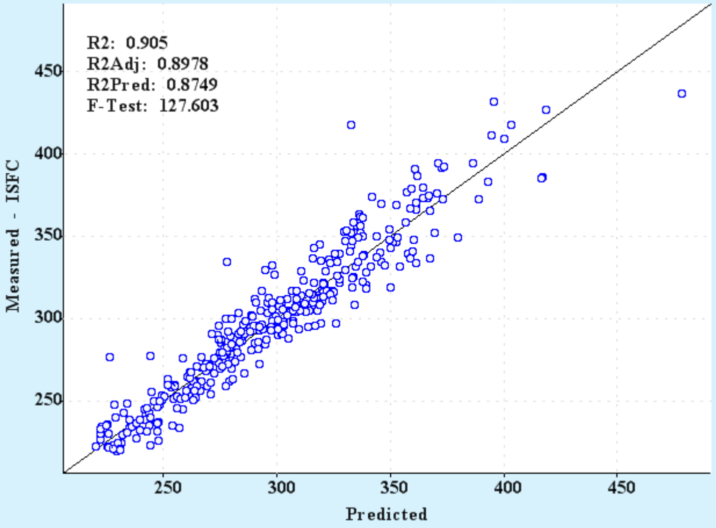

%_oxy vs. cetane


total_aro vs. T50_C

Measurements vs. predictions with AVL CAMEO©







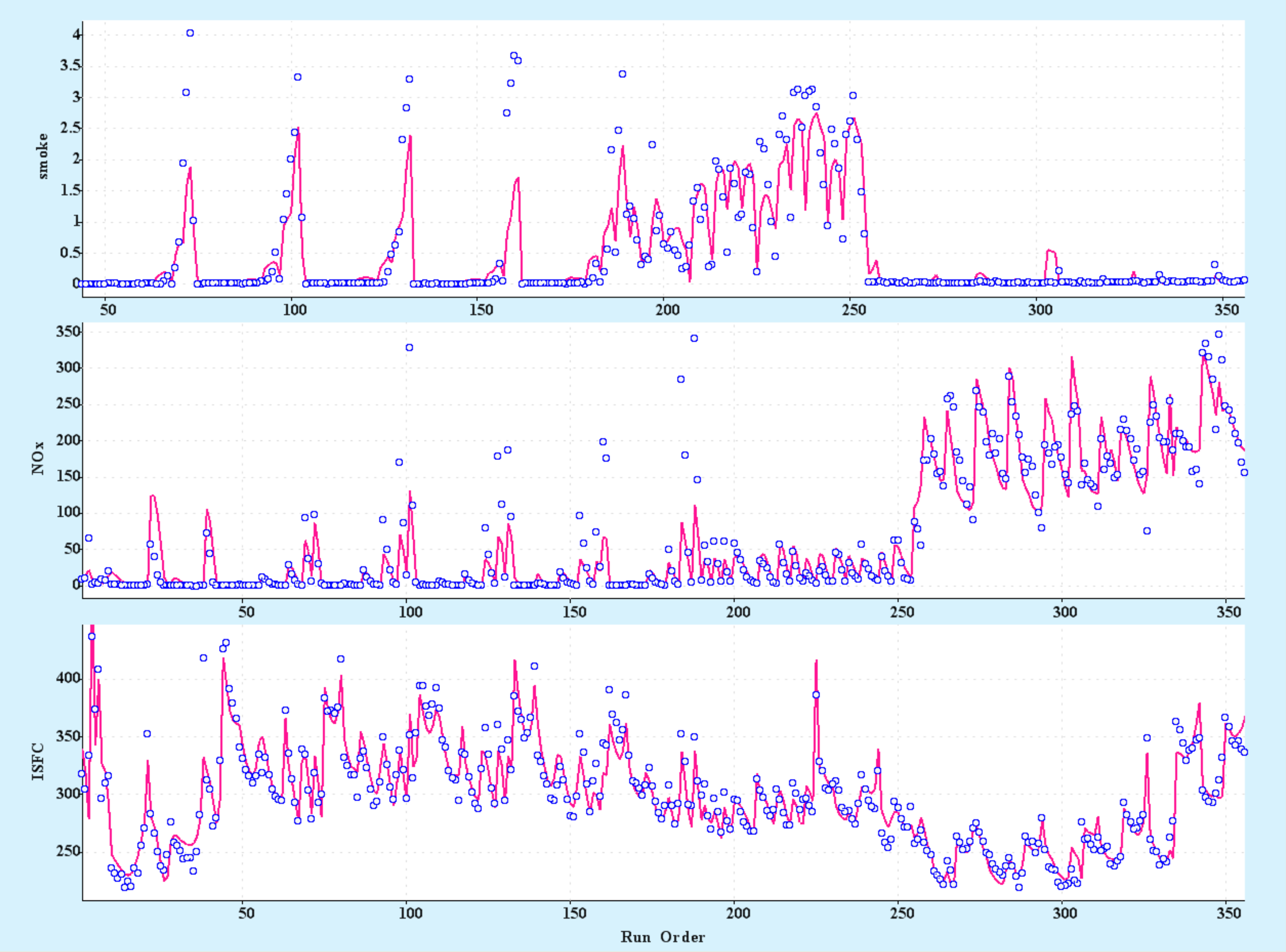
High R2 = models fit measurement data.

