Thermodynamic analysis of high temperature steam and carbon dioxide co-electrolysis

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Electronic supplementary information (ESI)

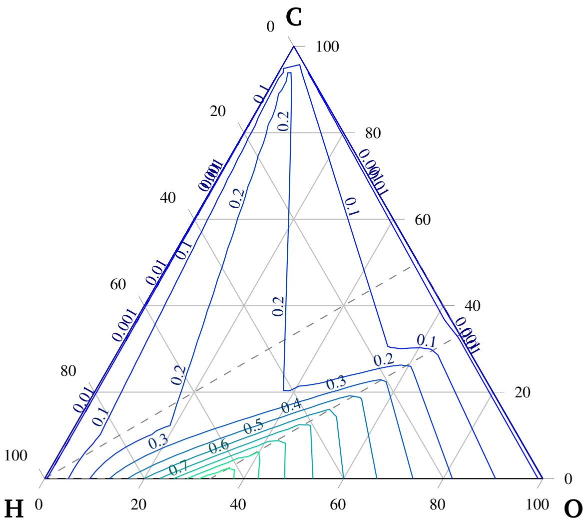
This electronic supplementary information provides the complementary ternary diagrams with equilibrium partial pressures of H_2O, CO and CH_4 to the manuscript†.

The equilibrium partial pressures of gases in the mixture depend on temperature, total pressure and C:H:O-ratio, therefore, ternary diagrams were chosen for the presentation of the results. The relative partial pressure of steam equilibrium is shown in the Figure S1. Amount of oxygen in the mixture is the main driving factor of the steam presence. If the mixture contains enough oxygen so that both carbon and hydrogen can be fully oxidized, i.e. C:H:O-ratio is in the triangle formed by H_2O, CO_2 and O_2, the elementary hydrogen is present exclusively in the form of steam.

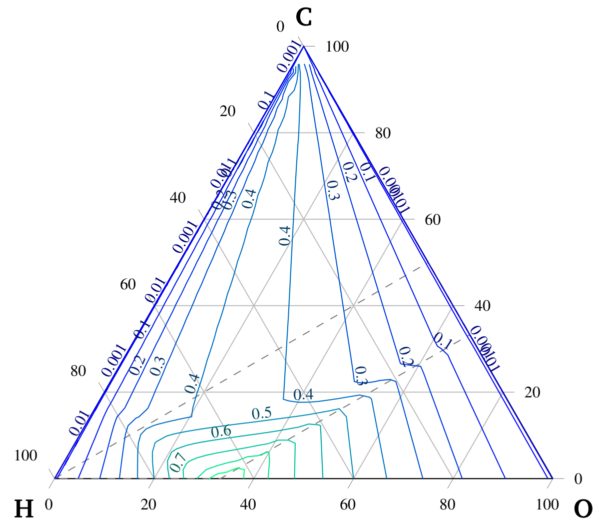
The equilibrium partial pressures of methane at 50 bar are shown in Figure S2. No methane is present in the if the C:H:O-ratio is inside the aforementioned triangle as follows from the steam. Elevated pressure sets stoichiometric preference of methane over carbon monoxide and hydrogen gas. Rising temperature serves detrimentally because of the methane-steam reforming reaction.

The equilibrium partial pressures of carbon monoxide are shown in Figure S3. Carbon monoxide is also absent in the gaseous mixture for C:H:O-ratio in the triangle of H_2O, CO_2 and O_2, where elementary carbon is present in the form of carbon dioxide. The temperature and pressure behavior of CO is opposite to the behavior of methane due to the methane steam reduction reaction.

