Computer Simulation of a Flex-Fuel Engine Running on Different Gasoline-Hydrous Ethanol Blends

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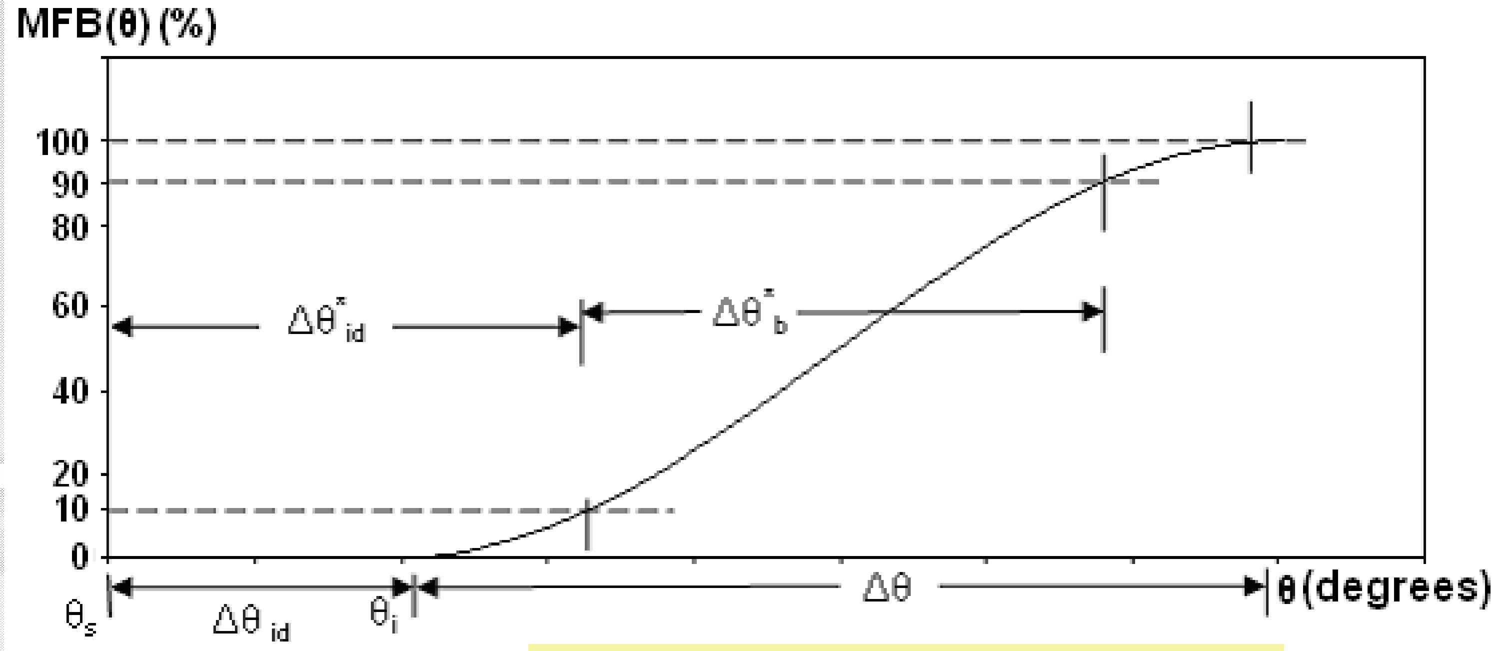
Introduction

- In 2003, Flex-Fuel vehicle was commercially introduced in the Brazilian market.
- Brazilian Flex-Fuel vehicles can work with gasohol (gasoline blended with 18-25% v/v of anhydrous ethanol), hydrous ethanol or any blends of these fuels.
- Since 2009, Flex-Fuel new vehicles sales are over 80% of total in the country.
- There are not so many published papers about Flex-Fuel engine simulation.
- There was a need to study engine simulations with a flex fuel engine for different blends of hydrous ethanol on gasoline using a commercial simulation software (AVL BOOST).

Combustion model

- Predefined heat release rate calculated by the Wiebe two zone equation (burned and unburned zones).
- Wiebe model is still used for quasi-dimensional combustion modeling.