High R2Adj = models do not overfit.

High R2Pred = model has good prediction power

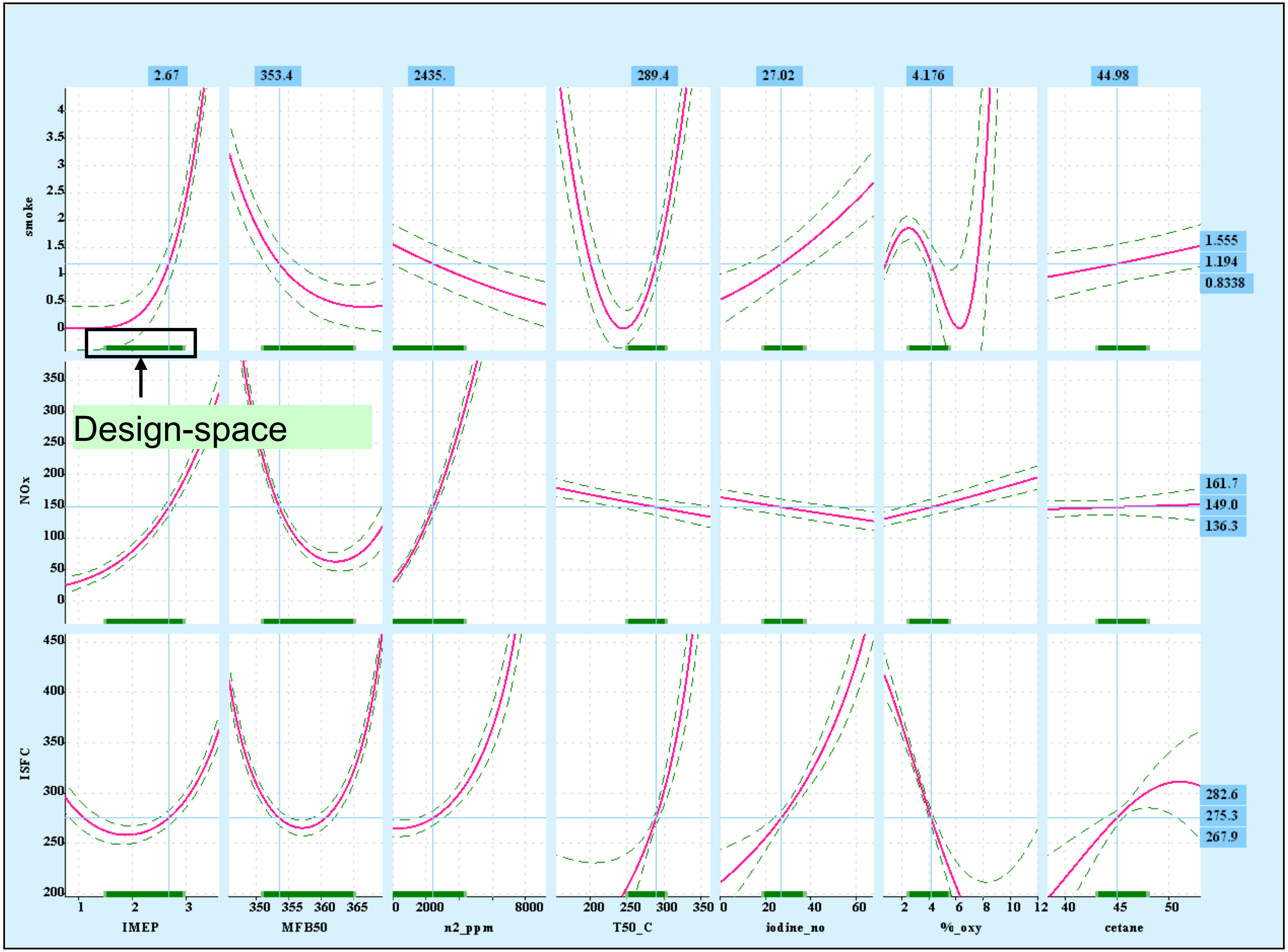
High F-Test = model terms are significant

Measurements vs run order with AVL CAMEO©



- **Blue = experimental points**
- **Red = model results**
- **Run order sequence shows**
  - **Timing sweeps**
  - **Characteristics of groups of fuels**
  - **Visualization of ability to model experiments**

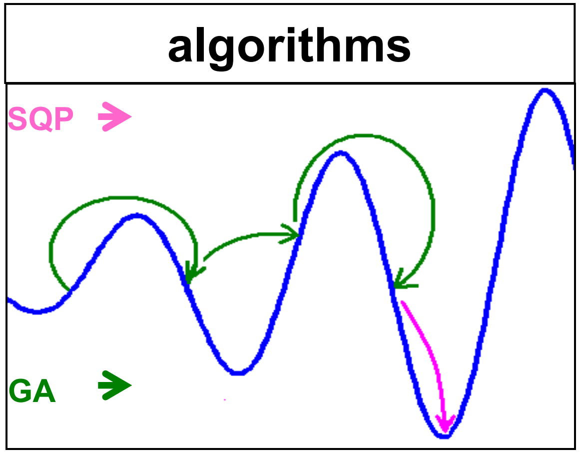
Models of ISFC, NOx, Smoke with AVL CAMEO©



