

Supplementary Materials

Mechanism investigations of EC/EMC electrolyte combustion suppression by phosphorus-iron agents via ReaxFF MD

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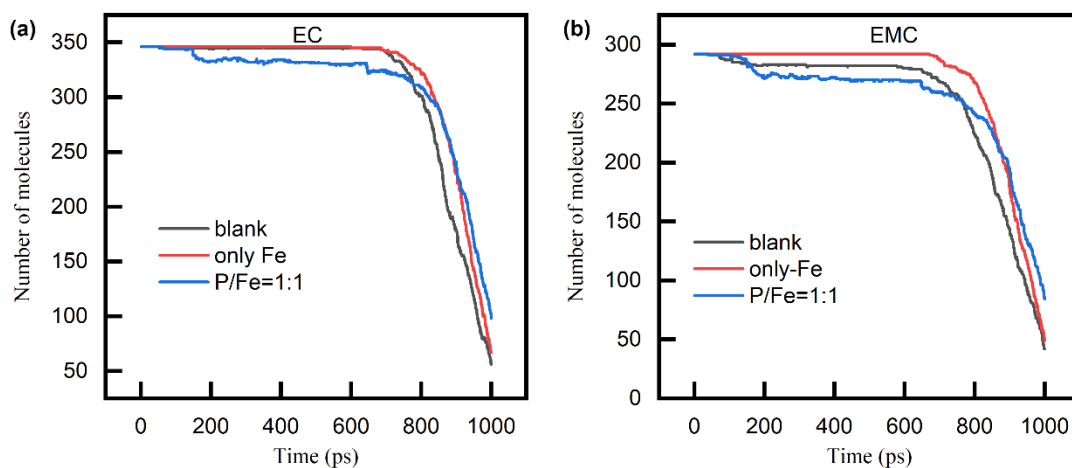


Figure S1. EC and EMC number of blank, only Fe and P/Fe=1:1 system

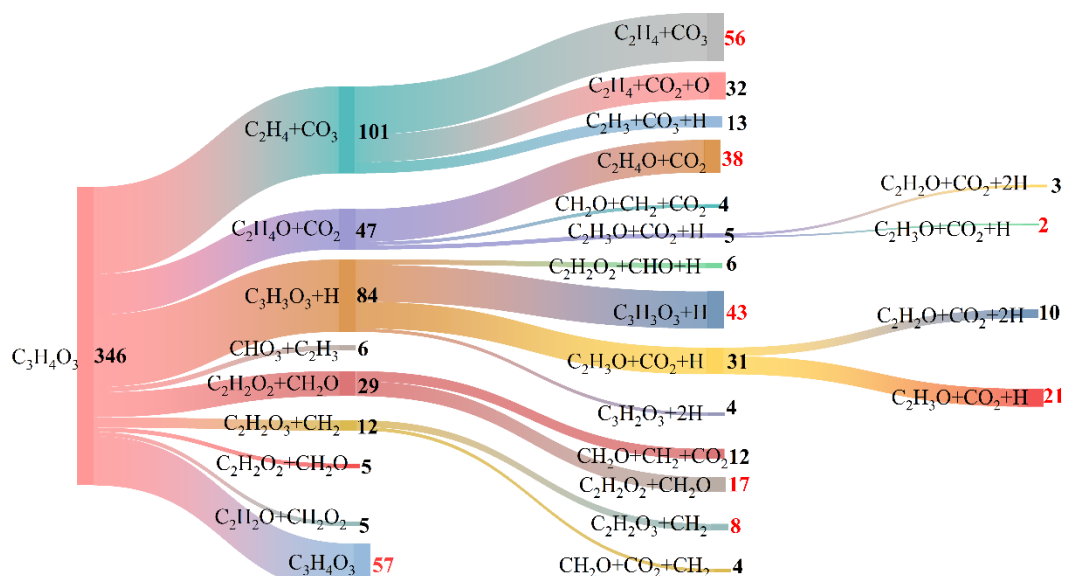


Figure S2. Reaction pathways of EC in the P/Fe = 1:2 system.

