



COMBUSTION MODELLING OF A GASOLINE ENGINE BY THE WEIBE FUNCTION

A thermodynamic simulation of a reciprocating-engine cycle is to be performed using a Weibe function to model the combustion process, with typical parameters for a spark-ignition internal-combustion-engine (SI-ICE): $a=5$, $m=3$, $\theta_{bs}=-10^\circ$, $\Delta\theta_{bs}=60^\circ$. The model is to be applied to an engine with the following characteristics (Yamaha YZ250FN motorcycle): single cylinder ($Z=1$), four-stroke ($S=4$), 250 cc ($V_d=249$ cm³ of displacement), bore $D=0.0770$ m, stroke $L=0.0526$ m, and compression ratio $r=12.5$. Only the compression and expansion strokes are to be simulated, with the crank angle (θ) as the independent variable, and only at the steady state corresponding to full load at $n=8500$ rpm. Assume the cylinder is supplied with an stoichiometric mixture at ambient conditions, with unit volumetric efficiency, and approximate gasoline properties by n-octane if needed. To do:

- Compute clearance volume, trapped mass of air and fuel, and chemical energy released per cycle.
- Compute chemical energy release as a function of θ , for the ideal Otto cycle and for the Weibe model, and make a plot.
- Establish the energy balance for the gas, and get a single differential equation to compute the pressure profile $p(\theta)$.
- Solve numerically for $p(\theta)$, $T(\theta)$ and the contribution to the shaft work at each step, and plot them.
- Find the mean effective pressure, the shaft power and the energy efficiency of the engine

🇪🇸 Se va a hacer una simulación termodinámica del proceso de combustión en un motor alternativo mediante la función de Weibe, con parámetros típicos de un motor de encendido provocado ($a=5$, $m=3$, $\theta_{bs}=-10^\circ$, $\Delta\theta_{bs}=60^\circ$), aplicándolo a un motor de las siguientes características (Yamaha YZ250FN): un sólo cilindro ($Z=1$), de cuatro tiempos ($S=4$), 250 cm³ ($V_d=249$ cm³ de desplazamiento), diámetro $D=0,0770$ m, carrera $L=0,0526$ m, y relación de compresión de $r=12,5$. Sólo se van a simular las carreras de compresión y expansión, con el ángulo de cigüeñal, θ , como variable independiente, y sólo en régimen estacionario a plena carga a $n=8500$ rpm. Suponer que el cilindro se llena con una mezcla estequiométrica en condiciones ambiente, con rendimiento volumétrico unidad, y aproximar las propiedades de la gasolina por las del n-octano. En particular, se pide:

- Calcular el volumen muerto, las masas de aire y combustible atrapadas, y la energía química liberada por ciclo.
- Calcular la energía química liberada en función de θ , para el ciclo Otto ideal y en el modelo de Weibe.
- Establecer el balance energético para el gas, y obtener una ecuación diferencial para el perfil de presiones, $p(\theta)$.
- Resolver numéricamente lo anterior, y hallar $p(\theta)$, $T(\theta)$ y la contribución al trabajo al eje en cada etapa del ciclo.
- Calcular la presión media efectiva, la potencia al eje, y el rendimiento energético del motor.

Solution.

- Compute clearance volume, trapped mass of air and fuel, and chemical energy released per cycle.

First, there is a redundancy in data, since $V_d = \pi D^2 L / 4$; the discrepancy is $V_d - \pi D^2 L / 4 = 249 \cdot 10^{-6} - \pi \cdot 0.0770^2 \cdot 0.0526 / 4 = 4 \cdot 10^{-6} \text{ m}^3$; i.e. a 1.6% attributable to data uncertainty. Let use the direct data $V_d = 249 \cdot 10^{-6} \text{ m}^3$.

Clearance volume V_{cl} is deduced from compression ratio: $r = (V_{cl} + V_d) / V_{cl}$; $V_{cl} = V_d / (r - 1) = 249 \cdot 10^{-6} / (12.5 - 1) = 22 \cdot 10^{-6} \text{ m}^3$ (22 cm³).

Trapped mass of mixture is deduced from ideal gas law:

$$m = \frac{pV}{RT} = \frac{p_0 (V_{cl} + V_d)}{R_a T_0} = \frac{10^5 \cdot (22 + 249) \cdot 10^{-6}}{287 \cdot 288} = 0.33 \cdot 10^{-3} \text{ kg} \quad (1)$$

(checking: ¼ litre approx. ¼ gram); this is roughly the mass of air, since air/fuel ratios are large.