(Wiebe Equation)

$$MFB(\theta) = \left(1 - \exp\left[-a\left(\frac{\theta - \theta_i}{\Delta\theta}\right)^{m+1}\right]\right) \times 100$$

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Heat Transfer Coefficient

- Newton heat transfer equation was used for the calculation of cylinder wall heat loss (Qw):
- $Qw = Ai \, . \, h \, (Tc - Tw)$
- The heat transfer coefficient (h) can be calculated as suggested by Woschni:
- $h_{woschni} = 0.013 D^{0.2} Pc^{0.8} Tc^{0.53} Vg^{0.8}$
- The wall temperature was constant and set to 120˚C

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NO_X Formation

Based on Zeldovich Mechanism (Pattas *et al.*, 1973; Heywood, 1988)

$$\frac{d[NO]}{dt} = NO\_POST \times NO\_MULT \times 2{,}0 \times (1-\varepsilon^2)\frac{R_1}{1+\varepsilon \times AK_2} \times \frac{R_4}{AK_4}$$

$$AK_2 = \frac{R_1}{R_2 + R_3}$$

$$AK_4 = \frac{R_4}{R_5 + R_6}$$

$$\varepsilon = \frac{[NO]}{[NO]_{eq}} \times \frac{1}{NO\_POST}$$

$R1 = k1 \times [O] \times [N_2]$
$R2 = k2 \times [N] \times [O_2]$
$R3 = k3 \times [N] \times [OH]$
$R4 = k4 \times [N_2O] \times [O]$
$R5 = k5 \times [O_2] \times [N_2]$
$R6 = k6 \times [OH] \times [N_2]$

- NO_POST and NO_MULT: BOOST Adjustment factors

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CO Formation

According to ONORATI *et al* (2001) and RAGGI (2005)

$$CO + OH \underset{k_{10}^{-}}{\overset{k_{10}^{+}}{\rightleftharpoons}} CO_2 + H \qquad R_{10} = k_{10}^{+} \times [CO]_{eq} \times [OH]_{eq}$$

$$CO_2 + O \underset{k_{11}^{-}}{\overset{k_{11}^{+}}{\rightleftharpoons}} CO + O_2 \qquad R_{11} = k_{11}^{-} \times [CO]_{eq} \times [O_2]_{eq}$$

$$\frac{d[CO]}{dt} = CO\_MULT (R_{10} + R_{11})(1 - \frac{[CO]}{[CO]_{eq}})$$

- CO_MULT - BOOST Adjustment factor

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HC Formation

1. Crevices - A fraction of the charge enters the crevice volumes
2. Fuel vapor is absorbed into the oil layer during the intake and desorbed later after combustion.
3. Quench layers on the combustion chamber wall since the flame extinguishes before reaching the walls.
4. Occasional partial burning or complete misfire occurring when combustion quality is poor
5. Direct flow of fuel vapor into the exhaust system during valve overlap in PFI engines

$$\frac{d[HC]}{dt} = -HC\_MULT \times HC\_POST \times HC\_PART \times 7{,}7 \times 10^{12} \times [O_2] \times [HC] \times \exp\left(\frac{18790}{T}\right)$$

- HC_MULT, HC_POST and HC_PART: BOOST Adjustment factors

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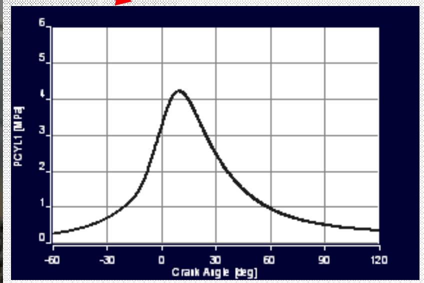
Engine Modeling – Experimental Data (FIAT FIRE 1.4 L, Tetrafuel)