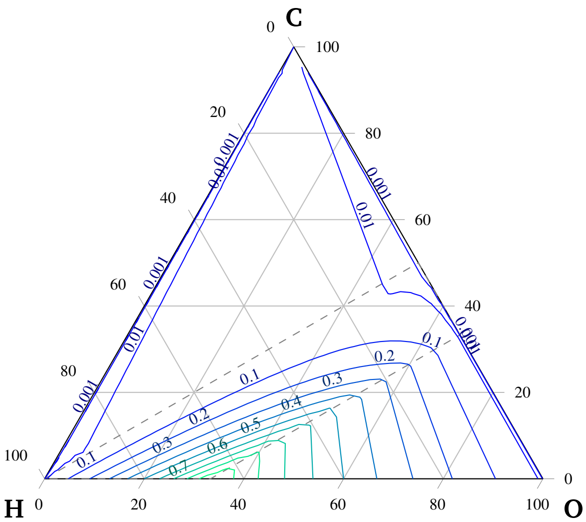
† Electronic Supplementary Information (ESI) RCE. See DOI: 10.1039/cXCP00000x/



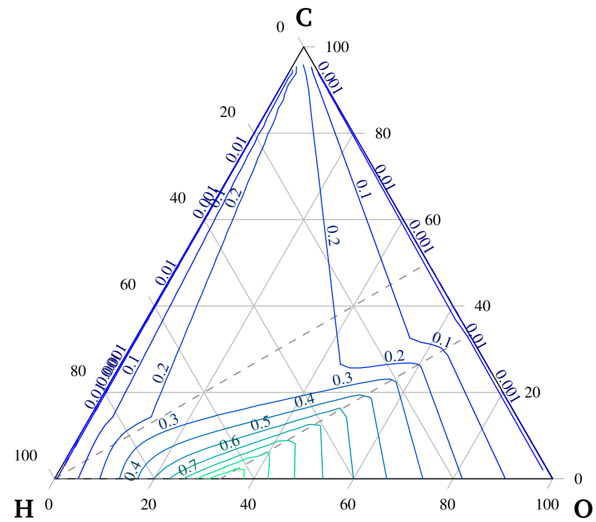
(a) Relative partial pressure of H_2O at 600 °C and 1 bar



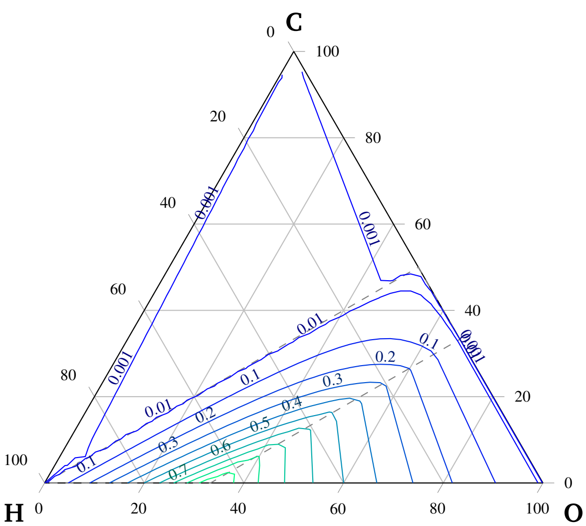
(b) Relative partial pressure of H_2O at 600 °C and 50 bar



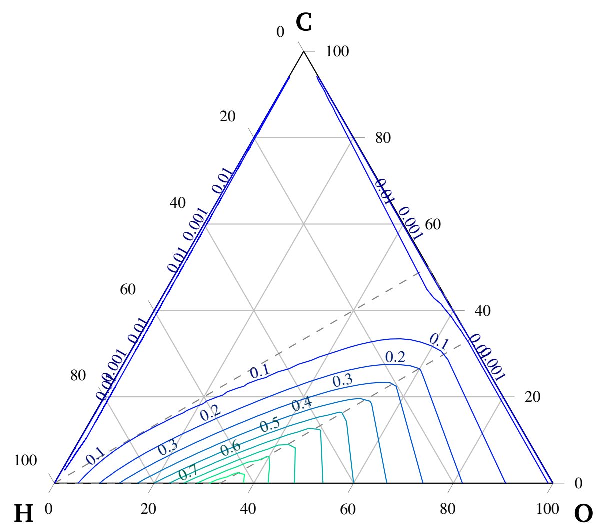
(c) Relative partial pressure of H_2O at 800 °C and 1 bar