For the stoichiometric air/fuel ratio, equating $\text{C}_8\text{H}_{18} + a\text{O}_2 = 8\text{CO}_2 + 9\text{H}_2\text{O}$ one gets $a = 8 + 9/2 = 12.5$ and thence $A = a/c_{21} = 12.5/0.21 = 59.5 \text{ mol}_{\text{air}}/\text{mol}_{\text{octane}} = 59.5(0.029/0.114) = 15.1 \text{ kg}_{\text{air}}/\text{kg}_{\text{octane}}$.

For the four-stroke cycle, to that mass of fuel, $m_F = m_a / A = 0.33 \cdot 10^{-3} / 15.1 = 0.022 \cdot 10^{-3} \text{ kg}$, corresponds a heating value of:

$$Q_{\text{cycle}} = m_F h_{\text{LHV}} = \frac{m_a}{A_0} h_{\text{LHV}} = \frac{0.33 \cdot 10^{-3}}{15.1} 46 \cdot 10^6 = 1010 \text{ J} \quad (2)$$

where a $h_{\text{HHV, gasoline}} = 46 \text{ MJ/kg}$ available from the fuel tables was used (the values for octane can be computed from standard thermochemical tables as $h_{\text{HV}} = -8h_{\text{fCO}_2}^{\ominus} - 9h_{\text{fCO}_2}^{\oplus} + 8h_{\text{fCO}_2}^{\ominus}$, what yields $h_{\text{HHV, n-octane}} = 48.0 \text{ MJ/kg}$ and $h_{\text{LHV, n-octane}} = 44.5 \text{ MJ/kg}$). In the air-standard Otto cycle, both for constant volume heat deposition and for finite heat-release rate, the real combustion process (of internal energy exchange from chemical energy to thermal energy) is be modelled as a simple heat flow, in the amount Q_{cycle} , to unreacting air.

b) Compute chemical energy release as a function of θ , for the ideal Otto cycle and for the Weibe model, and make a plot.

There is an instantaneous heat addition in the ideal Otto cycle at the top dead centre, TDC (constant volume process), i.e. the accumulated energy added is zero up to the TDC and $Q_{\text{cycle}} = 1010 \text{ J}$ after that, whereas in the Weibe model the accumulated energy added is a smooth function that starts at -10° crank-angle and prolongs during 60° for completion; the relative value, coincident with the fuel mass-fraction burnt, is:

$$y_{F, \text{burnt}} = \frac{Q_{\text{acc}}}{Q_{\text{cycle}}} = 1 - \exp \left[-a \left(\frac{\theta - \theta_s}{\Delta \theta_d} \right)^m \right] \quad (3)$$

and both, accumulated-heat and their derivatives, for the ideal-Otto and Weibe-function models, are shown in Fig. 1.

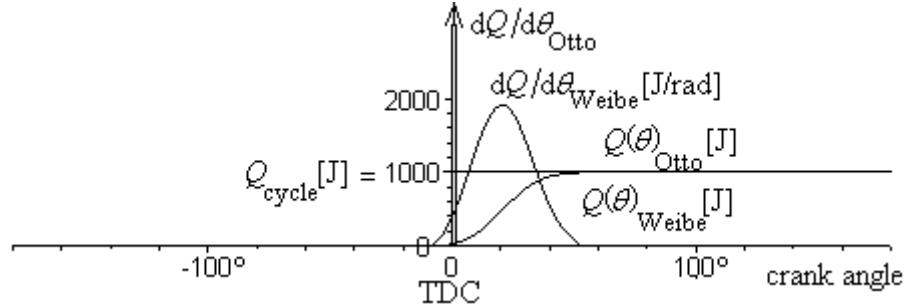


Fig. 1. Heating laws during the compression and expansion strokes, according to ideal Otto cycle and to Weibe function.

c) Establish the energy balance for the gas, and get a single differential equation to compute the pressure profile $p(\theta)$.

Once the intake valve closes (say at -140° TDC; it might have opened at about -185° TDC and have a crossing with the exhaust valve, that might close at about -178° TDC), the energy balance for the control mass in an infinitesimal evolution, assumed to have the air properties, is

$$mc_{va}dT/d\theta = dQ/d\theta - p dV/d\theta \quad (4)$$

where only one-zone model (uniform temperature in the whole mass) is used, with a constant thermal capacity at constant volume, c_v , and with the particular value for room air, instead of that of the mixture and at highly changing temperatures; moreover, the same simplification will be later done for γ ; i.e we take $\gamma=1.4$ in spite that for the air/fuel mixture is a little lower (in the case of large-molecule fuels), for the exhaust gases is always lower, and it further decreases with temperature (e.g. $\gamma=1.3$ at 1000 K).

