Supporting Information to: Adsorption for efficient low carbon hydrogen production – part 2: cyclic experiments and model predictions

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S1 Temperature profiles

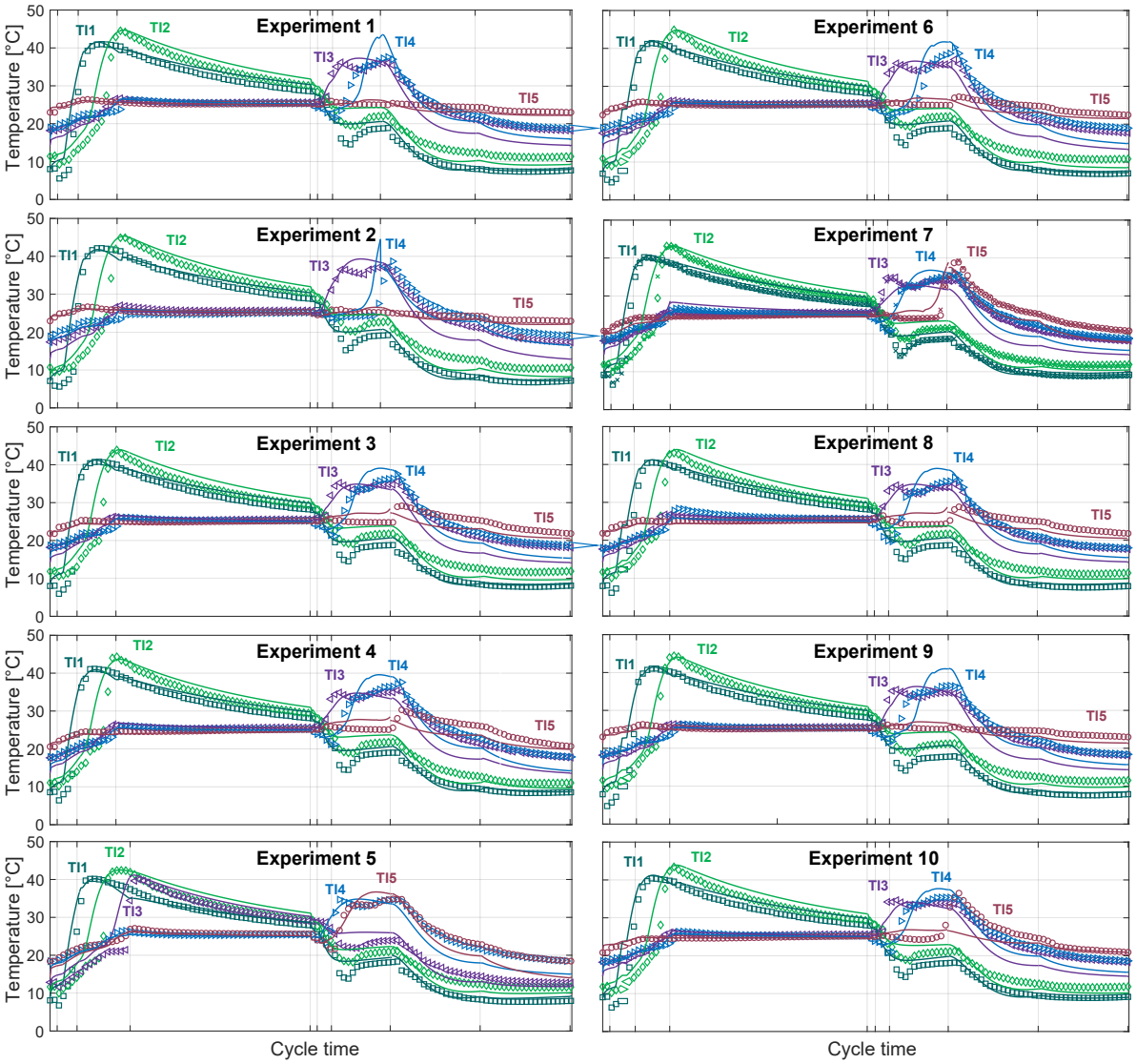

Figure S1: Measured (symbols) and simulated (lines) temperature profiles in cyclic steady state (CSS) for column 1 and Experiments 1-10. Multi-component adsorption is modeled using the real adsorbed solution theory (RAST) and $\overline{\lambda_i} = 4000$. TI1-TI5 are positioned at 10, 35, 60, 85 and 110 cm from the column bottom. The temperature profiles for the repetition of experiment 7 are shown with crosses showing excellent reproducibility

S2 Composition profiles experiment 5

Figure S2 shows the measured and simulated composition profiles for experiment 5. CH_4 breakthrough occurs at the end of the adsorption step. There is a time delay of a few seconds between the column outlet and the MS downstream of the column during adsorption, such that the simulated breakthrough occurs shifted in time by a few seconds. The H_2 produced during the last few seconds of Ads cannot be measured experimentally, which is why the model predicts a lower H_2 purity than seen in the experiment. Note that during HP, CO_2 breakthrough occurs at around the middle of the step (simulation) but is perceived only toward the end of the step with an rapid increase in measured CO_2 content, due to the time delay between column and MS.

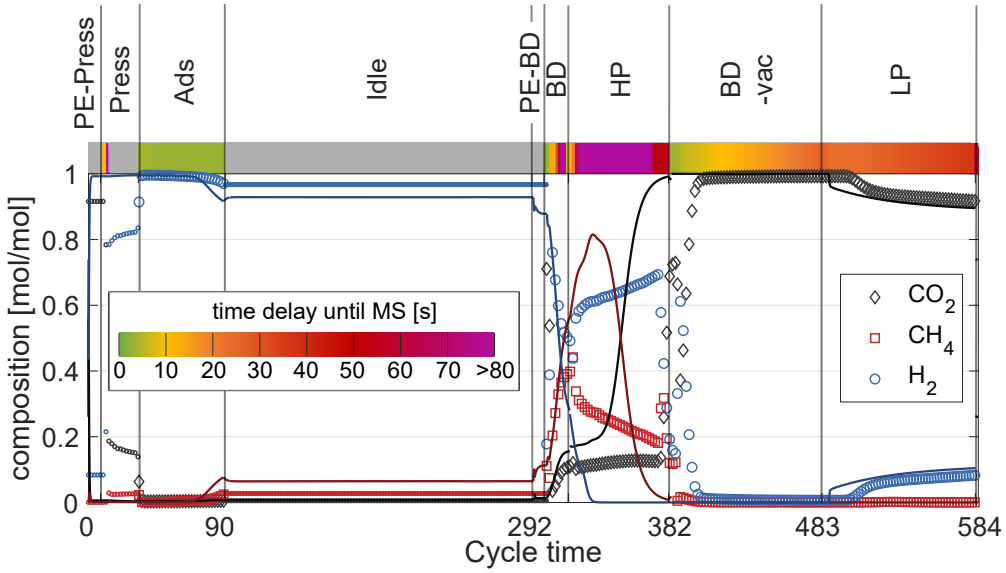

Figure S2: Measured (symbols) and simulated (lines) composition profiles in CSS for experiment 5. Multi-component adsorption is modeled using the real adsorbed solution theory (RAST) and $\overline{\lambda_i} = 4000$. The bar at the top indicates the time delay from the column outlet until the composition is measured at the MS