Supporting Information

Comparative analysis of aromatic compounds steam reforming over Rh supported on γ-Al_2O_3

Marinela D. Zhurka, Panagiotis N. Kechagiopoulos*

Chemical Processes & Materials Group, School of Engineering, University of Aberdeen, Aberdeen, AB24 3UE, UK

Corresponding author: p.kechagiopoulos@abdn.ac.uk

Contents

S1. Catalyst characterisation

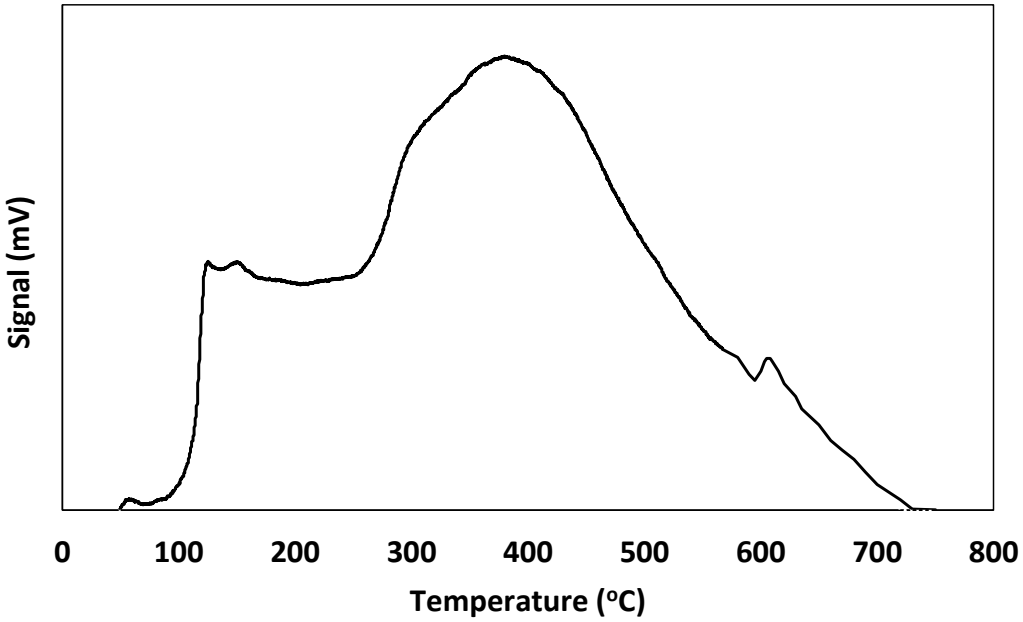

Figure S1. Temperature-programmed reduction (TPR) profile of calcined Rh/γ-Al_2O_3 catalyst.

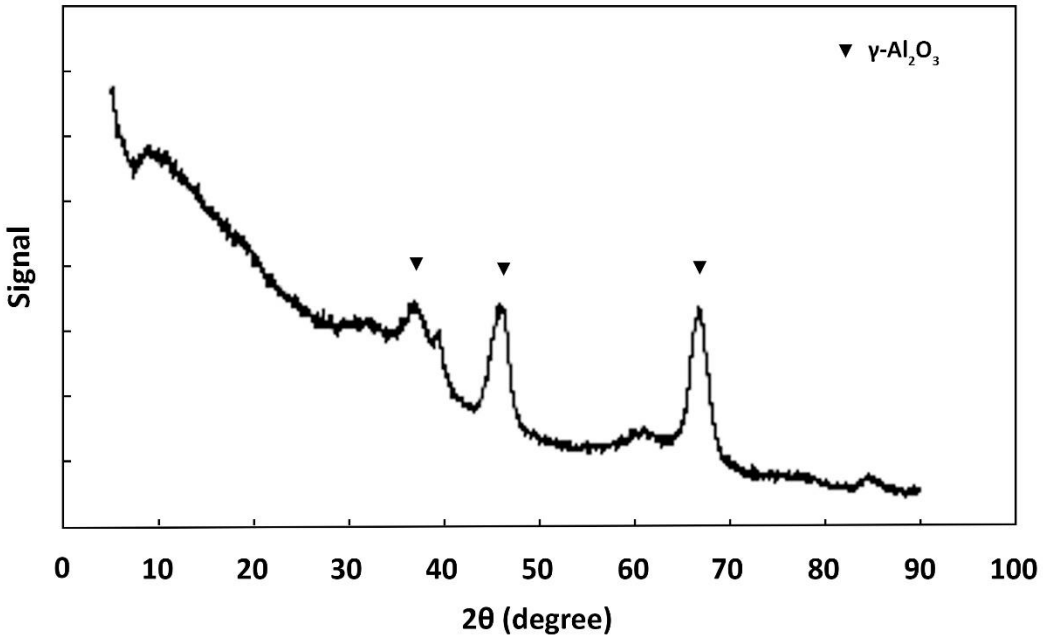

Figure S2. X-ray diffractogram of calcined Rh/γ-Al_2O_3 catalyst.

