

Experimental and numerical study of the impact of pressure on diethyl carbonate and ethyl methyl carbonate electrolytes pyrolysis

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Supplementary Material

1/ CO time-history profiles for the pyrolysis of DEC in 99.75% He/Ar

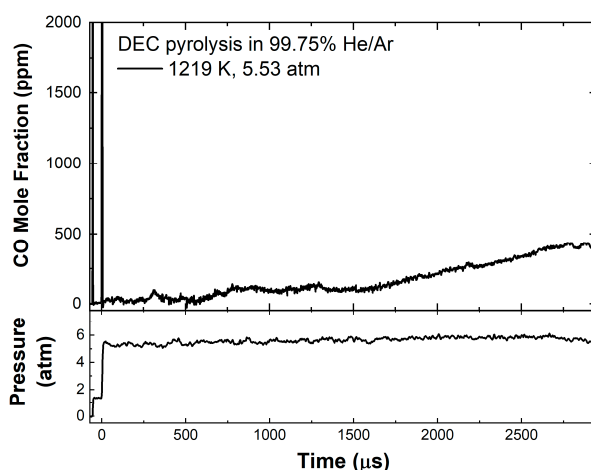


Figure S1: CO time-history profile for DEC in 99.75% He/Ar at 1219 K, 5.53 atm.

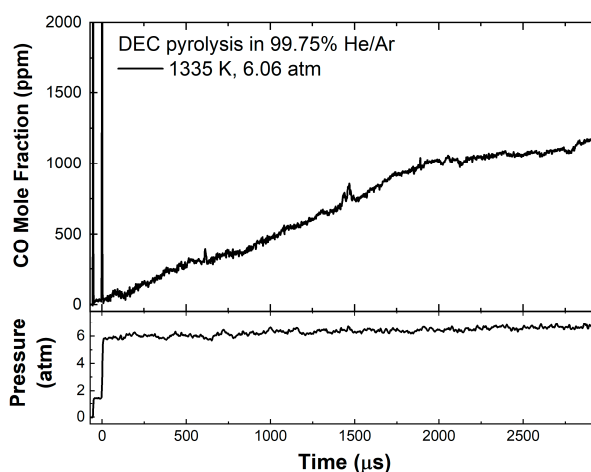


Figure S2: CO time-history profile for DEC in 99.75% He/Ar at 1335 K, 6.06 atm.

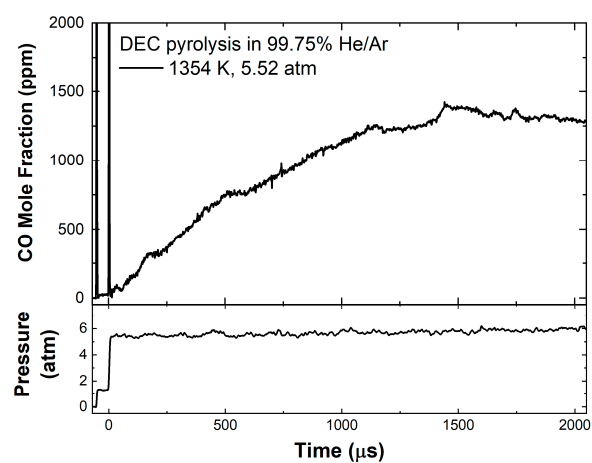


Figure S3: CO time-history profile for DEC in 99.75% He/Ar at 1354 K, 5.52 atm.

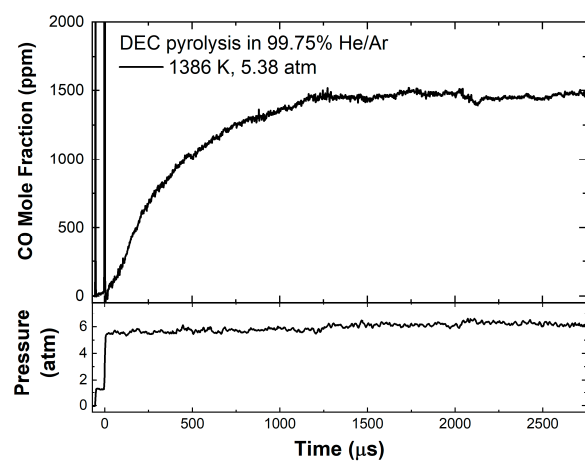


Figure S4: CO time-history profile for DEC in 99.75% He/Ar at 1386 K, 5.38 atm.

