ICEN Extension to SENKIN Code

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This document describes the zero-dimensional internal combustion engine model used in the ICEN (Internal Combustion ENgine) extension to SENKIN [1] code in Chemkin-II [2] based on Heywood.[3] Although the model and the input parameters were intended to be compatible with the similar extension in Chemkin-3/4, the calculation results are not assured to be the same as them.

1. Nomenclature

The symbols and abbreviation used in this document are listed below.

a	Crank radius	A	Surface area
$A_{\rm ch}$	Cylinder head surface area	A_p	Piston crown surface area
B	Cylinder bore	c_p	Isobaric specific heat capacity
$C_{p,\rm m}$	Isobaric molar heat capacity	h_c	Heat-transfer coefficient
k	Thermal conductivity	K	Compression ratio
l	Connecting rod length	L	Piston stroke
M_{air}	Molar mass of air	N	Crankshaft rotational speed (= $\omega / 2\pi$)
p	Pressure	Q	Heat
R	connecting rod length / crank radius	R_{gas}	Molar gas constant
s	Crank axis to piston pin distance	$\hat{S}_p$	Mean piston speed
t	Time	T	Temperature
T_w	Cylinder wall temperature	V_c	Clearance volume
V_d	Displaced cylinder volume		
δ_h	Thickness of thermal boundary layer	θ	Crank angle ATDC (after TDC)
μ	Viscosity	ρ	Density
ω	Crankshaft angular velocity (= $2\pi N$)		
BDC	Bottom dead center	Nu	Nusselt number (= h_cB / k)
Pr	Prandtl number (= $c_p\mu / k$)	Re	Reynolds number (= $\rho\hat{S}_pB / \mu$)
TDC	Top dead center		

2. Piston-Crank Mechanism

From a geometric consideration, as depicted in Fig. 1, the distance, s, between the crank axis and piston pin axis can be written as,

$$s = a\cos\theta + \sqrt{l^2 - a^2\sin^2\theta} \qquad (1)$$

Since the distance s at the TDC is $s_{\rm TDC} = a + l$, the cylinder volume is,

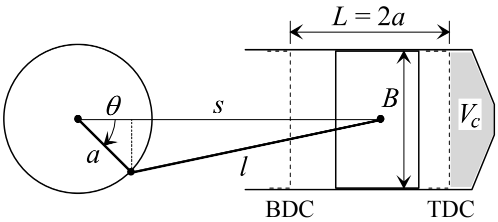

Fig. 1 Schematics of the Piston-Crank Mechanism

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[1] A. E. Lutz, R. J. Kee, and J. A. Miller, SENKIN: *A Fortran Program for Predicting Homogeneous Gas Phase Chemical Kinetics With Sensitivity Analysis*, SAND87-8248·UC-401, Sandia National Laboratories, 1995.

[2] R. J. Kee, F. M. Rupley, and J. A. Miller, *Chemkin-II: A Fortran Chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics*, SAND89-8009B·UC-706, Sandia National Laboratories, 1995.

[3] J. B. Heywood, *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988.

$$V = \frac{\pi B^2}{4}\left(s_{\mathrm{TDC}} - s\right) + V_c \qquad (2)$$

By using the ratio of connecting rot length to crank radius,

$$R = \frac{l}{a} \qquad (3)$$

and the compression ratio,

$$K = \frac{V_d + V_c}{V_c} = \frac{\pi B^2 a}{2V_c} + 1 \qquad (4)$$

eq. (2) can be rewritten as,

$$\frac{V}{V_c} = \frac{K-1}{2}\left(1 + R - \cos\theta - \sqrt{R^2 - \sin^2\theta}\right) + 1 \qquad (5)$$

For a constant angular velocity, the time variation is described with,

$$\theta = \theta_0 + \omega t \qquad (6)$$

where θ_0 is the crank angle at $t = 0$. Differentiation of eq. (5) with respect to θ gives,

$$\frac{1}{V_c}\frac{\mathrm{d}V}{\mathrm{d}\theta} = \frac{K-1}{2}\sin\theta\left(1 + \frac{\cos\theta}{\sqrt{R^2 - \sin^2\theta}}\right) \qquad (7)$$

The time derivative of the volume is given by,

$$\frac{\mathrm{d}V}{\mathrm{d}t} = \omega\frac{\mathrm{d}V}{\mathrm{d}\theta} \qquad (8)$$

Similarly, the cylinder surface area is given by,

$$A = A_{\mathrm{ch}} + A_p + \frac{2V_c(K-1)}{B}\left(1 + R - \cos\theta - \sqrt{R^2 - \sin^2\theta}\right) \qquad (9)$$

For flat-topped piston and cylinder,

$$A_p = \frac{\pi B^2}{4} \qquad (10)$$

$$A_{\mathrm{ch}} = \frac{\pi B^2}{4} + \frac{4V_c}{B} \qquad (11)$$

The mean piston speed is defined as,

$$\hat{S}_p = 2LN = \frac{8V_c(K-1)}{\pi B^2}N \qquad (12)$$

3. Heat Transfer

For a forced-convection condition, the rate of heat-transfer is described by,

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = h_c A(T - T_w) \qquad (1)$$

The heat-transfer coefficient h_c is related to the thermal conductivity k and the thickness of the thermal boundary layer δ_h by a simple boundary layer model,

$$h_c = \frac{k}{\delta_h} \qquad (2)$$

Thus the main problem of the forced-convection heat-transfer is in the estimation of δ_h or the Nusselt dimensionless number *Nu*,

$$Nu = \frac{B}{\delta_h} = \frac{h_c B}{k} \qquad (3)$$

Note that in this document, the *characteristic length* in a dimensionless number is taken to be the cylinder bore *B*. In many empirical correlations, *Nu* is written by Reynolds and Prandtl numbers, *Re* and *Pr*, respectively, as,

$$Nu = a Re^m Pr^n \qquad (4)$$

The Reynolds and Prandtl numbers are defined as,

$$Re = \frac{\rho \hat{S}_p B}{\mu} \qquad (5)$$

$$Pr = \frac{c_p \mu}{k} \qquad (6)$$

By assuming that the gas property is dominated by that of air, ρ, k, μ, and c_p are approximated as,

$$k \approx k(\text{air}) = 3.50\times10^{-4}\ T^{0.764}\ [\text{J m}^{-1}\ \text{s}^{-1}\ \text{K}^{-1}] \qquad (7)$$

$$= 35.0\ T^{0.764}\ [\text{erg cm}^{-1}\ \text{s}^{-1}\ \text{K}^{-1}] \qquad (7')$$

$$\mu \approx \mu(\text{air}) = 4.41\times10^{-7}\ T^{0.664}\ [\text{kg m}^{-1}\ \text{s}^{-1} = \text{Pa s} = \text{N s m}^{-2}] \qquad (8)$$

$$= 4.41\times10^{-6}\ T^{0.664}\ [\text{g cm}^{-1}\ \text{s}^{-1} = \text{dyn s cm}^{-2}] \qquad (8')$$

Widely used Woschni's correlation assumes that $a = 0.035$ and $n = 0$ in eq. (4),

$$Nu = 0.035 Re^m \qquad (9)$$

In many cases, the exponent *m* is chosen to be 0.8.