S2. Thermodynamic analysis

The Aspen plus software was used for the thermodynamic analysis of the steam reforming reaction of the aromatic compounds, using the R-Gibbs reactor with the Peng-Robinson property method. The carbon selectivities are presented as a function of temperature ranging from 300 to 800 ^{o}C and S/C ratio ranging from 0.25 to 2 mol_{H_2O} mol_{C}^{-1}. Based on experimental results, the possible products considered in the simulations consisted of H_2, H_2O, CO, CO_2, CH_4, C_6H_6 (benzene), $C_{10}H_8$ (naphthalene), C_5H_6 (cyclopentadiene), the aromatics under study, namely C_6H_6O (phenol), $C_6H_6O_2$ (hydroquinone), C_7H_8O (benzyl alcohol) and C_7H_8 (toluene), and carbon (graphite).

The equilibrium calculations indicate the complete conversion of all model compounds under the examined conditions, forming H_2, CO, CO_2, CH_4 and solid C (graphite). The general trends of the carbon selectivities are similar for all the model compounds. Specifically, at lower temperature and S/C ratio solid carbon and methane are the main products. However, increasing the temperature and S/C ratio the solid carbon and methane formation reduce, with CO and CO_2 being the main products.

S2.1. Hydroquinone steam reforming

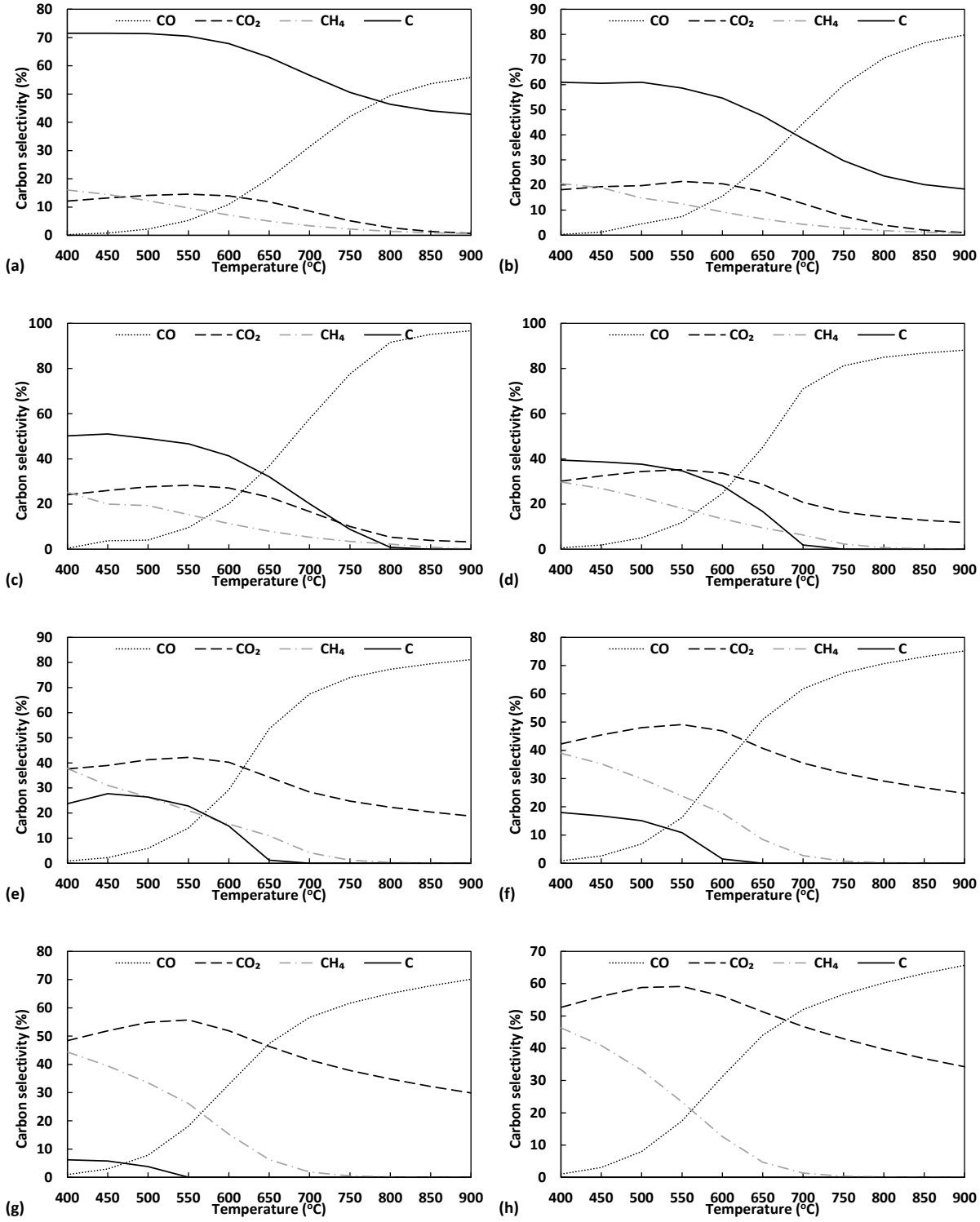

Figure S3. Temperature effect on the equilibrium product composition (CO, CO_2, CH_4 and C) during hydroquinone steam reforming at S/C = 0.25 (a), 0.5 (b), 0.75 (c), 1 (d), 1.25 (e), 1.5 (f), 1.75 (g) and 2 (h).