(d) Relative partial pressure of H_2O at 800 °C and 50 bar

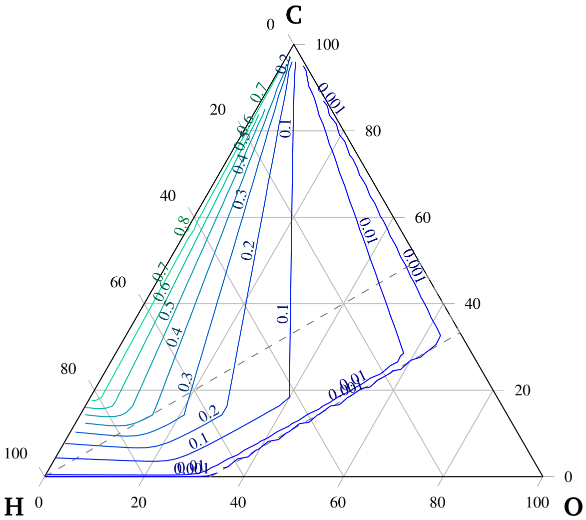


(e) Relative partial pressure of H_2O at 1000 °C and 1 bar

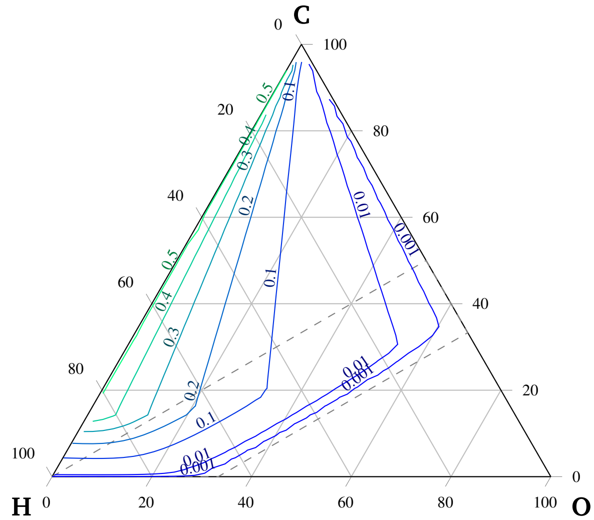


(f) Relative partial pressure of H_2O at 1000 °C and 50 bar

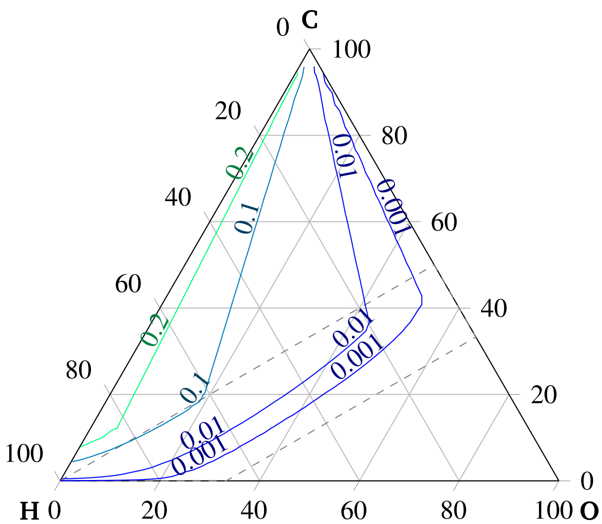
Figure S1 Relative partial pressures of H_2O.