Optimization with AVL CAMEO©

Standard algorithms (SQP, Genetic) allow the user to find :

- **Optimum of ISFC within design-space under constraints of emission limits**
- **Compromises NOx vs ISFC, Smoke vs NOx, …etc**
- **Optimum Engine Response Maps & Multiple Visualization Tools**



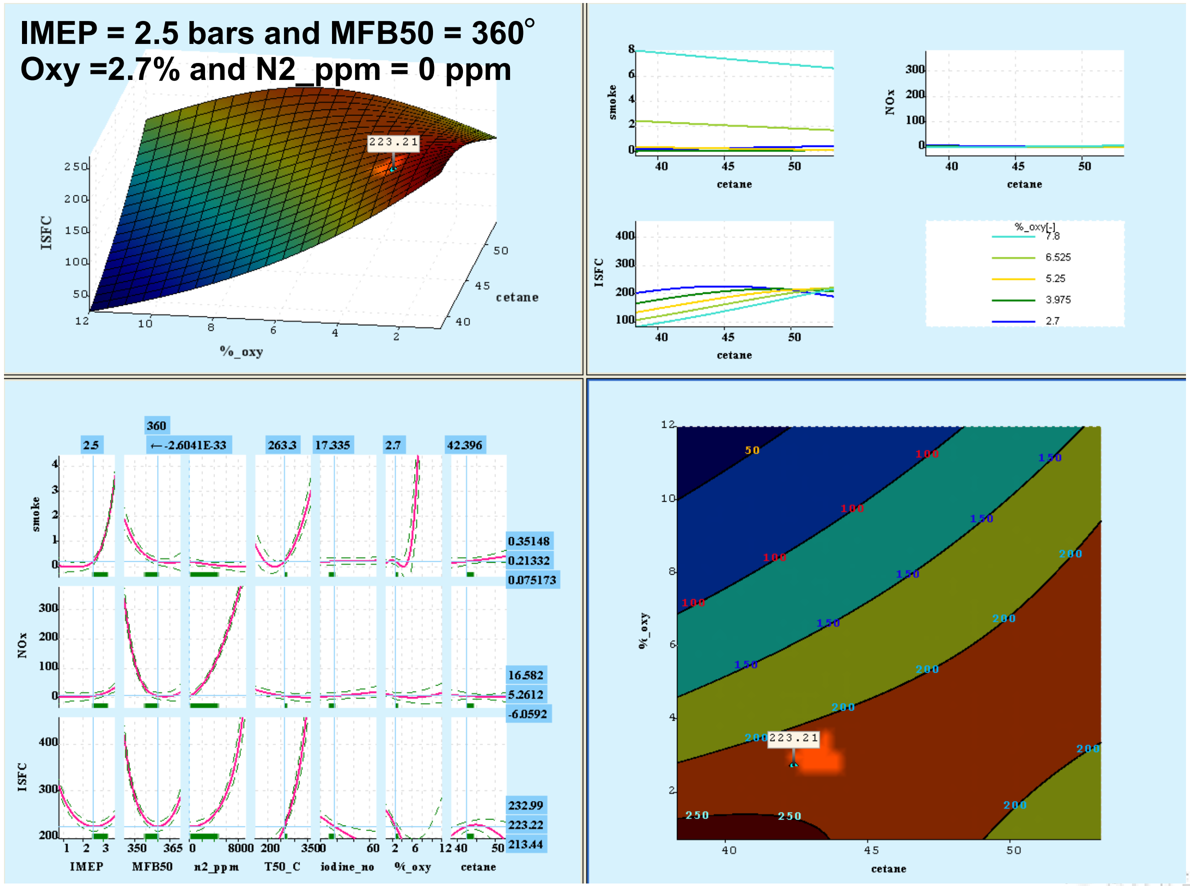
Example :

