

Table 1

Initial densities and ensemble of ReaxFF simulation about DR-2.

	Molecules	Initial density ($\rho / g \cdot cm^{-3}$)	Ensemble
Ref.[9]	50 DR-2	1.3595	NVT
Ref.[11]	150 DR-2 + 450 O ₂ (1)	0.015 (1)	NVT
	75 DR-2 + 450 O ₂ (2)		
	300 DR-2 + 450 O ₂ (3)		
Ref.[12]	150 DR-2 + 450 O ₂ (1)	0.015	NVT
	150 DR-2 + 450 O ₂ +37 H ₂ O (2)		
	150 DR-2 + 450 O ₂ +75 H ₂ O (3)		
	150 DR-2 + 450 O ₂ +112 H ₂ O (4)		
	150 DR-2 + 450 O ₂ +150 H ₂ O (5)		
This work	100 DR-2 + 50 O ₂ (1)	0.00538 (1) 1.36 (2-3)	NVT
	45 DR-2 (2)		
	45 DR-2 +5 O ₂ (3)		