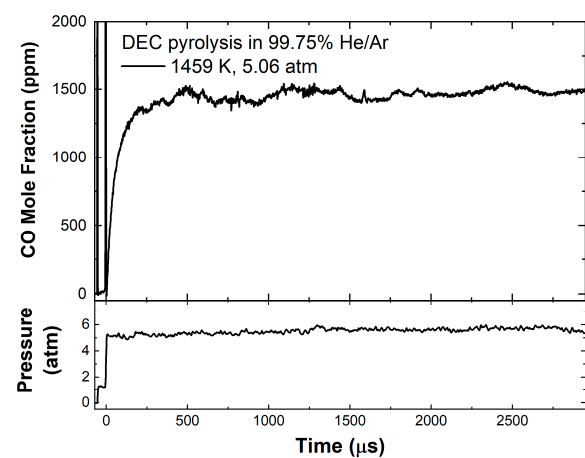


Figure S5: CO time-history profile for DEC in 99.75% He/Ar at 1459 K, 5.06 atm.

2/ CO time-history profile for the pyrolysis of EMC in 99.75% He/Ar

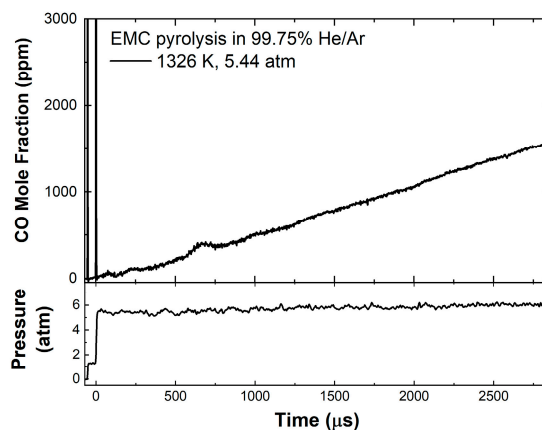


Figure S6: CO time-history profile for EMC in 99.75% He/Ar at 1326 K, 5.44 atm.

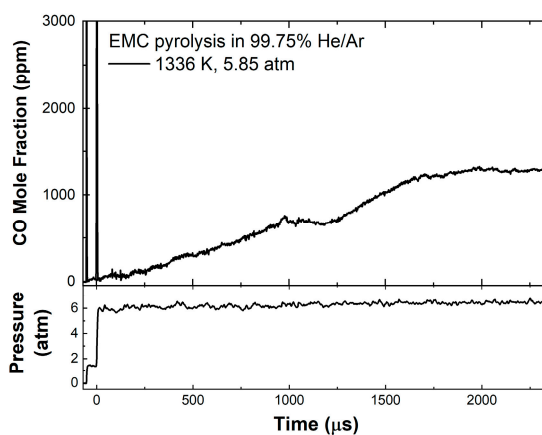


Figure S7: CO time-history profile for EMC in 99.75% He/Ar at 1336 K, 5.85 atm.

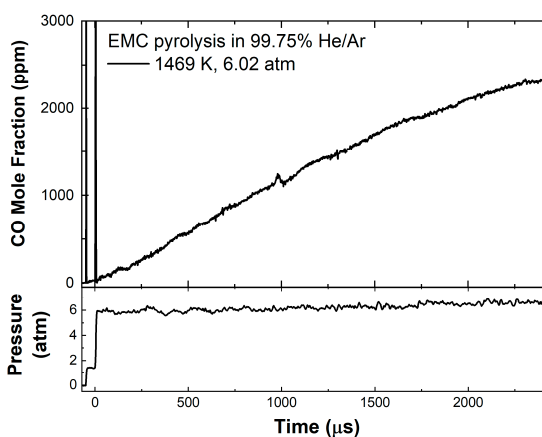


Figure S8: CO time-history profile for EMC in 99.75% He/Ar at 1469 K, 6.02 atm.