Target : Min ISFC in design-space

Constraint 1 : NOx < 20ppm

Constraint 2 :Smoke < 1 FSN

Optimization results based on models must be confirmed during verification tests

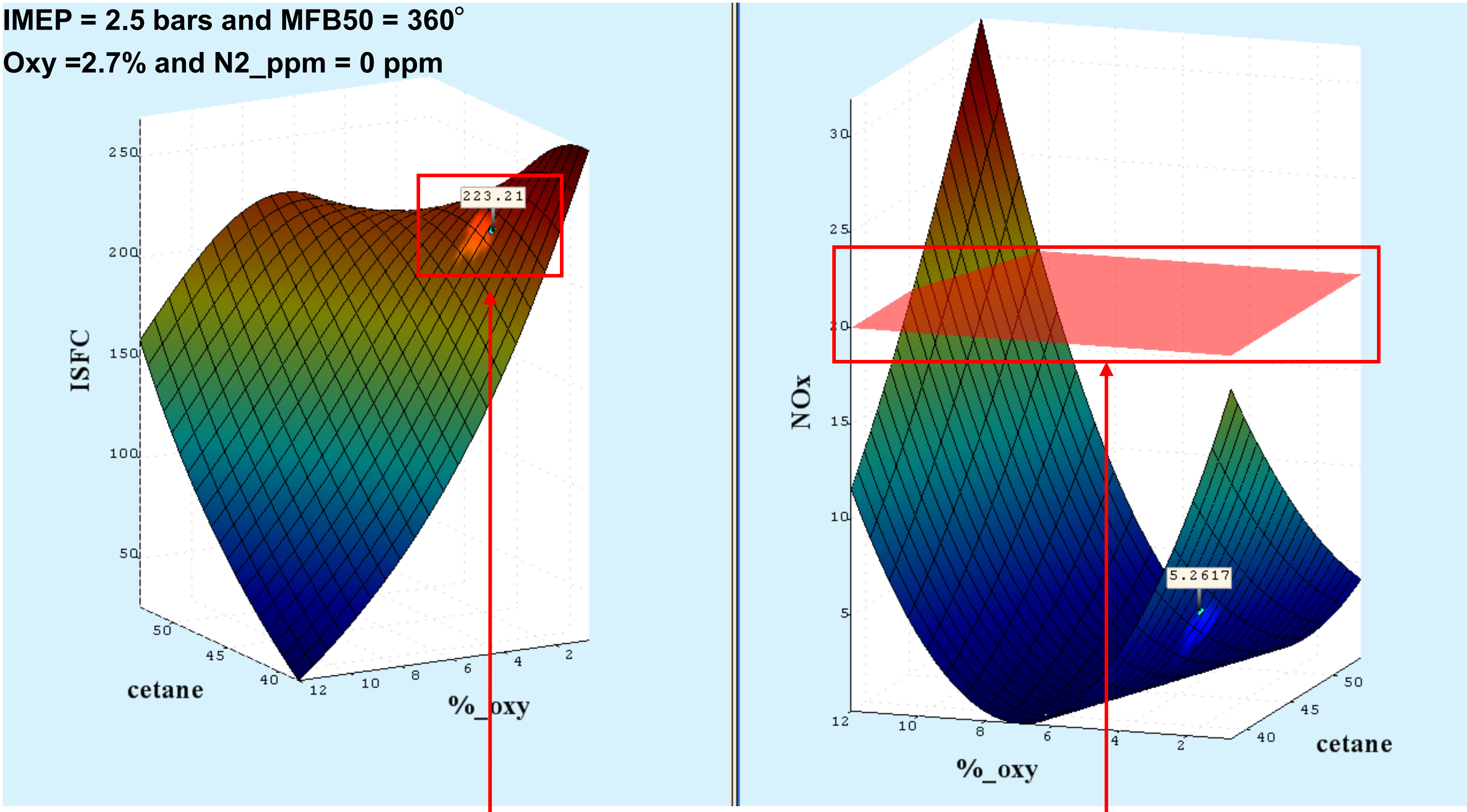


IMEP = 2.5 bars and MFB50 = 360°
Oxy =2.7% and N2_ppm = 0 ppm

Response Maps with AVL CAMEO© after optimization

example of a minimum of ISFC with NOx constraint under 20 ppm

Minimum ISFC fuel = 263 T50, 17.3 iodine, 2.7 oxygen, 42.3 cetane


IMEP = 2.5 bars and MFB50 = 360°

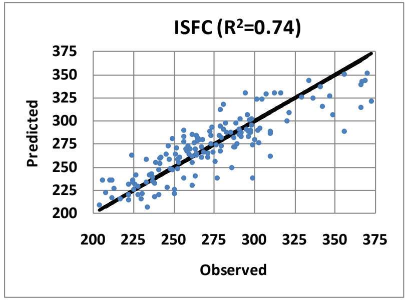
Oxy =2.7% and N2_ppm = 0 ppm

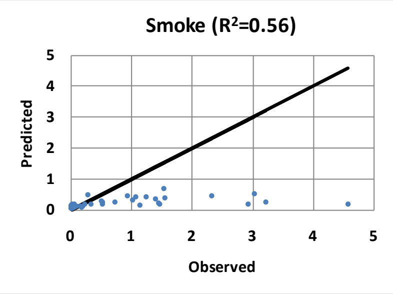
The result of the optimization must remain in the design-space (highlighted area of the response map)

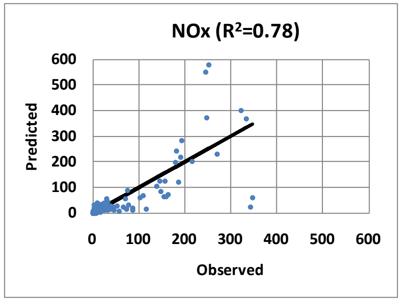
Limit of optimization NOx < 20 ppm

PCA based fuel modeling and statistical analysis

- Principal components (vectors) formulated from 11 selected fuel variables
  - T10, T50, T90, MonoArom, PolyArom, BioD, Oxy, Iodine, Nnat, Nadd, and SpGrv)
  - Any fuel can be represented by numeric vector values, which are used as input to the engine model
- Engine model
  - 5 vector values for fuels, 2 control variables for engine (IMEP, MFB50)
  - 9 variables representing test series to help assign systematic variation between experiments
- Models include:
  - Engine simulator: engine response to fuel and control variables
  - Fuel simulator: conversion between vector values and fuel variables
  - Models are embedded into excel workbooks for ease of use