The term $dQ/d\theta$ in (4) is the net heat transfer to the control mass, accounting for the real heat transfer to or from the walls, and the virtual heat transfer corresponding to the chemical energy release:

$$\frac{dQ}{d\theta} = \frac{hA(\theta)(T_w - T(\theta))}{d\theta/dt} + \frac{dQ_{acc}}{d\theta} \quad (5)$$

where h , the convective heat-transfer coefficient, can be estimated from a typical Nusselt correlation $Nu = aRe^n$ with the Reynolds number corresponding to the piston velocity. In spite of the very high temperatures involved, this real heat-transfer term is not too-high in practice, because at the steady state the walls reach an intermediate temperature, T_w , (with small fluctuations along the cycle), decreasing the temperature jump and giving back some heat to the cold gas during the initial phase of compression. No real heat transfer is incorporated in the present model ($h=0$).

The term $dV/d\theta$ is in (4) is given by the slide-rod / crank-shaft mechanism:

$$V(\theta) = V_{cl} + \frac{V_d}{2} \left(\sqrt{s^2 - \sin^2(\theta)} + 1 - s - \cos(\theta) \right) \quad (6)$$

in terms of the clearance volume $V_{cl}=22 \cdot 10^{-6}$, the displacement volume $V_d=249 \text{ cm}^3$, and the slide-rod /crank length-ratio, typically of order $s=3$ (has very small influence). As we want to go to a single equation in the pressure evolution, expressions for $dT/d\theta$ and $dQ/d\theta$ must be substituted in terms of $p(\theta)$. The former is found from the ideal gas equation:

$$m_a R_a T = pV, \quad m_a R_a dT/d\theta = V dp/d\theta + p dV/d\theta \quad (7)$$

and the $dQ/d\theta$ term is obtained deriving Q_{acc} from (3), taking care because of the piecewise character of the function. Combining (6) with (4) yields:

$$V dp/d\theta + p dV/d\theta = (R_a/c_{va})(dQ_{acc}/d\theta - p dV/d\theta) \quad (8)$$

an ordinary differential equation in $p(\theta)$ after substitution of the two explicit terms $dQ_{acc}/d\theta$ and $dV/d\theta$ from (3) and (5).

d) Solve numerically for $p(\theta)$, $T(\theta)$ and the contribution to the shaft work at each step, and plot them.

Equation (5) is a non-linear ordinary first-order differential equation, easily solved numerically by the Euler or better Runge-Kutta method, starting with the initial conditions prevailing at the inlet-valve-close position (say -140° TDC), with $dQ_{acc}/d\theta=0$ up to the spark (the delay to start burning is a few degrees and is neglected here), and with $dQ_{acc}/d\theta$ given by (1) from there up to the exhaust-valve-open position (say 130° TDC), although, in what follows, we do not take these valve events into consideration (i.e. we take them at -180° TDC and $+180^\circ$ TDC, or $-\pi$ and π , since we shall work in radians).

In the case of the ideal Otto cycle there is a closed solution, since the combination of the ideal gas equation and the energy equation for $Q_{acc}=0$ (except at the singularity) yields the isentropic relation $pV^\gamma=\text{constant}$, i.e.:

$$p(\theta) = p_0 \left(\frac{V_{cl} + V_d}{V(\theta)} \right)^\gamma \quad \text{and} \quad T(\theta) = T_0 \left(\frac{V_{cl} + V_d}{V(\theta)} \right)^{\gamma-1} \quad \text{during compression} \quad (9)$$

starting at $\theta=-\pi$ with $p_1=p_0=100 \text{ kPa}$, $T_1=T_0=288 \text{ K}$ and ending at the TDC $\theta=0$ with $p_2=3.4 \text{ MPa}$, $T_2=790 \text{ K}$. The constant-volume heat addition cause a jump in temperature and pressure:

$$T_3 = T_2 + \frac{m_F h_{LHV}}{m_a c_{va}} \quad \text{and} \quad p_3 = p_2 \frac{T_3}{T_2} \quad (10)$$

up to $p_2=22 \text{ MPa}$, $T_2=5000 \text{ K}$, followed by an isentropic expansion:

$$p(\theta) = p_3 \left(\frac{V_{cl}}{V(\theta)} \right)^\gamma \quad \text{and} \quad T(\theta) = T_3 \left(\frac{V_{cl}}{V(\theta)} \right)^{\gamma-1} \quad \text{during expansion} \quad (11)$$

to $p_4=640 \text{ kPa}$, $T_4=1800 \text{ K}$. Figures 2 and 3 present pressure and temperature evolution with both models.