S2.2. Phenol steam reforming

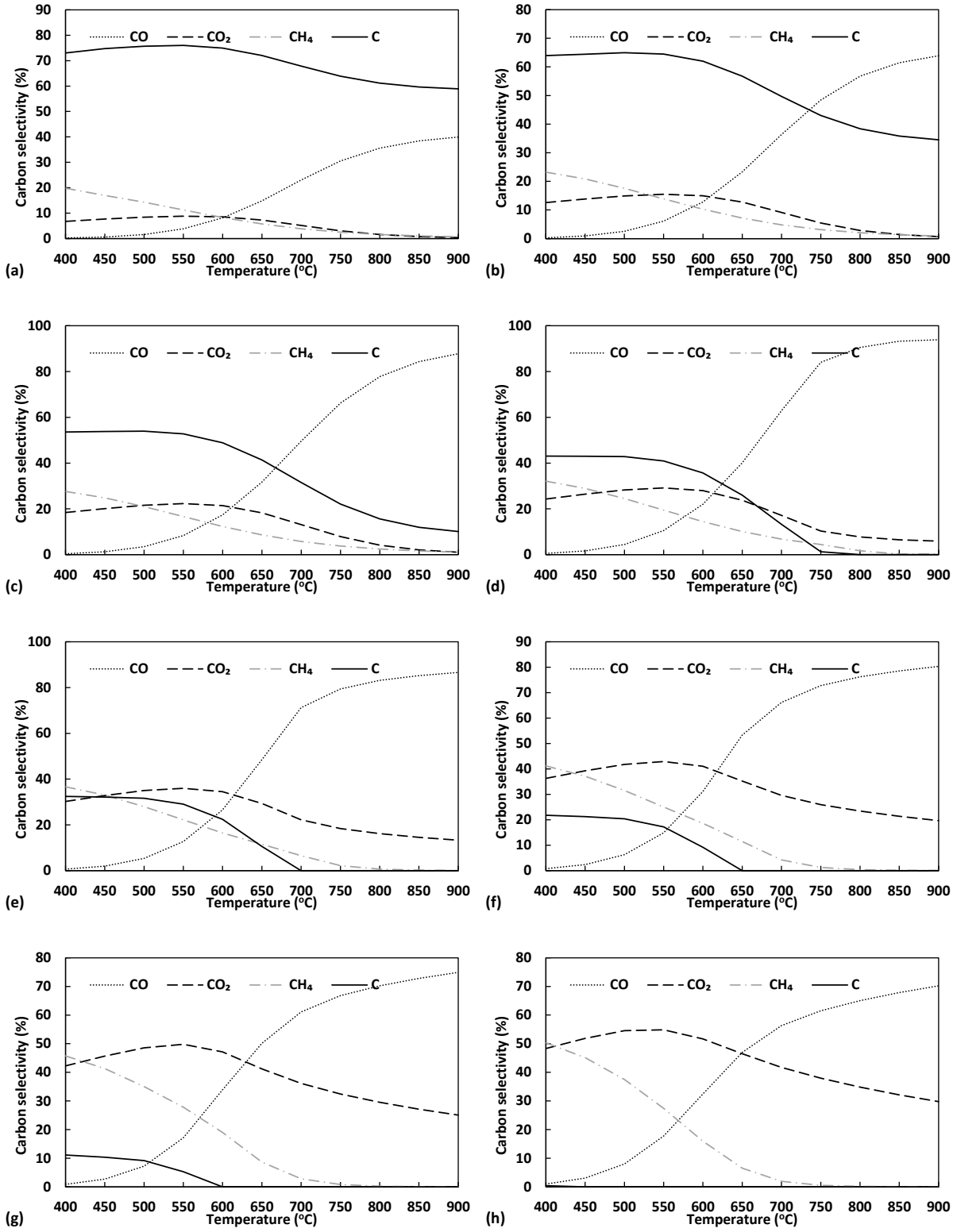

Figure S4. Temperature effect on the equilibrium product composition (CO, CO_2, CH_4 and C) during phenol steam reforming at S/C = 0.25 (a), 0.5 (b), 0.75 (c), 1 (d), 1.25 (e), 1.5 (f), 1.75 (g) and 2 (h).