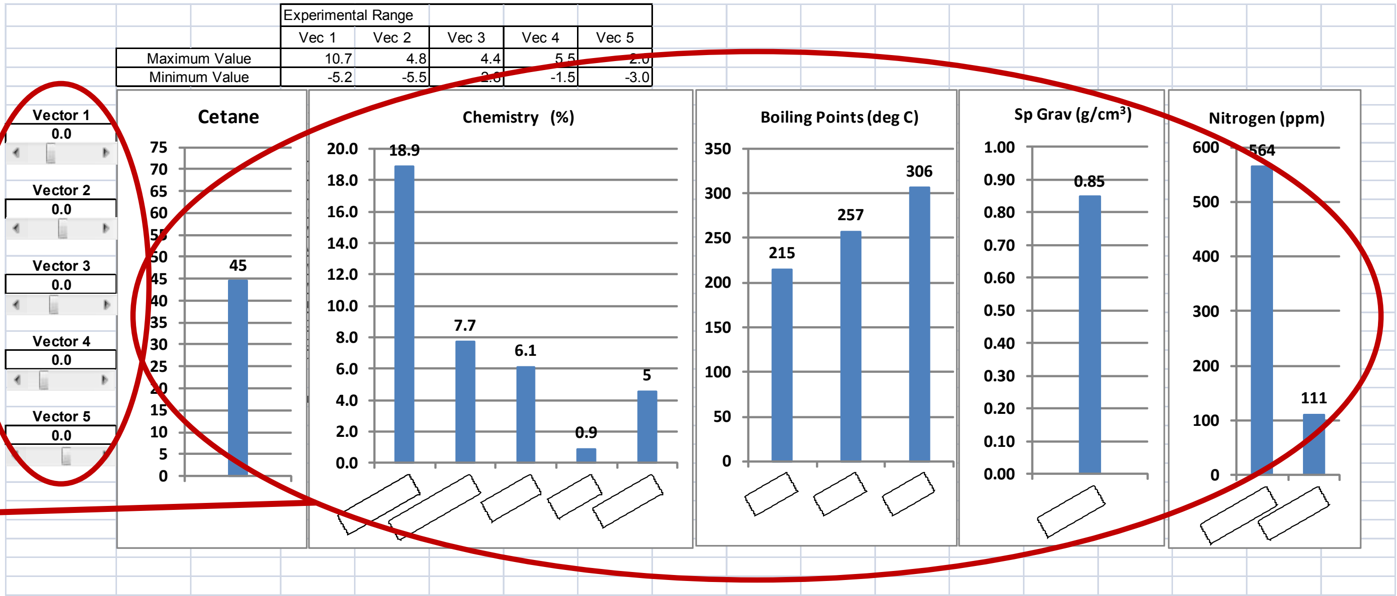

ISFC (R^2=0.74)


Smoke (R^2=0.56)


NOx (R^2=0.78)

Fuel and engine simulators

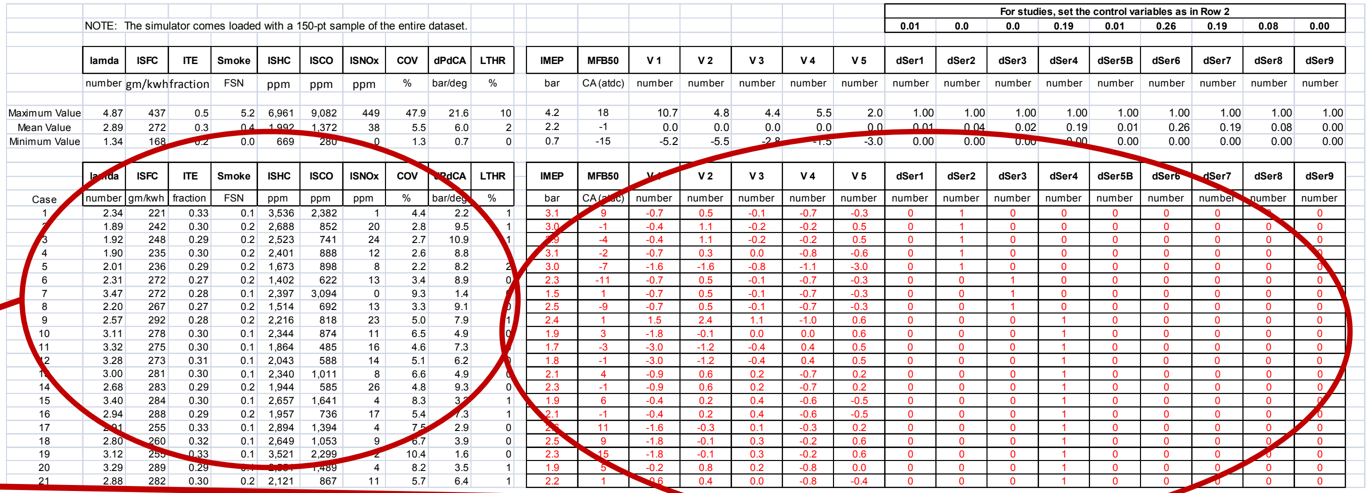
- **Fuel simulator, panel format shown, allows conversion from properties, chemistry, and vectors**
  - **Vector inputs**
  - **Property and chemistry outputs**



