## **Supporting Information**



Fig. A.1. Simplified scheme of the pilot unit.



**Fig. A.2.** Comparison of the basic N1 families intensities in the samples prepared with 0.5 mg/mL and 1 mg/mL of VGO.

## Table A.1

Sample	T, ℃	LHSV, h <sup>-1</sup>	HDN, %	d15, g/cm <sup>3</sup>	N total, wppm	N basic, wppm	N neutral, wppm	S, wppm	IBP, °C	FBP, °C
A1	T <sub>ref</sub> -20	LHSV <sub>ref</sub> -0.9	77	0.8960	305	81	224	723	210	592
A2	T <sub>ref</sub> -10	LHSV <sub>ref</sub> +2.1	44	0.9025	802	255	547	2435	223	595
A3	T <sub>ref</sub>	LHSV <sub>ref</sub> +2.1	53	0.9003	673	189	484	1612	201	592
A4	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +2.1	75	0.8946	360	66	294	541	148	590
A5	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +0.1	96	0.8867	61	<10	~51	78	137	586
B1	T <sub>ref</sub> -10	LHSV <sub>ref</sub> +2.1	40	0.9383	1640	569	1071	7190	222	588
B2	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +2.1	66	0.9231	939	235	704	2018	145	579
B3	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +0.1	88	0.9136	339	47	292	496	135	580
B4	T <sub>ref</sub> +30	LHSV <sub>ref</sub> +0.1	96	0.9055	123	<30	~93	159	120	572
C1	T <sub>ref</sub> -10	LHSV <sub>ref</sub> +2.1	44	0.9210	1980	562	1418	3294	194	582
C2	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +2.1	72	0.9110	999	198	801	1052	151	578
C3	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +0.1	91	0.9030	328	39	289	270	139	575
C4	T <sub>ref</sub> +30	LHSV <sub>ref</sub> +0.1	96	0.8983	132	<30	~102	86	123	573
C5	T <sub>ref</sub> +30	LHSV <sub>ref</sub> -0.4	98	0.8948	69	<30	~39	39	127	571
D1	T <sub>ref</sub> -10	LHSV <sub>ref</sub> +2.1	25	0.9231	2555	754	1801	1218	250	590
D2	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +2.1	50	0.9190	1730	443	1287	576	202	589
D3	T <sub>ref</sub> +20	LHSV <sub>ref</sub> +0.1	69	0.9138	1080	236	844	278	175	591
D4	T <sub>ref</sub> +20	LHSV <sub>ref</sub> -0.4	75	0.9115	868	171	697	183	171	585
D5	T <sub>ref</sub> +20	LHSV <sub>ref</sub> -0.9	85	0.9077	516	94	422	94	169	583
D6	T <sub>ref</sub> +20	LHSV <sub>ref</sub> -1.3	93	0.9017	244	32	212	27	167	583
D7	T <sub>ref</sub> +35	LHSV <sub>ref</sub> -1.3	97	0.8939	100	<10	~90	0	148	576

Operating conditions and physicochemical properties of the HDT effluents.

## Table A.2

Description of the used analyses.

Density at 15 °C	NF EN ISO 12185				
Refractive index	ASTM D1218-12				
Sulphur content	Internal IFPEN method based on X-ray				
	fluorescence spectrometry.				
Total nitrogen content	For samples containing 0.2-2500 mg/kg of N -				
	internal IFPEN method based on				
	chemiluminescence. For the samples with N>2500				
	mg/kg - internal IFPEN method based on				
	combustion.				
Basic nitrogen content	Internal IFPEN method based on potentiometry.				
Simulated distillation (determination of	Internal IFPEN method. Simulated distillation by				
the initial and final boiling points)	gas chromatography for distillates $35 - 650$ °C.				



Fig. A. 3. Simulated distillation curves of vacuum gas oils.



**Fig. A. 4.** Explanation of the planar limit approach using the example of quinoline (a – the slope is 0.75, a case of linear addition of aromatic rings to quinoline; b - the slope is above 0.75, a case of non-linear addition of aromatic rings to quinoline; c – the slope is below 0.75, a case of saturated ring addition).



Fig. A.5. The simple hypothetical structures of the most abundant species in VGOs A-D.













dibenzocarbazoles (DBE=16) in VGO B.









and dibenzocarbazoles (DBE=16) in VGO D.



Fig. A.12. The weighted arithmetic mean of DBE as a function of HDN in VGOs and gas oil.