S2.3. Benzyl alcohol steam reforming

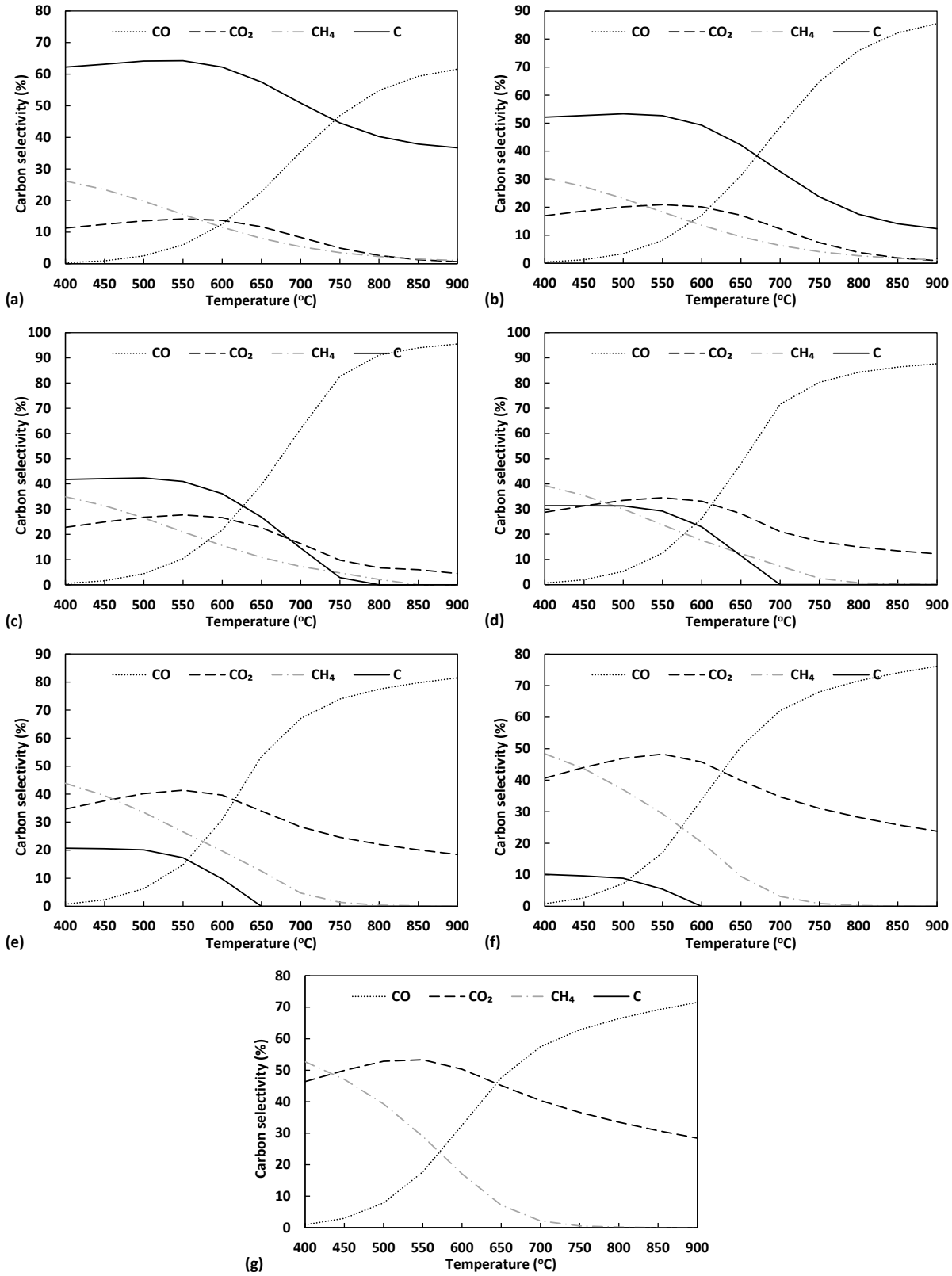

Figure S5. Temperature effect on the equilibrium product composition (CO, CO_2, CH_4 and C) during benzyl alcohol steam reforming at S/C = 0.5 (a), 0.75 (b), 1 (c), 1.25 (d), 1.5 (e), 1.75 (f) and 2 (g).