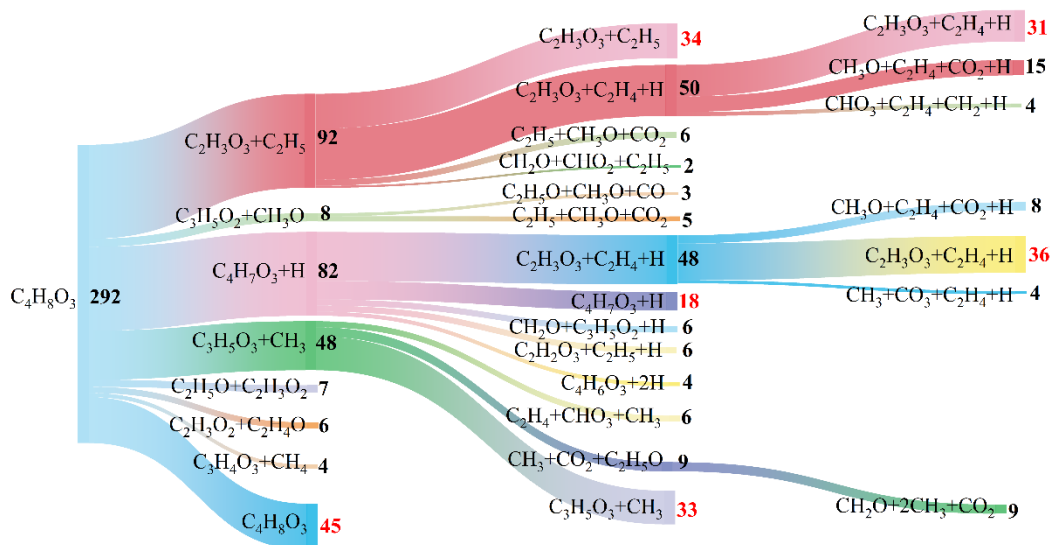


Figure S3. Reaction pathways of EMC in the P/Fe = 1:2 system.

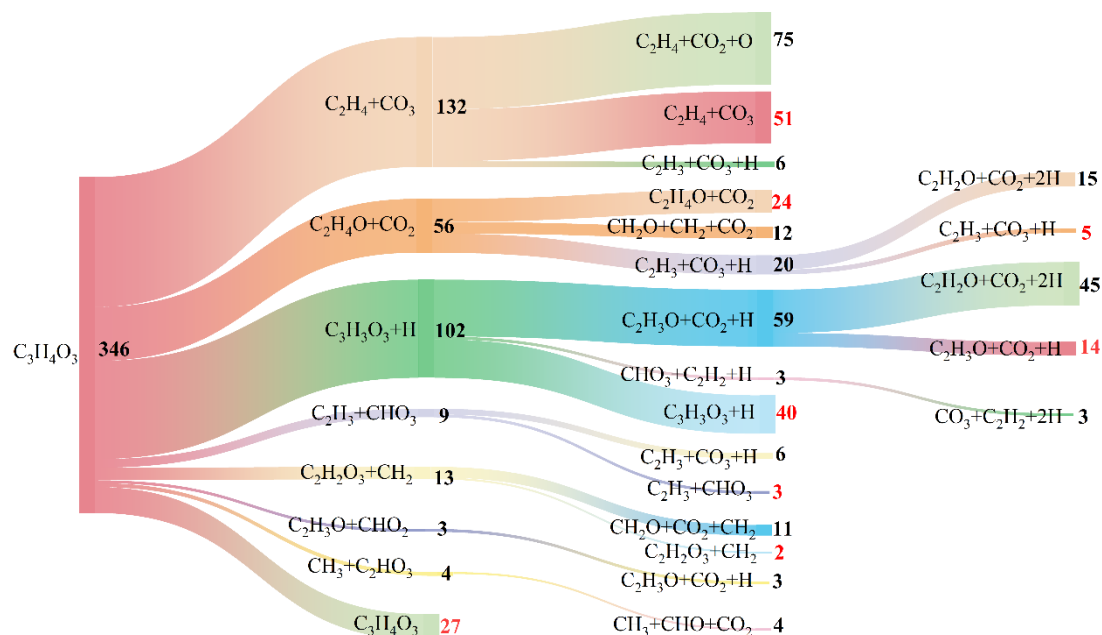


Figure S4. Reaction pathways of EC in the P/Fe = 1:3 system.