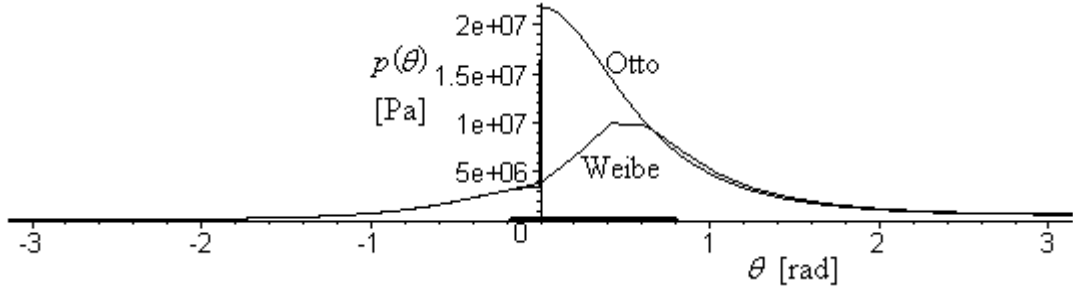


Fig. 2. Cylinder pressure p , versus crank-angle θ , for the ideal Otto cycle and Weibe model (thick line shows burning period).

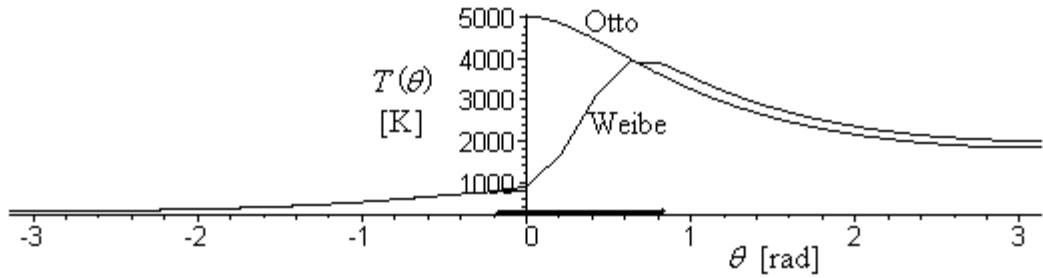


Fig. 3. Cylinder temperature T , versus crank-angle θ , for the ideal Otto cycle and Weibe model (thick line shows burning period).

If a very short burning period is introduced in the Weibe model, the numerical simulation recovers the ideal Otto cycle (instantaneous heat deposition). The most relevant difference between the instantaneous model and the 60° crank-angle burning-period is the lowering of the pressure (and to a lesser extent) temperature peaks, with a shift on the maximum position.

The contribution to the shaft work at each step is computed as follows. First, the shaft work is deduced from the pressure and volume change of the gases, $W_{\text{shaft}} = \int (p - p_0) dV$, where p_0 is crank-case pressure (assumed atmospheric), and thence applied to an infinitesimal time-step:

$$\dot{W}_{\text{shaft}} = \frac{dW_{\text{shaft}}}{dt} = \frac{(p - p_0) dV}{dt} = M \omega = \frac{Md\theta}{dt} \quad (12)$$

where M and ω are the torque and angular speed of the shaft. The contribution to the shaft work at each step is thus the shaft torque $M = dW_{\text{shaft}}/d\theta = (p - p_0)dV/d\theta$, that is represented in Fig. 4.

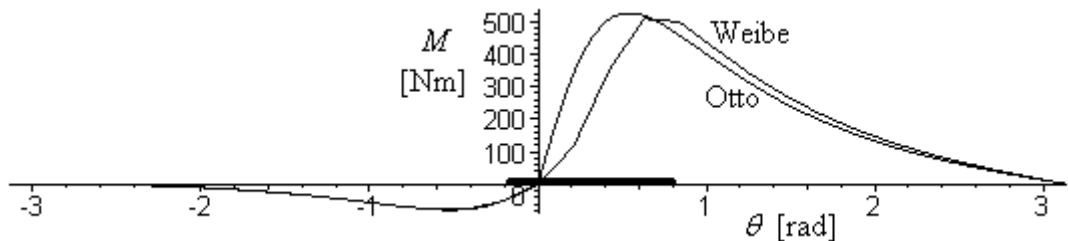


Fig. 4. Shaft torque $M = dW_{\text{shaft}}/d\theta = (p - p_0)dV/d\theta$, versus crank-angle θ , for the ideal Otto cycle and Weibe model (thick line shows burning period).