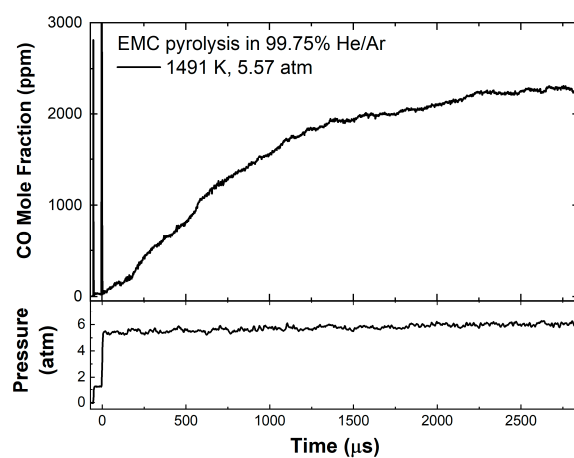


Figure S9: CO time-history profile for EMC in 99.75% He/Ar at 1491 K, 5.57 atm.

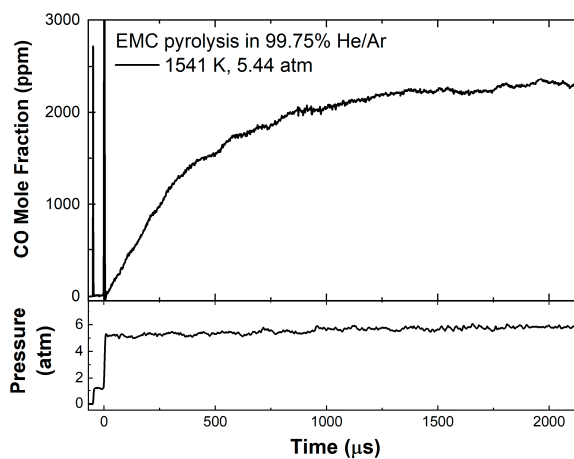


Figure S10: CO time-history profile for EMC in 99.75% He/Ar at 1541 K, 5.44 atm.

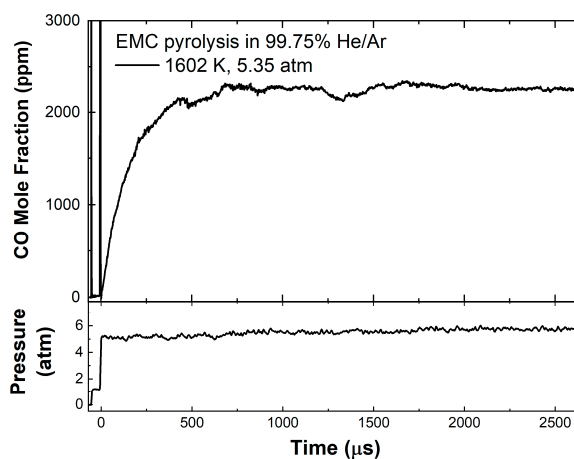


Figure S11: CO time-history profile for EMC in 99.75% He/Ar at 1602 K, 5.35 atm.

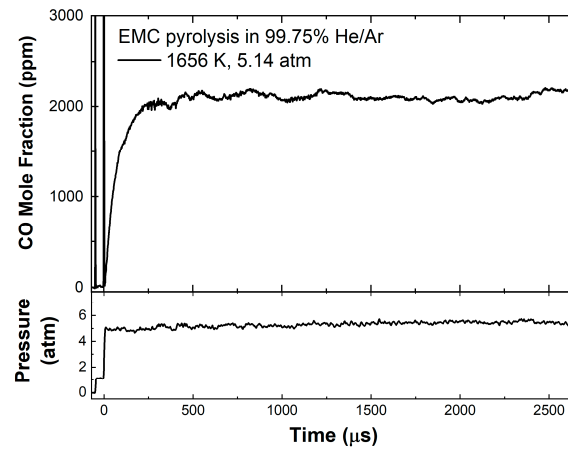


Figure S12: CO time-history profile for EMC in 99.75% He/Ar at 1656 K, 5.14 atm.