	Experimental Range				
	Vec 1	Vec 2	Vec 3	Vec 4	Vec 5
Maximum Value	10.7	4.8	4.4	5.5	2.0
Minimum Value	-5.2	-5.5	-2.8	-1.5	-3.0

Vector 1
0.0
Vector 2
0.0
Vector 3
0.0
Vector 4
0.0
Vector 5
0.0

- **Engine simulator, calculates engine response to control and fuel inputs**
  - **Output area**
  - **Input area**



NOTE: The simulator comes loaded with a 150-pt sample of the entire dataset.

For studies, set the control variables as in Row 2								
0.01	0.0	0.0	0.19	0.01	0.26	0.19	0.08	0.00

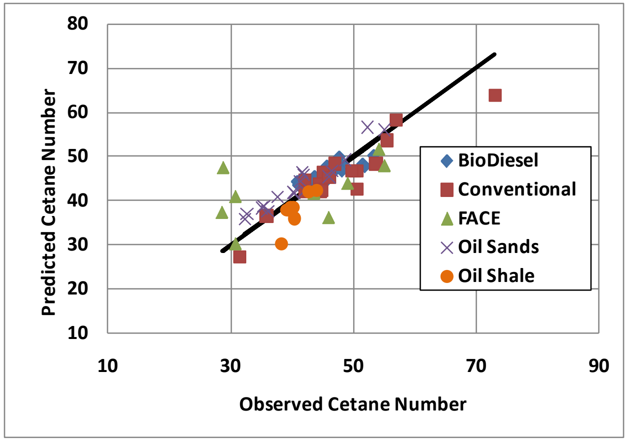
	lamda	ISFC	ITE	Smoke	ISHC	ISCO	ISNOx	COV	dPdCA	LTHR	IMEP	MFB50	V 1	V 2	V 3	V 4	V 5	dSer1	dSer2	dSer3	dSer4	dSer5B	dSer6	dSer7	dSer8	dSer9
	number	gm/kwh	fraction	FSN	ppm	ppm	ppm	%	bar/deg	%	bar	CA (atdc)	number	number	number	number	number	number	number	number	number	number	number	number	number	number
Maximum Value	4.87	437	0.5	5.2	6,961	9,082	449	47.9	21.6	10	4.2	18	10.7	4.8	4.4	5.5	2.0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Mean Value	2.89	272	0.3	0.4	1,992	1,372	38	5.5	6.0	2	2.2	-1	0.0	0.0	0.0	0.0	0.0	0.01	0.04	0.02	0.19	0.01	0.26	0.19	0.08	0.00
Minimum Value	1.34	168	0.2	0.0	669	280	0	1.3	0.7	0	0.7	-15	-5.2	-5.5	-2.8	-1.5	-3.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	lamda	ISFC	ITE	Smoke	ISHC	ISCO	ISNOx	COV	dPdCA	LTHR	IMEP	MFB50	V 1	V 2	V 3	V 4	V 5	dSer1	dSer2	dSer3	dSer4	dSer5B	dSer6	dSer7	dSer8	dSer9
Case	number	gm/kwh	fraction	FSN	ppm	ppm	ppm	%	bar/deg	%	bar	CA (atdc)	number	number	number	number	number	number	number	number	number	number	number	number	number	number
1	2.34	221	0.33	0.1	3,536	2,382	1	4.4	2.2	1	3.1	9	-0.7	0.5	-0.1	-0.7	-0.3	0	1	0	0	0	0	0	[illegible]	0
2	1.89	242	0.30	0.2	2,688	852	20	2.8	9.5	1	3.0	-1	-0.4	1.1	-0.2	-0.2	0.5	0	1	0	0	0	0	0	0	0
3	1.92	248	0.29	0.2	2,523	741	24	2.7	10.9	1	2.9	-4	-0.4	1.1	-0.2	-0.2	0.5	0	1	0	0	0	0	0	0	0
4	1.90	235	0.30	0.2	2,401	888	12	2.6	8.8	[illegible]	3.1	-2	-0.7	0.3	0.0	-0.8	-0.6	0	1	0	0	0	0	0	0	0
5	2.01	236	0.29	0.2	1,673	898	8	2.2	8.2	2	3.0	-7	-1.6	-1.6	-0.8	-1.1	-3.0	0	1	0	0	0	0	0	0	0
6	2.31	272	0.27	0.2	1,402	622	13	3.4	8.9	0	2.3	-11	-0.7	0.5	-0.1	-0.7	-0.3	0	0	1	0	0	0	0	0	0
7	3.47	272	0.28	0.1	2,397	3,094	0	9.3	1.4	0	1.5	1	-0.7	0.5	-0.1	-0.7	-0.3	0	0	1	0	0	0	0	0	0
8	2.20	267	0.27	0.2	1,514	692	13	3.3	9.1	0	2.5	-9	-0.7	0.5	-0.1	-0.7	-0.3	0	0	1	0	0	0	0	0	0
9	2.57	292	0.28	0.2	2,216	818	23	5.0	7.9	1	2.4	1	1.5	2.4	1.1	-1.0	0.6	0	0	0	1	0	0	0	0	0
10	3.11	278	0.30	0.1	2,344	874	11	6.5	4.9	0	1.9	3	-1.8	-0.1	0.0	0.0	0.6	0	0	0	1	0	0	0	0	0
11	3.32	275	0.30	0.1	1,864	485	16	4.6	7.3	0	1.7	-3	-3.0	-1.2	-0.4	0.4	0.5	0	0	0	1	0	0	0	0	0
12	3.28	273	0.31	0.1	2,043	588	14	5.1	6.2	0	1.8	-1	-3.0	-1.2	-0.4	0.4	0.5	0	0	0	1	0	0	0	0	0
13	3.00	281	0.30	0.1	2,340	1,011	8	6.6	4.9	0	2.1	4	-0.9	0.6	0.2	-0.7	0.2	0	0	0	1	0	0	0	0	0
14	2.68	283	0.29	0.2	1,944	585	26	4.8	9.3	0	2.3	-1	-0.9	0.6	0.2	-0.7	0.2	0	0	0	1	0	0	0	0	0
15	3.40	284	0.30	0.1	2,657	1,641	4	8.3	3.2	1	1.9	6	-0.4	0.2	0.4	-0.6	-0.5	0	0	0	1	0	0	0	0	0
16	2.94	288	0.29	0.2	1,957	736	17	5.4	7.3	1	2.1	-1	-0.4	0.2	0.4	-0.6	-0.5	0	0	0	1	0	0	0	0	0
17	2.01	255	0.33	0.1	2,894	1,394	4	7.5	2.9	0	[illegible]	11	-1.6	-0.3	0.1	-0.3	0.2	0	0	0	1	0	0	0	0	0
18	2.80	260	0.32	0.1	2,649	1,053	9	6.7	3.9	0	2.5	9	-1.8	-0.1	0.3	-0.2	0.6	0	0	0	1	0	0	0	0	0
19	3.12	255	0.33	0.1	3,521	2,299	2	10.4	1.6	0	2.3	15	-1.8	-0.1	0.3	-0.2	0.6	0	0	0	1	0	0	0	0	0
20	3.29	289	0.29	0.1	[illegible]	1,489	4	8.2	3.5	1	1.9	5	-0.2	0.8	0.2	-0.8	0.0	0	0	0	1	0	0	0	0	0
21	2.88	282	0.30	0.2	2,121	867	11	5.7	6.4	1	2.2	1	-0.6	0.4	0.0	-0.8	-0.4	0	0	0	1	0	0	0	0	0