(a) Relative partial pressure of CH_4 at 600 °C and 50 bar

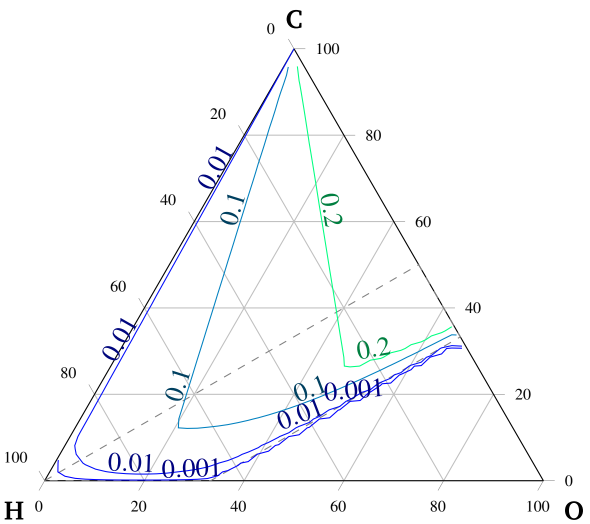


(b) Relative partial pressure of CH_4 at 800 °C and 50 bar

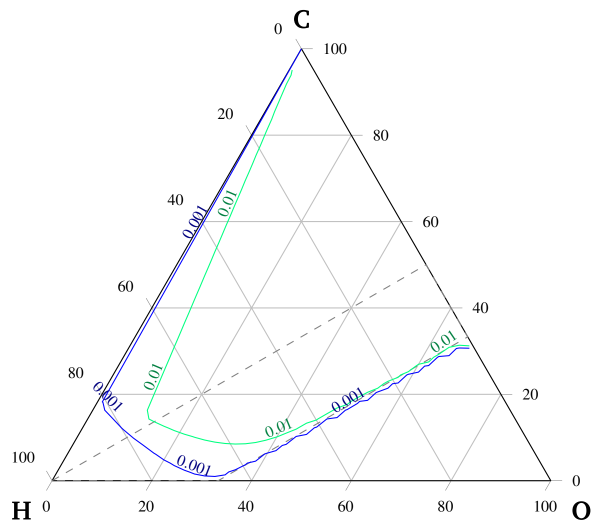


(c) Relative partial pressure of CH_4 at 1000 °C and 50 bar

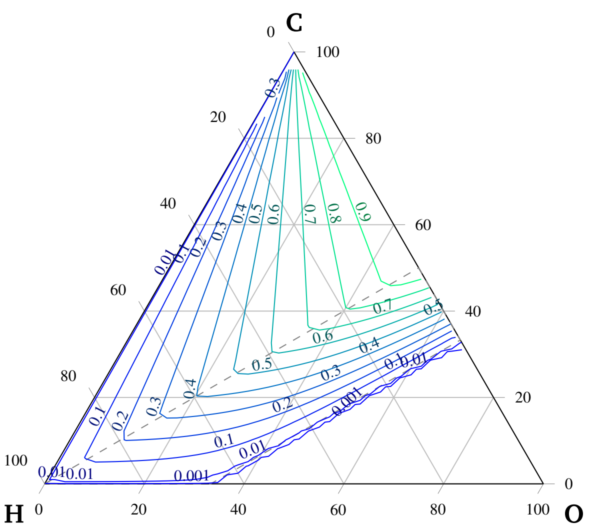
Figure S2 Relative partial pressures of CH_4 at 50 bar



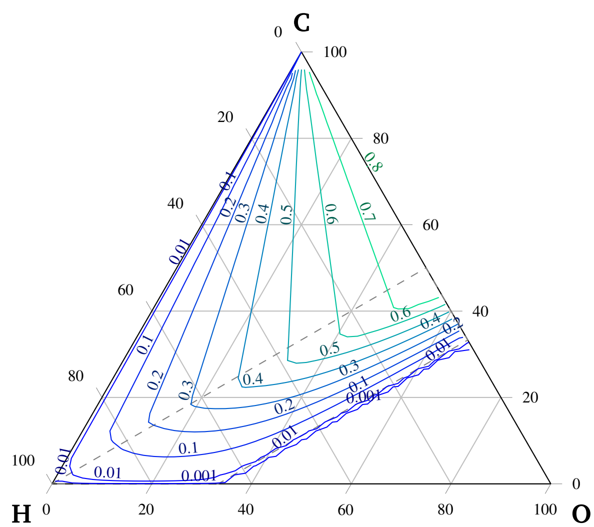
(a) Relative partial pressure of CO at 600 °C and 1 bar



(b) Relative partial pressure of CO at 600 °C and 50 bar



(c) Relative partial pressure of CO at 1000 °C and 1 bar



(d) Relative partial pressure of CO at 1000 °C and 50 bar

Figure S3 Relative partial pressures of CO.