3/ Effect of pressure on the pyrolysis of DEC in 99.75% He/Ar

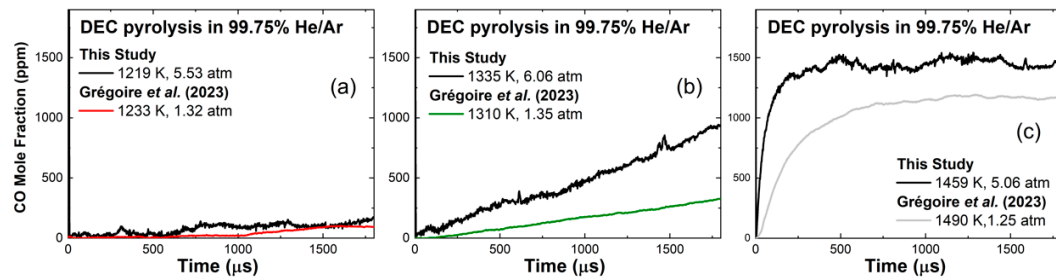


Figure S13: Effect of pressure on the pyrolysis of DEC in 99.75% He/Ar using CO time histories from this study near 5.5 atm and measurements in similar conditions from Grégoire *et al.* (1) obtained near 1.3 atm. Results are near a) 1226 ± 7 K and b) 1325 ± 15 K, and 1474 ± 16 K.

4/ Effect of pressure on the pyrolysis of EMC in 99.75% He/Ar

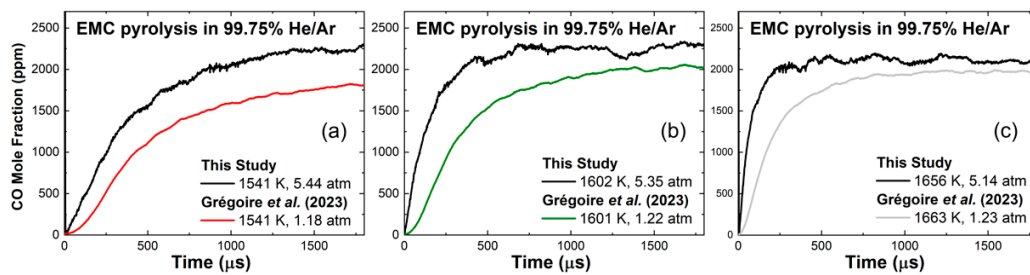


Figure S14: Effect of pressure on the pyrolysis of EMC in 99.75% He/Ar using CO time histories from this study near 5.5 atm and measurements in similar conditions from Grégoire *et al.* (1) obtained near 1.3 atm. Results are near a) 1541 K and b) 1601 ± 1 K, and 1660 ± 4 K.

5/ Effect of pressure on the pyrolysis of DEC and EMC in 99.75% He/Ar

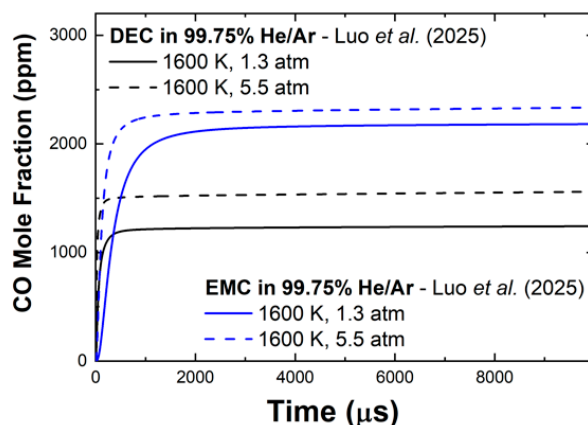


Figure S15: Predictions of CO for the pyrolysis of DEC and EMC in 99.75% He/Ar at 1600 K, 1.3-5.5 atm using the Luo *et al.* model (2). A higher pressure leads to the increase of reactivity for the electrolytes and larger CO concentrations at the plateau.