PCA fuel model

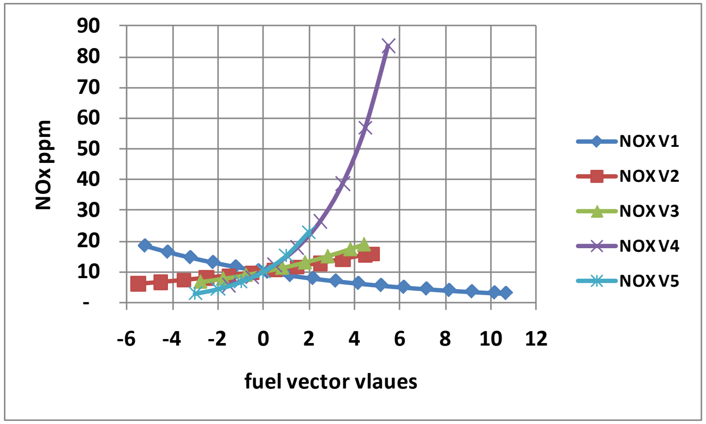
		Mean	Std Dev	Prin1	Prin2	Prin3	Prin4	Prin5
T10	deg C	216	34	0.391	0.118	0.300	-0.022	-0.163
T50	deg C	258	34	0.400	0.209	0.187	-0.192	-0.226
T90	deg C	306	34	0.343	0.313	0.012	-0.337	-0.190
MonoArom	wt %	18.7	7.8	-0.299	0.133	0.288	0.083	0.493
PolyArom	wt %	7.5	6.9	0.158	0.473	-0.271	0.263	0.378
BioD	vol %	6.3	14.3	0.350	-0.379	-0.242	0.062	0.138
Oxy	wt %	0.9	1.8	0.345	-0.388	-0.198	0.120	0.179
Iodine	number	4.9	11.3	0.310	-0.365	0.153	0.275	0.107
Nnat	ppm	653	2,112	0.034	-0.056	0.717	0.407	-0.056
Nadd	ppm	118	700	-0.014	0.247	-0.286	0.710	-0.466
SpGrv	gm/cm3	0.848	0.023	0.341	0.332	0.030	0.092	0.466