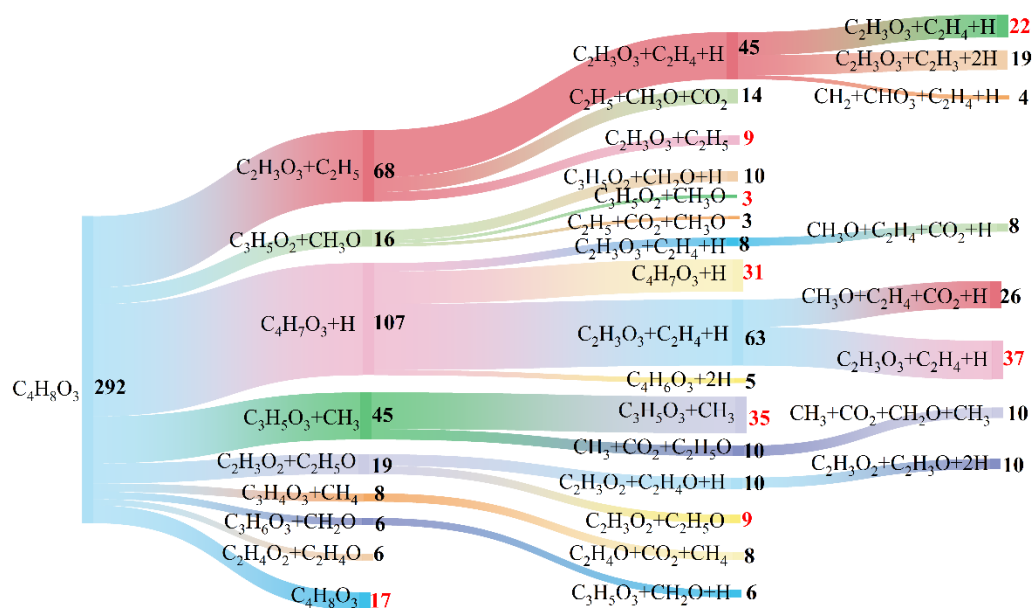


Figure S5 Reaction pathways of EMC in the P/Fe = 1:3 system.