- **Fuels: H0 (E25); H30; H50; H80; H100 at 60 & 105 Nm, 3875 rpm**



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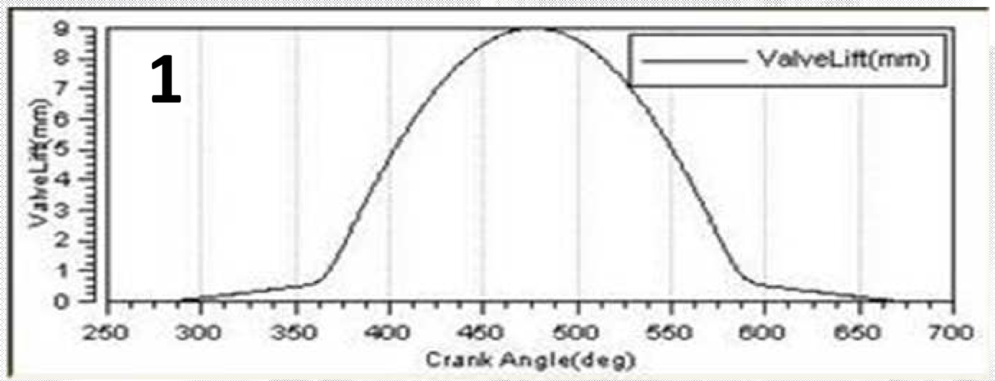
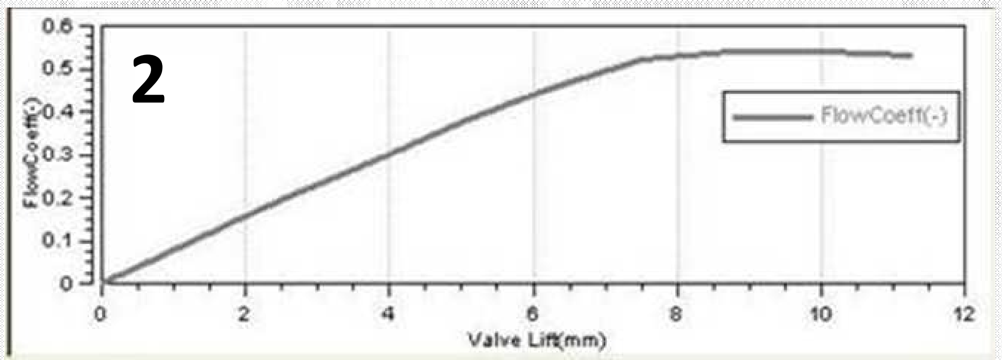
Engine Modeling

