Dry reforming of steelworks off-gases in a pilot plant integrated into a steel mill: influence of operating parameters

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Supplementary Material

The relative deviation σ_i on the left side and the absolute deviation θ_i on the right side of the measured species i from the gas analysis to the simulation with the DETCHEM[CHANNEL] model are shown in Figure S1. Not included in the evaluation are the deviations due to calibration uncertainties, uncertainties in temperature measurement, and the high sensitivity of temperature to the reactions. For example, the shape of the simulated curve of H_2O, shown in Figure 3, shows that temperature variations can have a significant impact on the concentration.

The three species with the largest deviation are O_2, C_2H_4, and C_2H_6 with a measured total contribution to the gas composition of about 0.4% in the gas analysis. Here, especially the small absolute deviations lead to high relative deviations. For O_2 and C_2H_6, the simulation showed proportions of about 0%, while these were somewhat higher in the measurement. The C_2H_4 content was also underestimated by the model compared to the gas analyser results. These deviations, especially for the species with low volume fractions of the measured gas, may be caused by calibration uncertainties of the analyser for these gases, since the species with a low content of less than 0.2% on average require a very fine calibration. CO and H_2 have the highest contribution to the syngas composition and are very well predicted by the model. The conversion of CO_2 and CH_4 with an average relative deviation of less than 13% and 2% respectively, also shows good agreement with the simulation for the pilot plant.
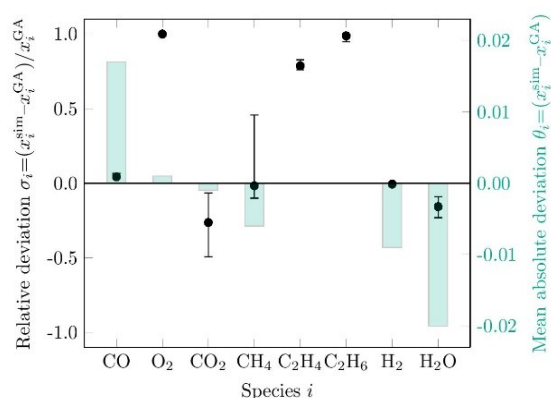

Figure S1. Relative deviation σ_i and absolute deviation θ_i from gas analysis (GA) results to kinetic simulation (sim) for the measured species i.