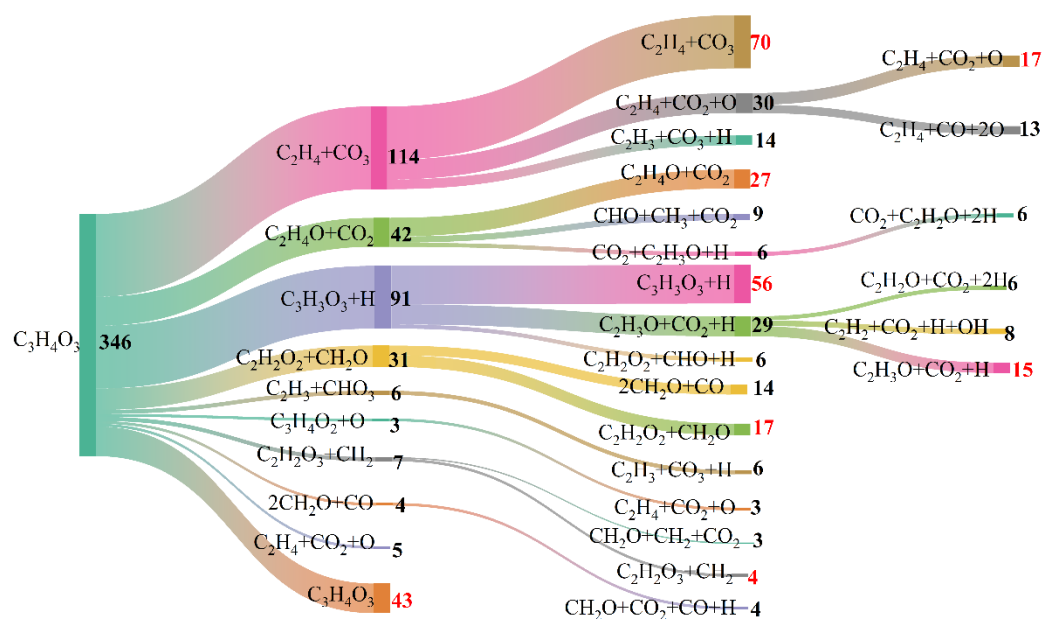
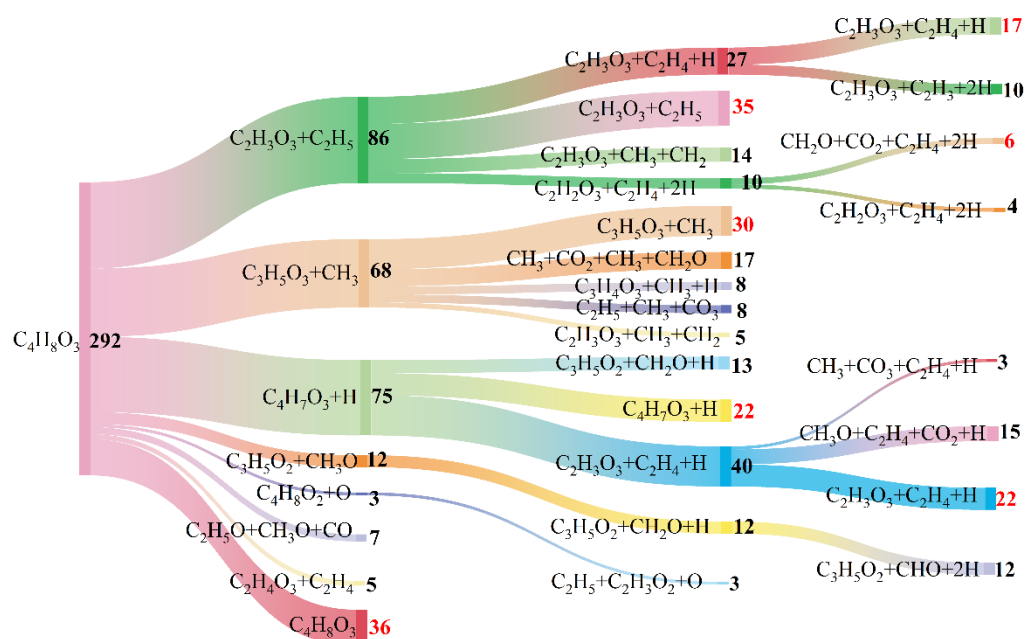


Figure S6. Reaction pathways of EC in the P/Fe = 2:1 system.