S2.4. Toluene steam reforming

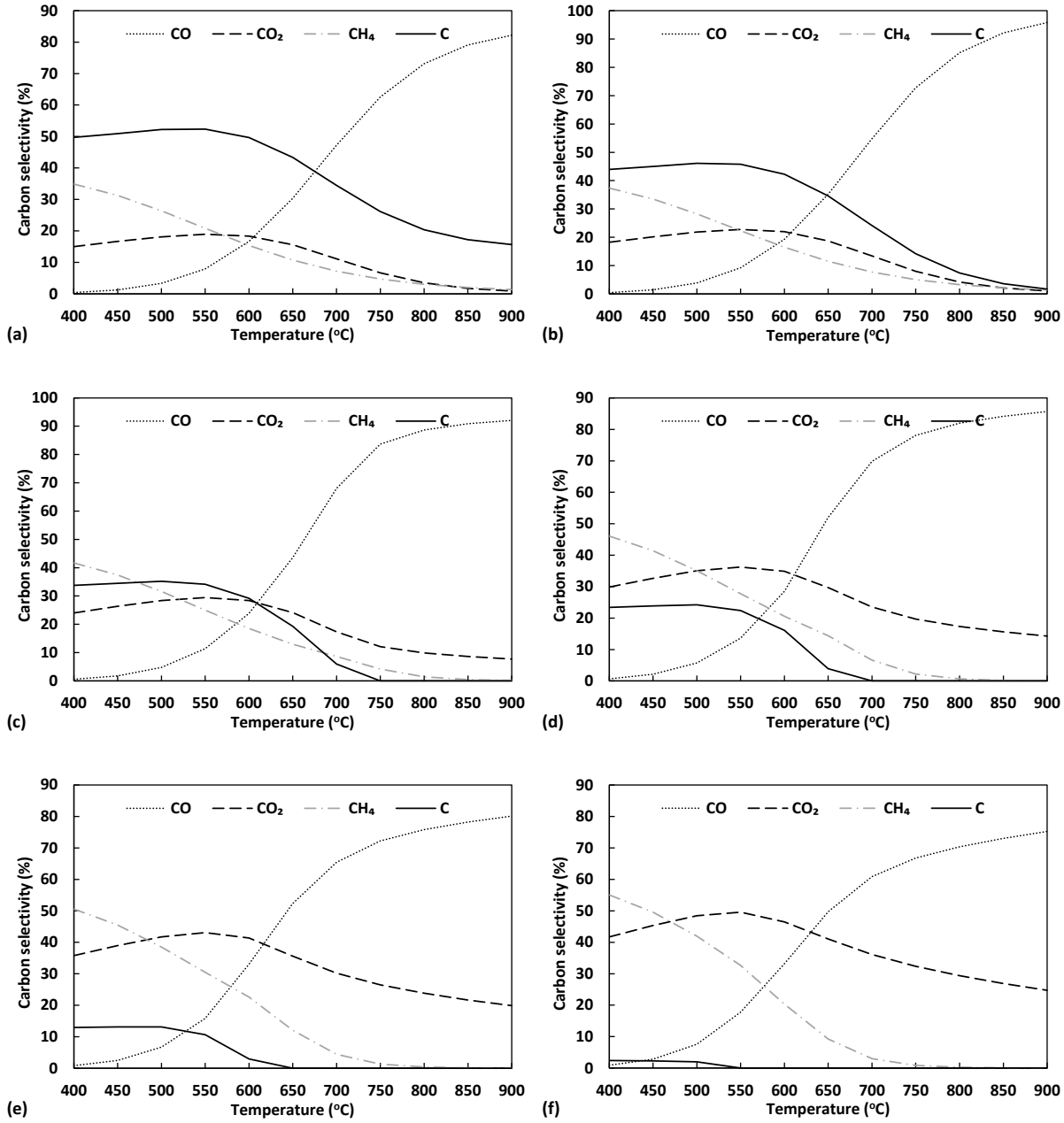

Figure S6. Temperature effect on the equilibrium product composition (CO, CO_2, CH_4 and C) during toluene steam reforming at S/C = 0.85 (a), 1 (b), 1.25 (c), 1.5 (d), 1.75 (e) and 2 (f).

