Supplementary Materials

Table S1. The σ (Å) and ϵ (kcal/mol) parameters for the components of Aviation Hydraulic Oil No. 15 model.

Force or Charge Site	σ(Å)	ϵ (kcal/mol)	q (e)
Nitrogen gas (TraPPE-UA model)			
N	3.310		-0.482
M			0.964
2-Dodecen-1-ylsuccinic anhydride (OPLS-AA model)			
CH_3	3.012	0.0561	
CH_2	2.958	0.0445	
C-O	3.297	0.121	
Undec-10-ynoic acid, tetradecyl ester (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-H (-CH)	2.738	0.0714	
C-O	3.125	0.134	
O-H	2.676	0.0561	
2-Hexyl-1-decanol (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	
O-H	3.125	0.134	
Tetradecyl chloroacetate (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	
O-H	3.125	0.134	
C-Cl	0	0	-0.191
Decyl methacrylate (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	
Eicosyl vinyl carbonate (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	
O-H	3.125	0.134	
2-Methyldecyl acrylate (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	
Pentadecyl 2-chloroacetate (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	
O-H	3.125	0.134	

C-Cl	0	0	-0.191
2(1H)-Benzocyclooctenone,decahydro-4a-methyl (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	
Butylated Hydroxytoluene (OPLS-AA model)			
C-H(-CH_3)	3.012	0.0561	
C-H(-CH_2)	2.958	0.0445	
C-O	3.297	0.121	

Table S2. Molecular simulation experimental design.

Chemical Compound	Molecular Formula	Temperature(K); Pressure(MPa)	Number
N_2	N_2	373;15	1378
		373;20	1786
		373;25	2164
		373;30	2514
		373;35	2834
		313;20	2174
		343;20	1958
		403;20	1646
		433;20	1528
2-Dodecen-1-ylsuccinic anhydride	$C_{16}H_{26}O_3$	373;15	127
		373;20	127
		373;25	128
		373;30	128
		373;35	129
		313;20	134
		343;20	130
		403;20	124
		433;20	121
Undec-10-ynoic acid, tetradecyl ester	$C_{25}H_{46}O_2$	373;15	60
		373;20	60
		373;25	60
		373;30	60
		373;35	61
		313;20	63
		343;20	61
		403;20	59
		433;20	57
2-Hexyl-1-decanol	$C_{16}H_{34}O$	373;15	58
		373;20	58
		373;25	58
		373;30	58
		373;35	58
		313;20	61
		343;20	59
		403;20	57
		433;20	55

phytol	$C_{20}H_{40}O$	373;15	54
		373;20	54
		373;25	55
		373;30	55
		373;35	55
		313;20	57
		343;20	56
		403;20	53
		433;20	52
Tetradecyl chloroacetate	$C_{16}H_{31}CLO_2$	373;15	44
		373;20	44
		373;25	44
		373;30	44
		373;35	45
		313;20	46
		343;20	45
		403;20	43
		433;20	42
Decyl methacrylate	$C_{17}H_{32}O_2$	373;15	41
		373;20	41
		373;25	41
		373;30	41
		373;35	41
		313;20	43
		343;20	42
		403;20	40
		433;20	39
Eicosyl vinyl carbonate	$C_{23}H_{44}O_3$	373;15	35
		373;20	35
		373;25	36
		373;30	36
		373;35	36
		313;20	37
		343;20	36
		403;20	35
		433;20	34
2-Methyldecyl acrylate	$C_{14}H_{26}O$	373;15	28
		373;20	28
		373;25	28
		373;30	28
		373;35	28
		313;20	29
		343;20	29
		403;20	27
		433;20	27
		373;15	26
		373;20	26

Pentadecyl 2-chloroacetate	$C_{17}H_{33}CLO_2$	373;25	26
		373;30	26
		373;35	26
		313;20	28
		343;20	27
		403;20	26
		433;20	25
2(1H)-Benzocyclooctenone,decahydro-4a-methyl-, trans-(-)-	$C_{13}H_{22}O$	373;15	23
		373;20	23
		373;25	23
		373;30	24
		373;35	24
		313;20	25
		343;20	24
		403;20	23
		433;20	22
Butylated Hydroxytoluene	$C_{15}H_{24}O$	373;15	13
		373;20	13
		373;25	13
		373;30	13
		373;35	13
		313;20	14
		343;20	13
		403;20	13
		433;20	12

Table S3. Density at different times during the data acquisition stage.

t (ns)	N_2		Oil	
	MD (g/cm³)	NIST (g/cm³)	MD (g/cm³)	EXP (g/cm³)
0.5 ns	0.139	0.141	0.772	0.770
1 ns	0.142		0.776	
2 ns	0.144		0.780	
3 ns	0.140		0.775	

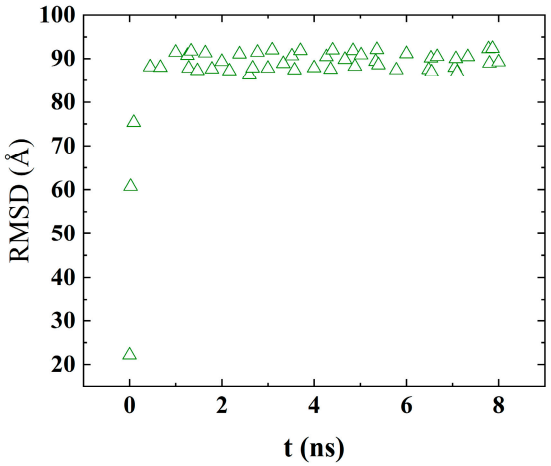


Figure S1. The curves of N_2, oil, and overall in the N_2-oil system during relaxation.

According to the review opinions, we first added the root-mean-square displacement (RMSD) of the N_2-oil system and each component to prove that the structure of the simulated system tends to a steady state after relaxation for a certain period. The RMSD quantifies the deviation in atomic coordinates from their initial positions. It tracks the displacement of individual components relative to their initial states and provides insights into the motion of substances within the system. RMSD values were used to assess the thermodynamic equilibrium of the system and were calculated using the following formula: As shown in Figure 1, during the relaxation process of 8 ns, the overall RMSD of the nitrogen-oil system quickly stabilized, proving that the binary system quickly converges to a steady state.