1. Intake and exhaust valves lift curves measured by laser alignment technique.

2. Discharge coefficient – determined experimentally on a flow bench.





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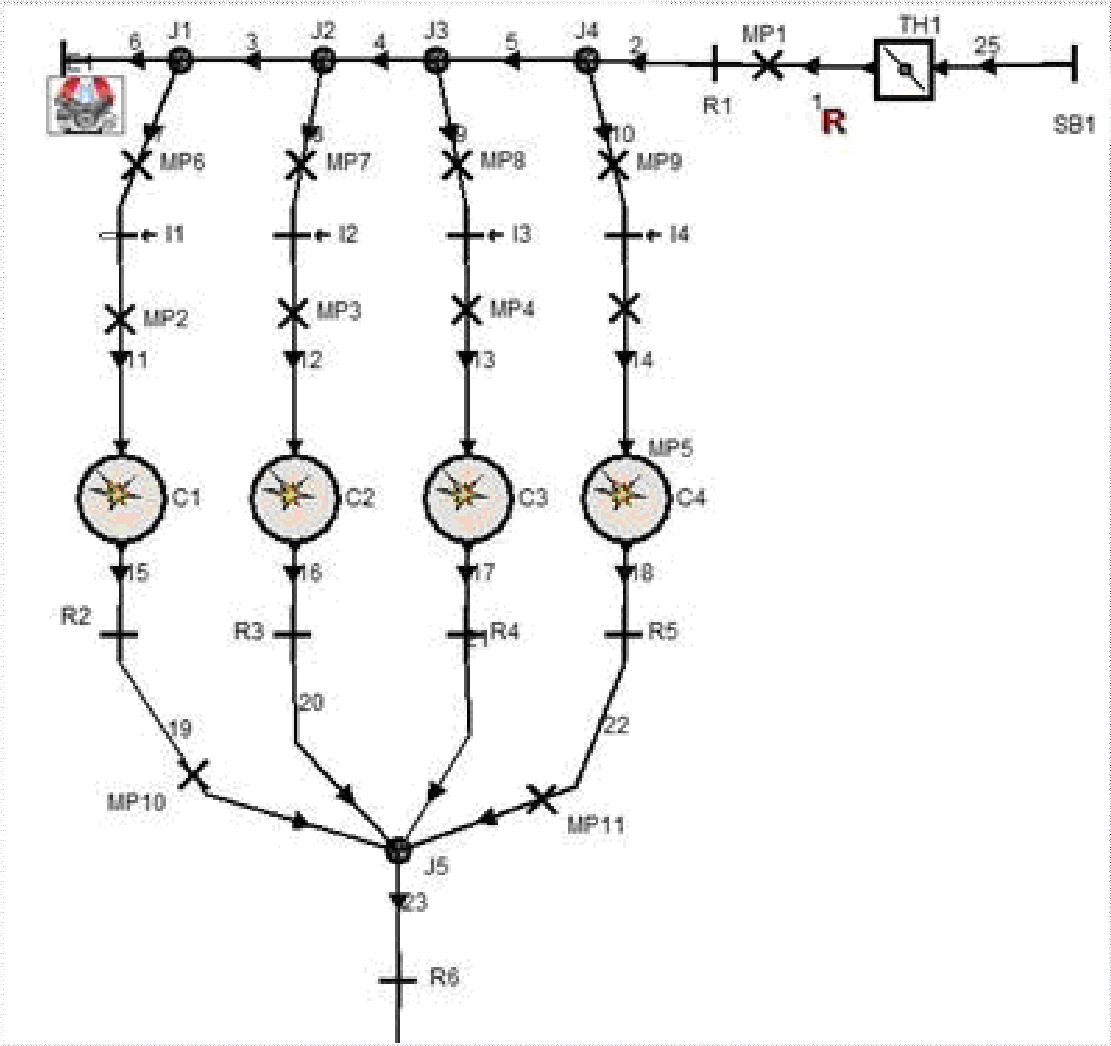
Engine Modeling



- **AVL BOOST TOOLS**: Modeling the cylinders, the intake and exhaust manifolds, the ducts and pipes, etc.

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Fuels Modeling

Properties	BOOST Gasoline	Gasoline Type A	Dif (%)
Molecular Weight (kg/kmol)	106	111	4,7
LHV (MJ/kg)	43,5	45,1	3,7
Carbon (% w/w)	87,6	86	1,8
Stoichometric Air-Fuel Ratio	14,5	14,8	2,1

- ✓ AVL BOOST - NASA algorithm for c_p (T) :

$$\frac{c_{p_k}}{R} = a_{1k} + a_{2k}T + a_{3k}T^2 + a_{4k}T^3 + a_{5k}T^4$$

- ✓ Blends of gasoline, ethanol and water allowed
- ✓ Real LHV and specific mass of the tested fuels
- ✓ Used BOOST gasoline

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Combustion Input Data – Wiebe 2 zones– 3875 rpm / 60 Nm

Fuel	Throttle Angle (Deg)	1% MFB (Deg BTDC)	(1-99%) MFB (Deg TDC)
H0	34.5	-3	49
H30	33.5	-9	48
H50	34.0	-14	54
H80	34.7	-15	55
H100	35.4	-13	56

Increased with ethanol

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Combustion Results – Wiebe 2 zones– 3875 rpm / 60 Nm

Fuel	H0	H30	H50	H80	H100
a	3.8	4.8	5.1	5.5	3.8
m	1.00	1.00	1.00	1.00	1.00
1-99% MFB	49	48	54	55	56

Fuel	Pmax EXP (MPa)	Pmax SIM (MPa)	Dif (%)	IMEP EXP (MPa)	IMEP SIM (MPa)	Dif (%)	Vair (kg/h)	Vair SIM (kg/h)	Dif(%)
H0	2.64	2.68	1.5	0.62	0.62	0.0	24.59	24.47	-0.5
H30	3.34	3.41	2.1	0.62	0.62	0.0	23.22	23.24	0
H50	3.77	3.79	0.5	0.63	0.64	1.6	23.89	23.74	-0.6
H80	4.01	4.09	2.0	0.63	0.63	0.0	24.7	24.61	-0.4
H100	4.10	4.09	-0.2	0.63	0.64	1.6	25.34	25.49	0.6