S3. Product yields

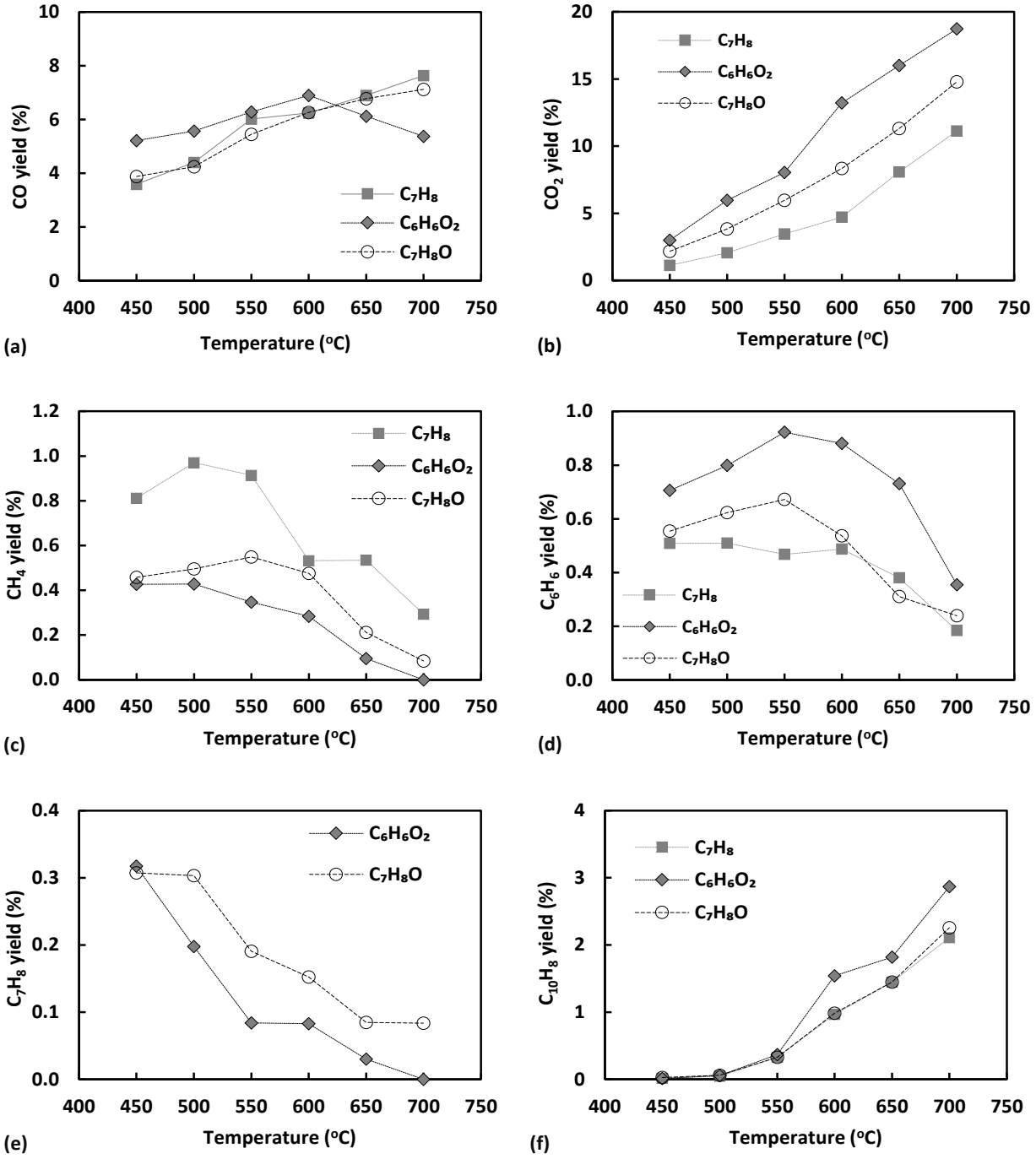

Figure S7. Temperature effect on yields of CO (a), CO_2 (b), CH_4 (c), C_6H_6 (d), C_7H_8 (e) and $C_{10}H_8$ (f) during the steam reforming of toluene, hydroquinone and benzyl alcohol ($W/F_{0,Aromatics}$ = 50 g_{cat} s $g_{Aromatics}^{-1}$, P = 1.9 bar, S/C = 2, aromatics ratio = 3 $mol_{Compound}/mol_{Phenol}$).

