Thesis Title	An alternative approach for the determination of retention indices and equivalent chain length of lipids in isothermal and temperature-programmed gas chromatography
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Candidate	Miss Kanisa Kittirattanapiboon
Supervisors	Assoc. Prof. Dr. Kanit Krisnangkura
	Assoc. Prof. Narumon Jeyashoke
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Abstract

Gas chromatographic identification of lipids can be preformed by several methods. Among these, the Kovats' retention indices (I) and the equivalent chain length (ECL) have been widely accepted as a general identification system. These equations require n-alkanes and fatty acid methyl esters (FAMEs) as references. Recently, Krisnangkura et al. [*Journal of Chromatographic Science* vol. 35 (1997) pp. 329 –332] have demonstrated that retention factor (k'), ECL(n) of FAMEs and the absolute temperature (T) are inter-related as described in equation 1.

$$\ln k' = a + bn + \frac{c}{T} + \frac{dn}{T} \qquad \text{Eq. 1}$$

Where a, b, c and d are thermodynamically related column constants.

In this study, equation 1 is utilized to convert the ECL into Kovats' retention index (I) and vice versa. The retention indices of FAMEs, n-alkanes and fatty alcohols separated on OV-101 capillary column can be calculated directly from their retention times and from their ECLs. The calculated retention indices are agreed well with those reported in the literature and the greatest differences is about 1%.

By rearranging Eq. 1 to Eq. 2 and combining the method of column slicing of Calvalli and Guinchard [*Journal of Chromatographic Science* vol. 33 (1995) pp.370-376], the

retention time of FAMEs in the temperature-programmed gas chromatography (TPGC) can be estimated.

$$t_R = \sum_{i=1}^{m} \frac{t_M}{m} \left(1 + e^{\left(\frac{c + dn}{\theta_t} + (a + bn) \right)} \right) \qquad \text{Eq.2}$$

When Eq. 2 is used to forecast the TPGC retention time of FAMEs separated on an OMEGAWAX capillary column, the difference between the observed and calculated values are –2.6 to 3.4 %. The greatest difference is found with high programming rate and longer carbon chain length. When a flow-adjustment term is incorporated into equation, the greatest difference between the observed and calculated retention time is reduced to appproximated 2.7 %. This equation can also accurately forecast the TPGC retention time of saturated and unsaturated FAMEs from cauliflower oils.

In addition, Eq. 2 can also be utilized to forecast the TPGC retention time and carbon number of n-alkane separated on the (polyimide clad and aluminium clad) HT5 capillary columns (25 m. x 0.32 mm. i.d. and film thickness 0.1 μm.) with the same column constants. The experimental and forecasted retention times from the polyimide clad and the aluminium clad are very close. Thus, it may be concluded that Eq. 1 can be transformed to other equations and used to convert the ECL to retention indices and to forecast the TPGC retention times.

Keywords : Carbon number / Fatty acid methyl esters / Gas chromatography / Retention time / Kovats' retention indices / Temperature programmed gas chromatography / Equivalent chain length