Supporting Information

Supercritical water oxidation VS supercritical water gasification: Which process is better for explosive wastewater treatment?

Jinli Zhang[a], Jintao Gu[a], You Han[a,*], Wei Li[a], Zhongxue Gan[b] and Junjie Gu[c]

[a]*School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China*

[b]*State Key Laboratory of Low Carbon Energy of Coal, ENN Group, Langfang 065001, Hebei Province, China*

[c]*Mechanical and Aerospace Engineering, Carleton University, 1125 Colonel By Drive, Ottawa, Ontario K1S5B6, Canada*

* *yhan@tju.edu.cn*

Table S1 The constant rate (k) of SCWG and SCWO systems.

Temperature (T)	$k_{SCWG}\times10^{-10}$	$k_{SCWO}\times10^{-10}$
1700	3.18	4.23
1800	4.38	5.41
1900	5.29	6.75
2000	6.94	8.60
2100	8.43	11.56
2200	10.67	14.58

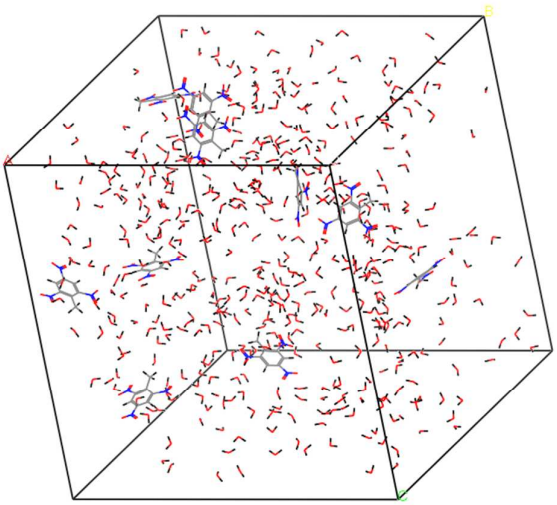

Figure S1. The constructed simulation cell obtained by Amorphous module using Materials Studio.

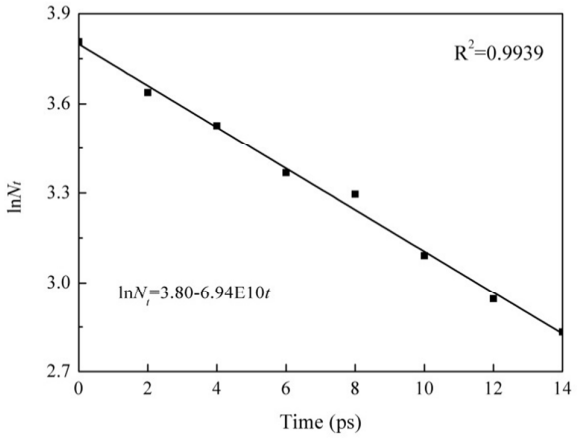

Figure S2 Napierian logarithm of TNT's molecular number in the initial 14 ps of the whole simulation at 2000 K of SCWG.