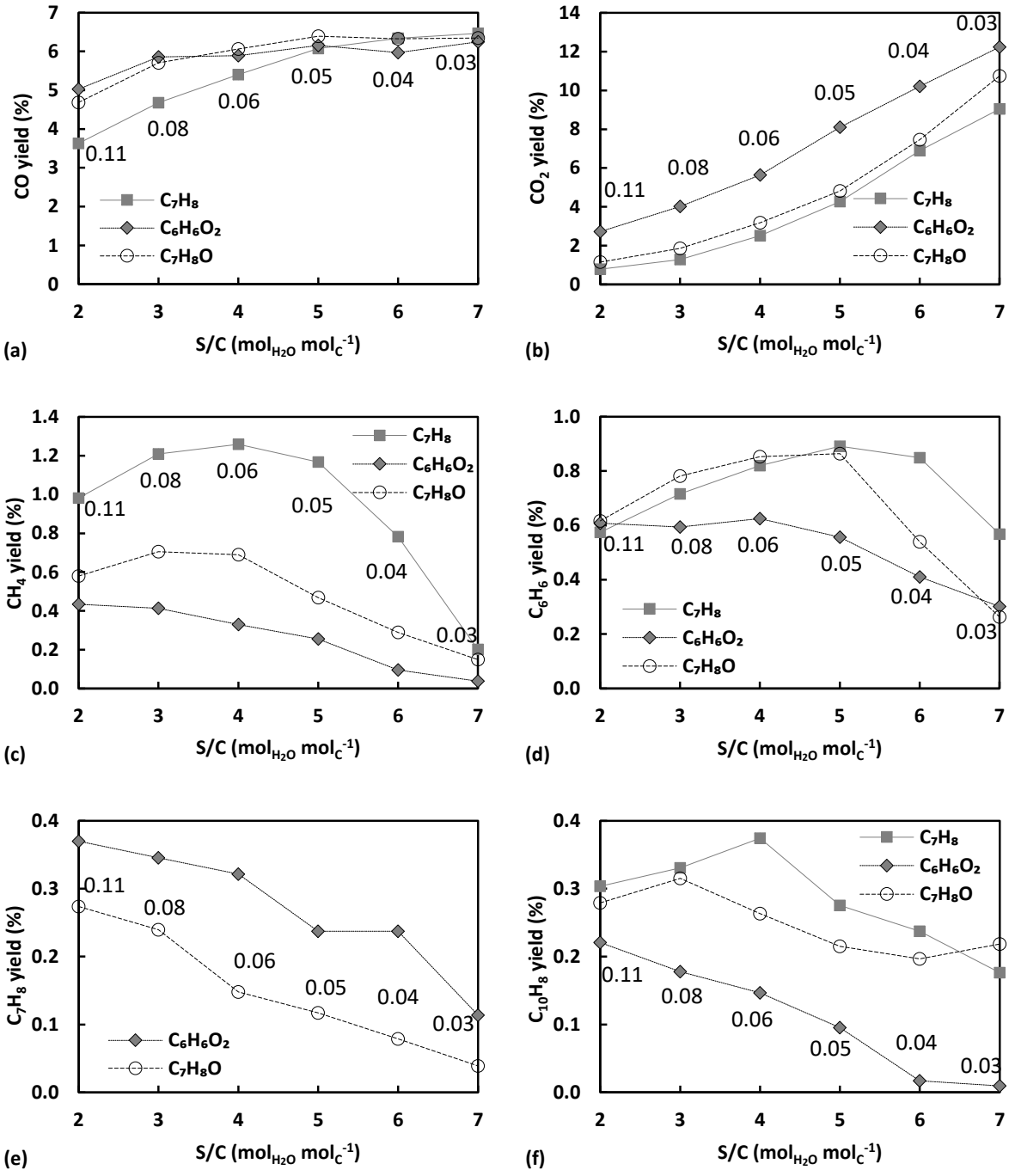

Figure S8. Partial pressure effect of aromatic compounds on yields of CO (a), CO_2, (b), CH_4 (c), C_6H_6 (d), C_7H_8 (e) and $C_{10}H_8$ (f) at 600 °C presented as a S/C variation with numbers on plot annotating the equivalent partial pressures of phenol in bar (P = 1.9 bar, Q_{tot} = 210 NmL min^{-1}, aromatics ratio = 3 $mol_{Compound}/mol_{Phenol}$).