Differences < 2.0%

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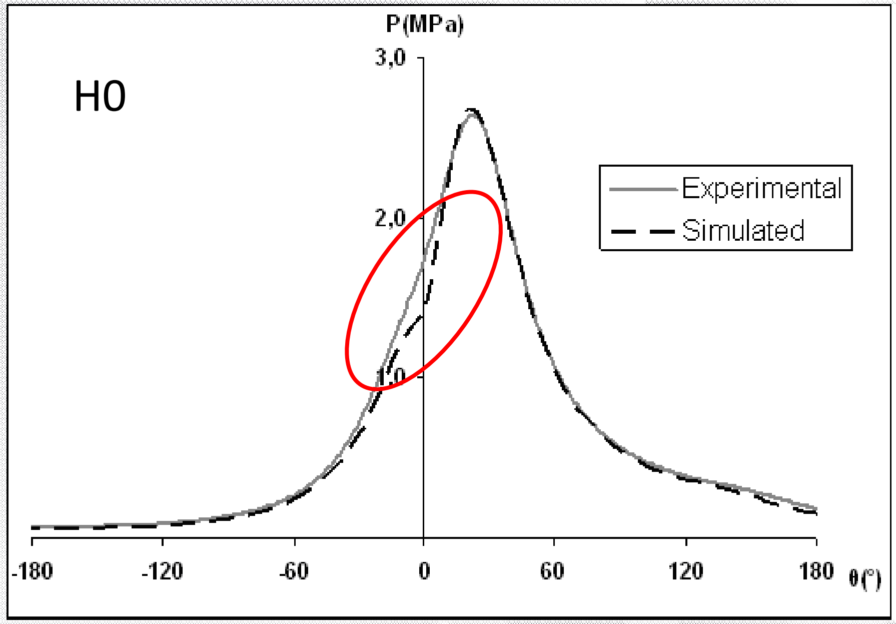
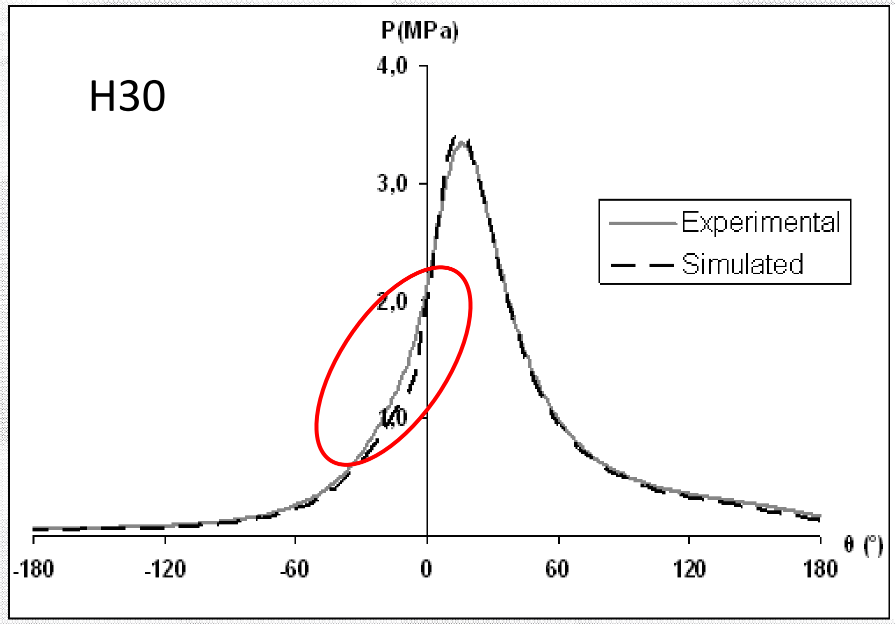
Experimental x Simulated Pressure Curves – 60 Nm





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Emission Input Data – Wiebe 2 zones– 3875 rpm / 60 Nm

