

A three dimensional semi-quantitative method to monitor the evolution of polycyclic aromatic hydrocarbons from vacuum gas oil feedstocks to lighter products

Carole Reymond^a, Agnès Le Masle^{a,*}, Cyril Colas^{b,c}, Nadège Charon^a

^a IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize, France

^b Institut de Chimie Organique et Analytique, Université d'Orléans, CNRS UMR 7311, Rue de Chartres, 45067 Orléans, France

^c Centre de Biophysique Moléculaire, CNRS UPR 4301, Université d'Orléans, rue Charles Sadron, 45071 Orléans, France

*Corresponding author. E-mail address: agnes.le-masle@ifpen.fr (A. Le Masle)

Table S1: Comparisons of the response factors of alkylated and non-alkylated pyrene, and coronene and 1-methylcoronene. Responses factors (a) were estimated using linear calibration curves ([Concentration] = a × Aire) for concentrations comprised between 0 and 200 mg/L.

Standards	Response factor (a)	Difference with the non-alkylated PAH (%)
Pyrene	7.78E-07	[Reference]
1-methylpyrene	7.19E-07	6
4-methylpyrene	7.16E-07	7
4,5-dimethylpyrene	7.73E-07	-1
2,7-dimethylpyrene	5.75E-07	25
1-ethylpyrene	7.04E-07	8
1-propylpyrene	7.30E-07	5
1-butylpyrene	7.54E-07	2

Coronene	8.03E-07	[Reference]
1-methylcoronene	7.75E-07	-2

Figure S1: Calibration curves of PAHs standards demonstrating the similar response of PAHs with a same DBE

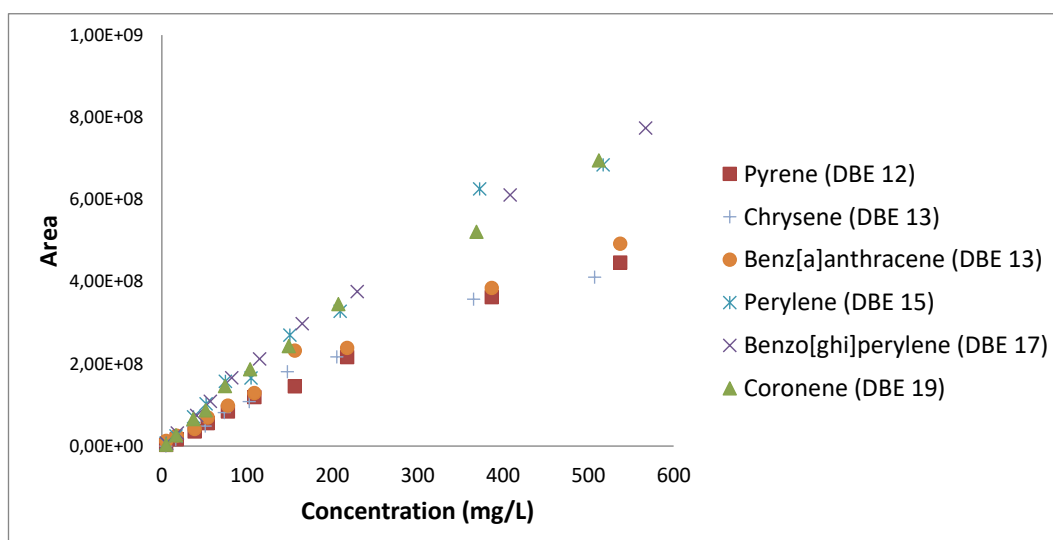


Figure S2: PAH concentration as a function of the number of carbon atoms for DBE 12 to DBE 20 in the six studied VGOs.

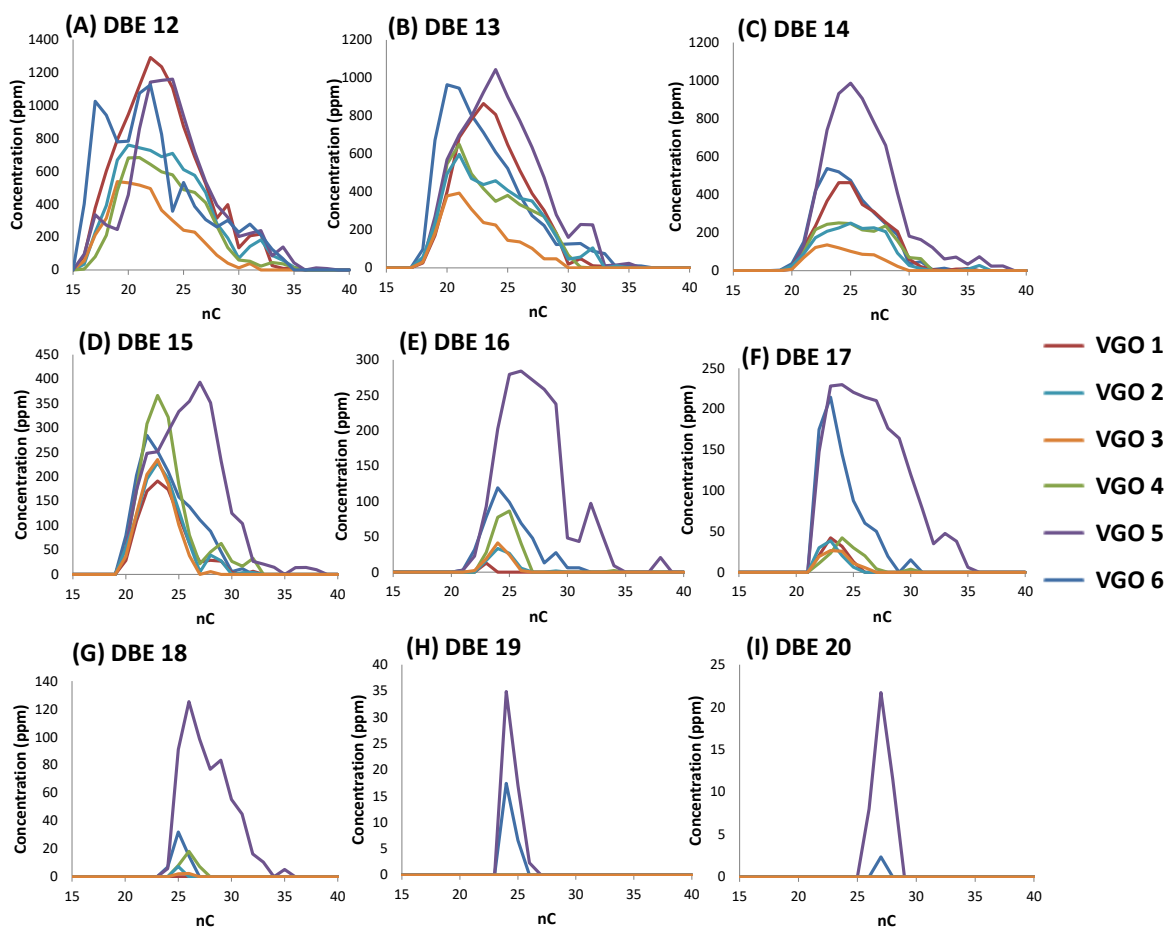


Figure S3: Mass spectra of main compounds belonging to pyrene family (DBE 12) in VGO 1 with one, two and three carbons in the alkyl chain