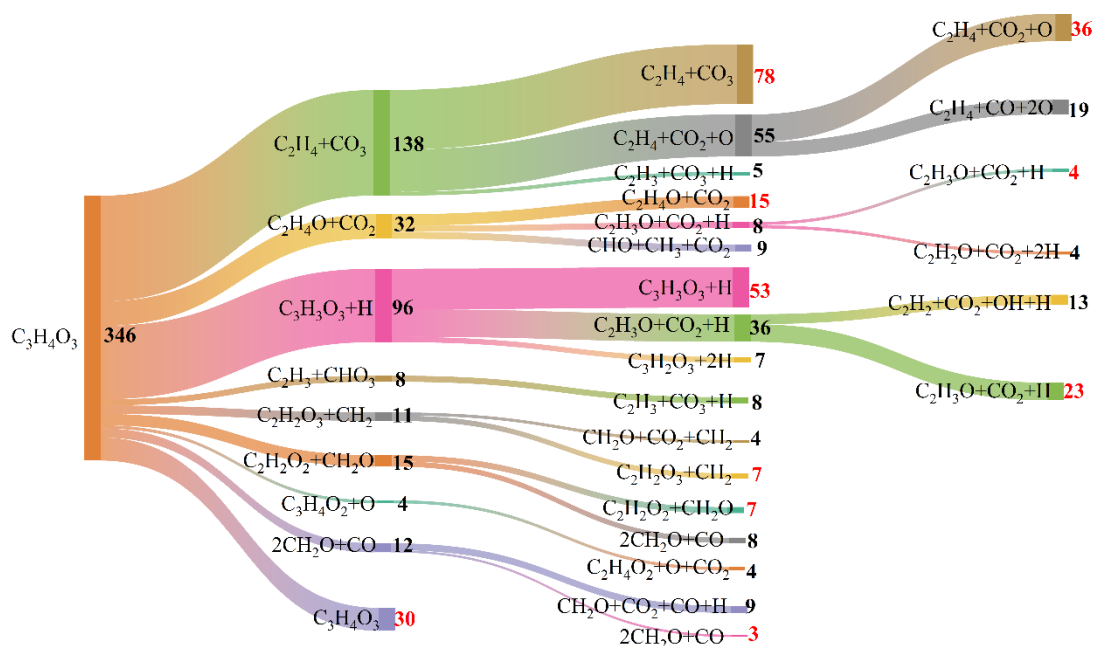


Figure S8. Reaction pathways of EC in the P/Fe = 3:1 system.

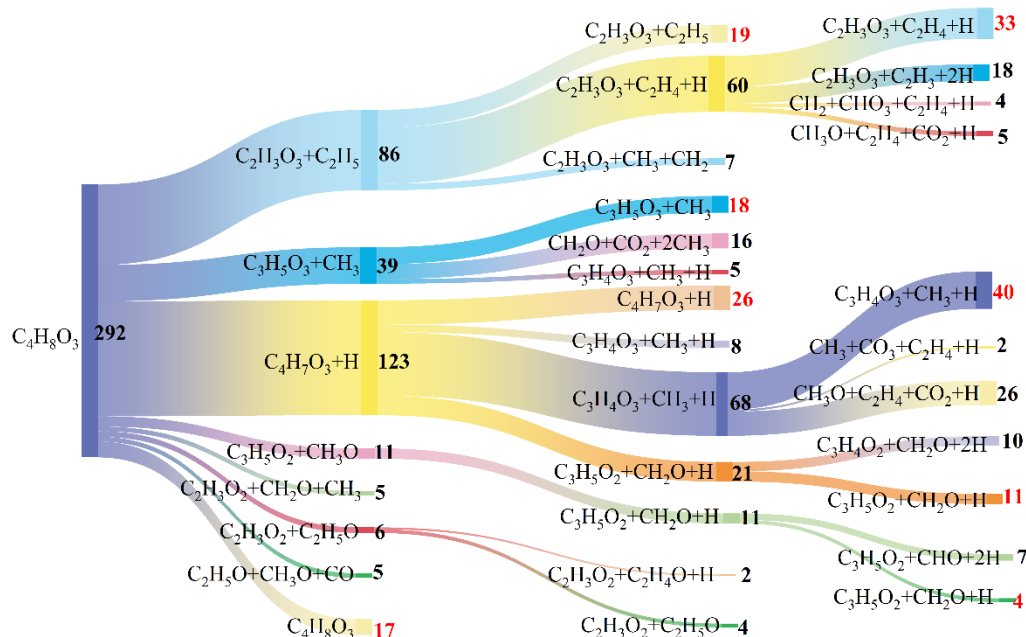


Figure S9. Reaction pathways of EMC in the P/Fe = 3:1 system