AVL BOOST emission parameters used in the simulation

Fuel	CO_MULT	NOX_MULT	NOX_POST	HC_MULT	HC_POST	HC_PARTIAL
H0	0.03	1	0.5	1	0.5	1
H30	0.018	1	0.4	1	0.6	1
H50	0.013	1	0.34	1	0.8	1
H80	0.0003	1	0.29	1	2	1
H100	0.0003	1	0.31	1	2	1

Very Low

- NO_X and HC – Only adjusted NO_POST and HC_POST (Post Oxidation)

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Emission Results – Wiebe 2 zones– 3875 rpm / 60 Nm

Fuel	CO EXP (%)	CO SIM (%)	Dif (%)	THC EXP (ppm)	THC SIM (ppm)	Dif (%)	NOX EXP (ppm)	NOX SIM (ppm)	Dif (%)
H0	0.512	0.520	1.6	598	604	1.0	2096	2091	-0.2
H30	0.505	0.503	-0.4	703	694	-1.3	2638	2615	-0.9
H50	0.478	0.476	-0.4	666	666	0	2766	2778	0.4
H80	0.485	0.481	-0.8	614	617	0.5	2650	2657	0.3
H100	0.475	0.284	-40.2	688	677	-1.6	2521	2511	-0.4

Impossible to simulate

Differences < 2,0% with exception of <u>H100</u>

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Combustion Input Data – Wiebe 2 zones– 3875 rpm /105 Nm

Fuel	Throttle Angle (Deg)	1% MFB (BTDC)	(1-99%) MFB (TDC)
H0	46,1	-6	48
H30	45	-8	51
H50	46,5	-12	53
H80	48,5	-13	54
H100	51	-14	56

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Combustion Results –Wiebe 2 zones– 3875 rpm /105 Nm

	H0	H30	H50	H80	H100
a	5.9	7.3	7.3	6.5	6.4
m	1.00	1.00	1.00	1.00	1.00
1-99% MFB	48	51	53	54	56

→ Similar Behavior of 60 Nm

Fuel	Pmax EXP (MPa)	Pmax SIM (MPa)	Dif (%)	IMEP EXP (MPa)	IMEP SIM (MPa)	Dif (%)	Vair EXP (kg/h)	Vair SIM (kg/h)	Dif (%)
H0	4.85	4.94	1.9	1.02	1.02	0.0	141.75	142.42	0.5
H30	5.21	5.29	1.5	1.02	0.97	-4.9	137.51	137.88	0.3
H50	5.88	5.93	0.9	1.03	0.99	-3.9	140.59	141.39	0.6
H80	5.99	6.11	2.1	1.03	1.04	1.0	145.07	145.28	0.1
H100	6.22	6.38	2.6	1.03	1.08	4.8	149.26	149.68	0.3