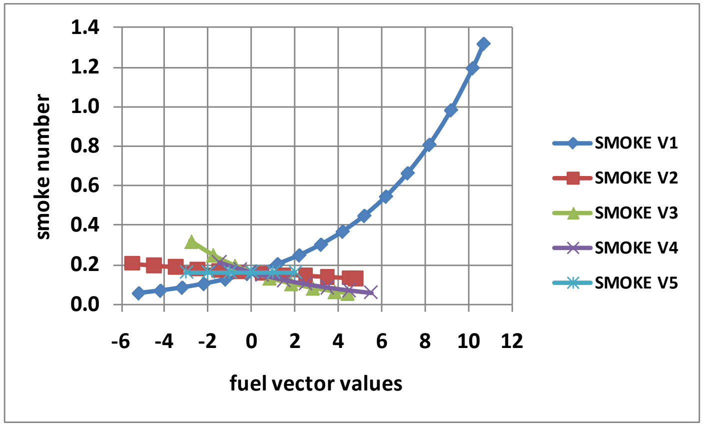
- Each of the 5 principal components above (vectors) is a linear combination of 11 fuel variables using coefficients shown
  - Each vector is orthogonal
  - There are 11 vectors in total, but these first 5 describe 90% of fuel variability
- This fuel model was developed to calculate cetane, and does not contain cetane as an input variable
  - Cetane model predicts about as well as ASTM D613 reproducibility (within ≈ 3.3, 19 of 20 measurements)

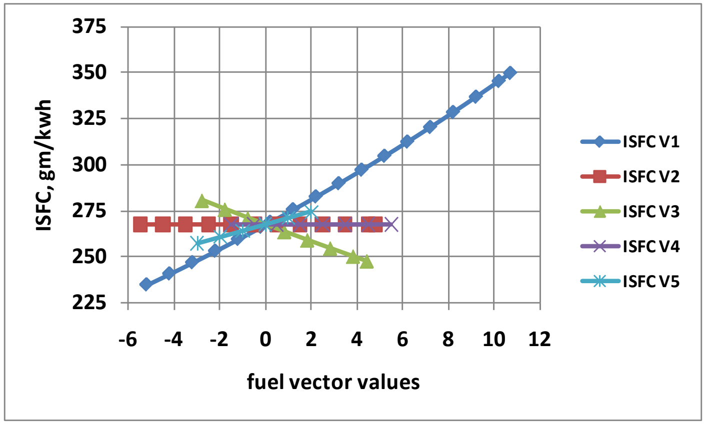


- Fuel vector values are used as input to the engine simulator

Optimization of fuels using PCA and corresponding engine simulator







- Engine simulator set for 2.5 bar IMEP, 360 MFB50, ‘average’ test series
- Since fuel vectors are independent, each can be exercised separately
- In this case, each vector was exercised over its range, with other vectors held at mid points
- Examining graphs,
  - Vector 4 and 5 must be less than 2 to meet NOx restraint of 20 ppm
  - Vector 1 must be less than 9 to meet smoke restraint of 1
  - Vector 1 must be minimum, vector 3 must be maximum, vector 5 minimum to minimize ISFC
- ¿¿¿ So ????
  - Now, we use fuel simulator to translate

Use of fuel simulator

- Use fuel simulator to create 1000 random fuels, covering vector range of all fuels
- Then, for this particular study, choose only conventional fuels (i.e., no biodiesel, no oxygen, no iodine, no nitrogen)
  - This reduces 1000 fuels to 11 fuels
- Rank fuels by V1 (minimize to reduce ISFC)
- Use engine simulator to confirm performance for these fuels
- Choose fuels providing lowest ISFC and meeting NOx and smoke constraints
- Optimum fuel:
  - Below average for cetane, distillation, and specific gravity
  - Above average for mono-aromatics, very low poly-aromatics

Cetane	T10	T50	T90	MonoArom	PolyArom	BioD	Oxy	Iodine	Nnat	Nadd	SpGrv
39.5	137	188	259	29.73	2.65	0	0	0	0	0	0.813
39.8	142	194	264	29.75	3.53	0	0	0	0	0	0.817

Conclusions

- Statistical analysis can help unlock complex data sets, allowing determination of relationships and effects
- ‘Messy’ data sets can be fully mined for information, as long as one is careful with model behavior and extrapolation
- Variables used to represent fuels included:
  - Cetane, T50, oxygen, iodine, nitrogen (CAMEO, for oxygen containing fuels)
  - T10, T50, T90, mono-aro, poly-aro, bio-diesel, oxygen, iodine, nitrogen (both), SG (PCA, all fuels)
- A large data set like this offers too many degrees of freedom for a single optimization, one must fix some engine and fuel variables
- Models can be used to find fuels meeting desired performance targets under a wide variety of chemistry or property targets
  - Examples given for biofuels and conventional diesel fuels

Accomplishments for 2010, plans for 2011

- Combined and analyzed multiple data sets of diesel range fuels
  - Gasoline range data would logically be next
- Evaluated two commercial codes for statistical analysis
  - This presentation highlights AVL CAMEO
- Developed generalized PCA modeling capability for fuels
  - This presentation also highlights PCA representation of fuels
- Completed funds-in project for CRC on gasoline HCCI fuel effects (AVFL13C)
- SAE paper on HCCI engine response for FACE diesel fuels
- 2011 plans – on hold pending funding decisions
  - Technical paper covering results in more detail
  - Similar analysis for gasoline range fuels
  - Other funds-in projects