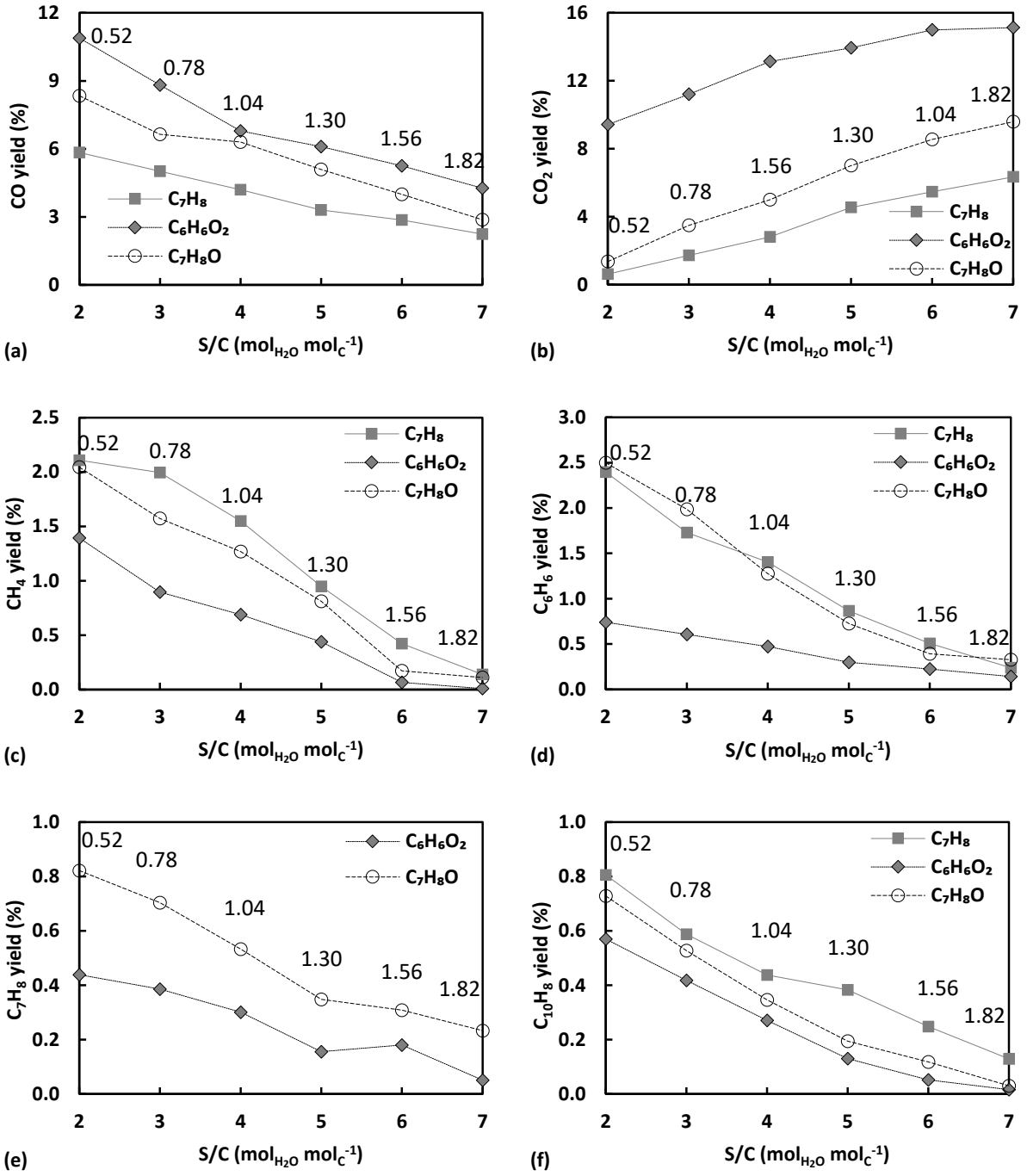

Figure S9. Partial pressure effect of water on yields of CO (a), CO_2, (b), CH_4 (c), C_6H_6 (d), C_7H_8 (e) and $C_{10}H_8$ (f) at 600 °C presented as a S/C variation with numbers on plot annotating the equivalent partial pressures of water in bar (P = 1.9 bar, Q_{tot} = 230 NmL min^{-1}, aromatics ratio = 3 mol$_{Compound}$/mol$_{Phenol}$).

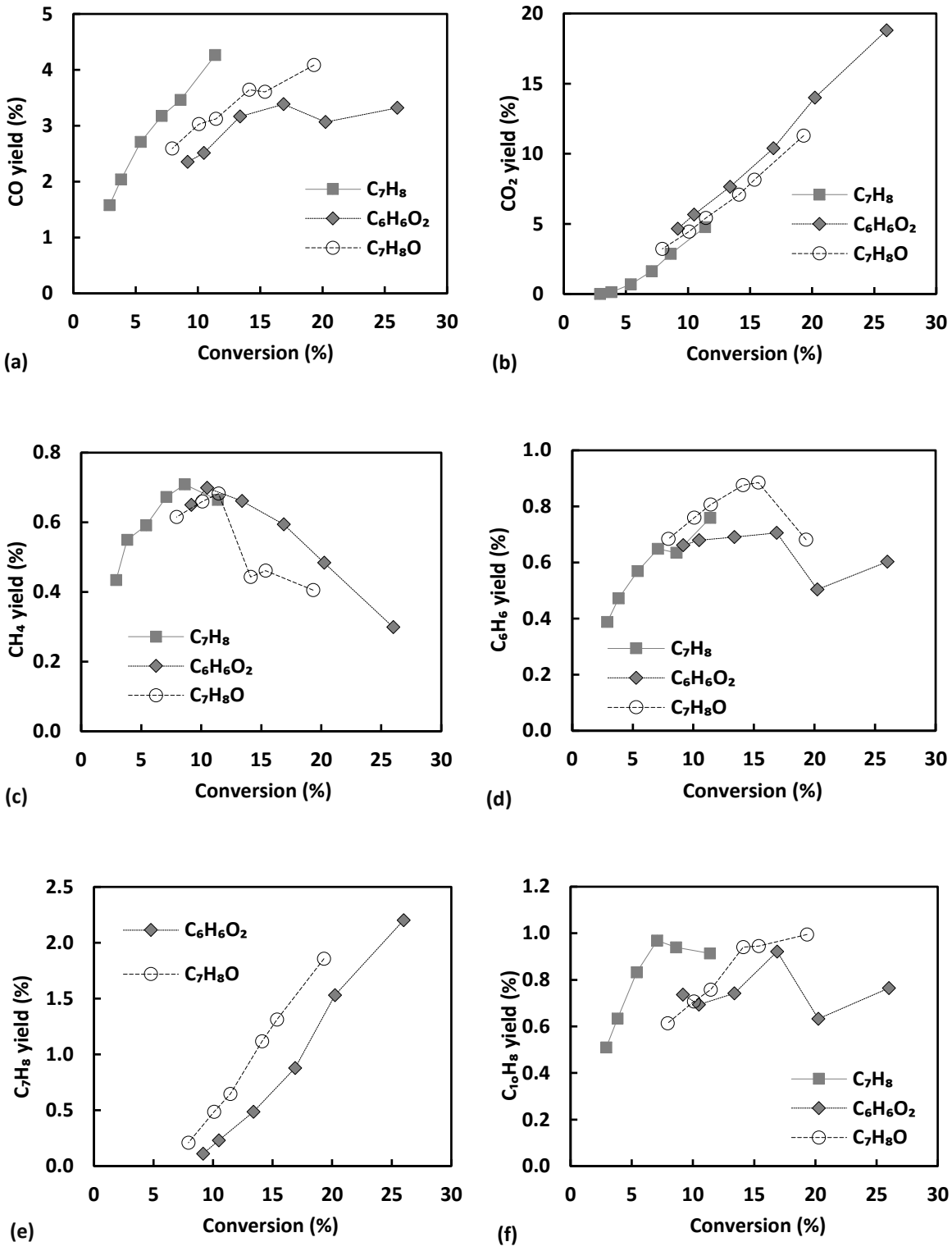

Figure S10. Yields of CO (a), CO_2, (b), CH_4 (c), C_6H_6 (d), C_7H_8 (e) and $C_{10}H_8$ (f) versus the total conversion observed during W/F_0 variation at 600 °C (P = 1.8 bar, S/C = 2, aromatics ratio = 3 $mol_{Compound}/mol_{Phenol}$).