6/ Comparison between the Luo *et al.* (2) and the Khan-Ghauri *et al.* (3) models

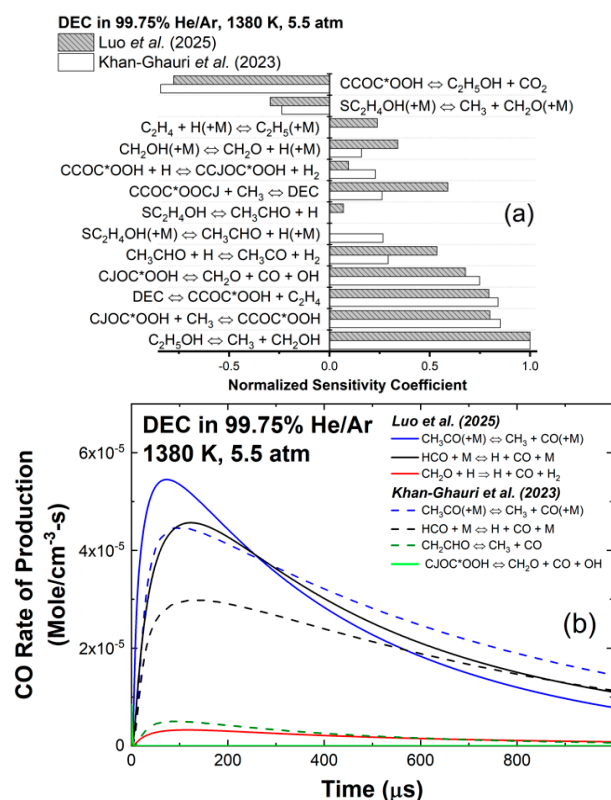


Figure S16: CO sensitivity (a) and rate-of-production (b) analyses for the pyrolysis of DEC in 99.75% He/Ar at 1380 K, 5.5 atm using two different mechanisms (2,3).

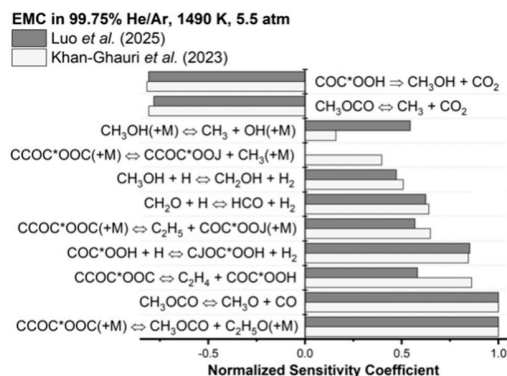


Figure S17: CO sensitivity analyses for the pyrolysis of EMC (CCOC*OOC in the model) in 99.75% He/Ar, 5.5 atm at 1490 K using two different mechanisms (2,3).

References

1. C. Grégoire, Cooper, S., Khan-Ghauri, M., Alturaifi, S., Petersen, E. and Mathieu, O. Pyrolysis Study of Dimethyl Carbonate, Diethyl Carbonate, and Ethyl Methyl Carbonate using Shock-Tube Spectroscopic CO Measurements and Chemical Kinetics Investigation. *Combust. Flame* **2023**, 249, 112594.
2. Q. Luo, Zheng, L., Wang, J., Jia, H., Wang, X., Zhang, S., Wang, D. and Lu, J. Investigation of chemical kinetic models for electrolyte solvent vapors released from thermal runaway lithium-ion batteries. *Journal of Energy Storage* **2025**, 107, 114932.
3. M. Khan-Ghauri, Grégoire, C. M., Kanayama, K., Diévar, P., Takahashi, S., Tezuka, T., Almarzooq, Y. M., Nakamura, H., Catoire, L., Maruta, K., Petersen, E. L. and Mathieu, O. Experimental and Detailed Kinetics Modeling Study of Bis(2,2,2-trifluoroethyl) Carbonate, a Fire Suppressant for Lithium-Ion Battery. *Energ. Fuel* **2025**, 39, 4893-4908.