Notice that the large difference on peak pressure between the instantaneous model and the 60° crank-angle burning-period, seen in Fig. 2, does not manifest in the instantaneous work (Fig. 4), because it

occurs near TDC, and volume variation with crank-angle there is very small, yielding a negligible contribution to $(p-p_0)dV$.

The p - V plot is also worth (the traditional ‘indicated’ diagram); for the ideal Otto model it is directly drawn with equations (8--10), whereas for the Weibe model a parametric representation $p(\theta)$ - $V(\theta)$ is used.

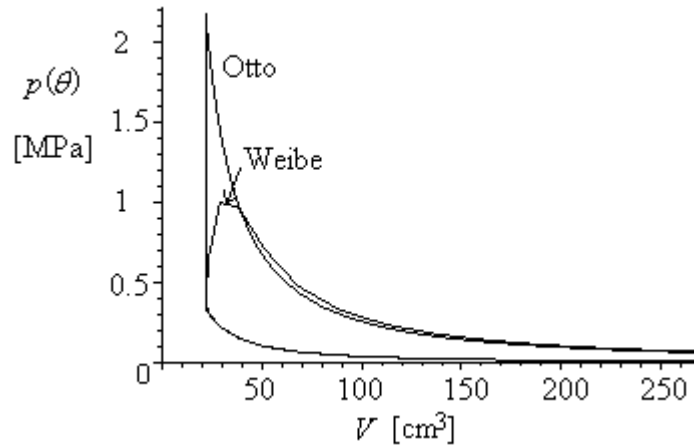


Fig. 5. Pressure-volume diagram for both the ideal Otto cycle and Weibe simulation.

e) Find the mean effective pressure, the shaft power and the energy efficiency of the engine.

The mean effective pressure, p_{MEF} , is the average effective pressure of the cylinders as they progress through all strokes, i.e. the average overpressure that, times the total displacement-volume, would yield the same work:

$$\dot{W}_{\text{shaft}} = p_{MEF} V_d Z n \frac{2}{S} \rightarrow p_{MEF} = \frac{2\dot{W}_{\text{shaft}}}{V_d n} = \frac{W_{\text{shaft,cycle}}}{V_d} = \frac{\int (p - p_0) dV}{V_d} = \eta_e \frac{h_{LHV}}{(\gamma - 1) A c_{va} T_0} \quad (13)$$

In the case of the ideal Otto cycle there is a closed solution for the energy efficiency in the conversion of heat to work:

$$\eta \equiv \frac{W_{\text{net}}}{Q_{\text{positive}}} \stackrel{\text{ideal Otto}}{=} 1 - \frac{1}{r^{\gamma-1}} = 1 - \frac{1}{12.5^{1.4-1}} = 0.64 \quad (14)$$

and, upon substitution of the values, one gets $p_{MEF} = \int (p-p_0)dV/V_d = 2.35$ MPa for the ideal Otto cycle, with $W_{\text{shaf,cycle}} = 630$ J, whereas the numerical solution for the Weibe model yields $W_{\text{shaf,cycle}} = 590$ J, $p_{MEF} = 2.37$ MPa and $\eta_e = 0.59$.

Of course, those values for the energy conversion efficiency are unrealistic, the reasons being that we did not consider heat transfer through the cylinder walls (>10%), engine friction (some 10% at full load, much more at partial loads), unburnt fuel (some 5% in SI-engines), fluid pumping work to renovate gases (some 5%), and fluid losses around piston rings (blow-by, some 1%).

Heat transfer inside the cylinder is difficult to model because of the turbulent motion and because of the different temperature zones. Air enters from the intake manifold that is at some 60 °C, through the inlet valve that is at some 250 °C, impinging on the piston head that is at some 300 °C (being refrigerated

somehow by oil at 70 °C), whereas the cylinder walls are at some 180 °C (being refrigerated by water at 100 °C), the sparkplug at 600 °C, the exit valve at about 650 °C.

Comments. Notice that the compression ratio for this engine, $r=12.5$, is in the upper limit for SI-engines, where typical values are about $r=9..10$; similarly, the speed (8500 rpm) is in the upper limit (typical values of full load regime for SI-engines are 5000..6000 rpm).

ADDITIONAL data for this Yamaha engine: rough external measurement of 0.35 x 0.41 x 0.51 meters, not including the exhaust system, i.e. some 73 litres in volume, with an approximate dry weigh of 27 kg including a 5-speed transmission and cooling pump. Its specific fuel consumption is $SFC=330$ g/kWh, and maximum power is 30.5 kW.

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