Differences < 5%

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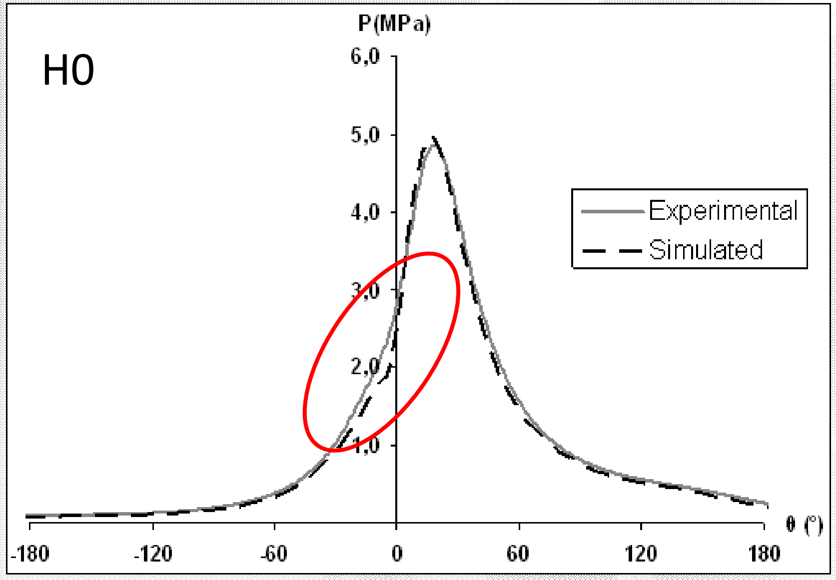
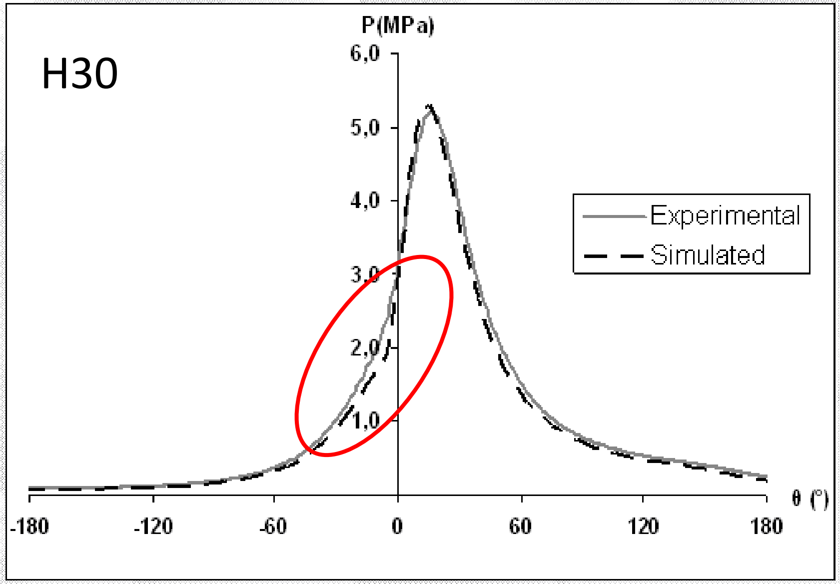
Experimental x Simulated Pressure Curves – 105 Nm





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Emission Input Data –Wiebe 2 zones– 3875 rpm /105 Nm

AVL BOOST emission parameters used in the simulation

Fuel	CO_MULT	NOx_MULT	NOx_POST	HC_MULT	HC_POST	HC_PARTIAL
H0	0,0003	1	1.06	1	3.7	1
H30	0,00001	1	0.56	1	0,8	1
H50	0,000001	1	0,35	1	0,4	1
H80	0,000001	1	0,25	1	0.14	1
H100	0,000001	1	0,19	1	0.1	1

Very Low

NO_X and HC – Only adjusted NO_POST and HC_POST (As at 60 Nm)

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Emission Results –Wiebe 2 zones– 3875 rpm /105 Nm

Fuel	CO EXP (%)	CO SIM (%)	Dif (%)	THC EXP (ppm)	THC SIM (ppm)	Dif (%)	NOX EXP (ppm)	NOX SIM (ppm)	Dif (%)
H0	1.94	1.96	1	1064	1056	-0.1	1940	1938	-0.1
H30	1.98	1.01	-44	1011	1006	-0.5	1897	1968	3.7
H50	1.69	0.73	-57	1056	1038	-1.7	1955	1907	-3.4
H80	1.63	0.49	-70	1091	1147	5.1	1892	1980	4.7
H100	1.5	0.42	-72	1110	1052	-5.2	1888	1850	-2

Impossible to simulate

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Conclusion

- Simulation results of maximum pressure and IMEP presented differences below 5%, compared to experimental results, for all tested fuels.

- Wiebe parameter *a* presented a non linear pattern variation with ethanol addition, when keeping *m* parameter fixed and equal to 1.

- Emission simulation using fixed emission parameters for NOx, THC and CO was not satisfactory, when changing fuels.

- Using specific adjustments for the pos-oxidation mechanism (THC and NOx) and kinetic reaction (CO) for each fuel, it was possible to achieve good results with exception of CO at 105 Nm for fuels from H30 to H100 and CO at 60 Nm for H100.

- The results showed that the model can not have a predictive behavior for ethanol addition, when using the same emission parameter adjustment.

- It is necessary other studies to improve the model and the software for ethanol use.

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