ARTICLE

Electronic Supplemental Information (ESI)

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Predicting thermal excursions during *in-situ* oxidative regeneration of packed bed catalytic fast pyrolysis catalyst

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GradientCheck Reports

Tables S1 and S2 show the full reports from the GradientCheck web tool for the nominal 2FBR and TCPDU cases summarized in Tables 3 and 4 in the main body of the paper. While this analysis is useful, it is not strictly applicable for the reasons mentioned before:

1. Carbon in coke is a fixed, non-diffusing reactant.
2. The regeneration process is transient, not steady state.
3. For most practical combustion rates, the reaction is confined to a combustion zone which is generally much smaller than the entire reactor.

2FBR Modelled Temperatures at the Outlet Face Center Point

Figure S1 shows the modelled 2FBR temperature profiles using the center point of the outlet face, for the four effective conductivities. The profiles based on the lowest, most realistic values of 0.25 W/(m.K) and 0.675 W/(m.K) do not match measured temperatures with any value of wall heat transfer coefficient. The 1.725 W/(m.K) profile does not match the shape of the measured profile very well. While the highest (bulk) value of 11.9 W/(m.K) gives a reasonable match, a very low wall heat transfer coefficient of 30 W/(m2.K) is required. While not definitive, these results point to the average modelled outlet temperature as the better choice for this study.

Tube Wall Heat Flow Profiles for TCPDU Parametric Sweep

For reference, Figure S2 shows the tube wall heat flow profiles corresponding to the outlet temperature curves in Figure 14. The spread between the heat transfer parameter pairs increases with reduced N_2 flow and increased cooling air flow. Integrating these curves over the entire regeneration produced the values regressed in Figure 15.

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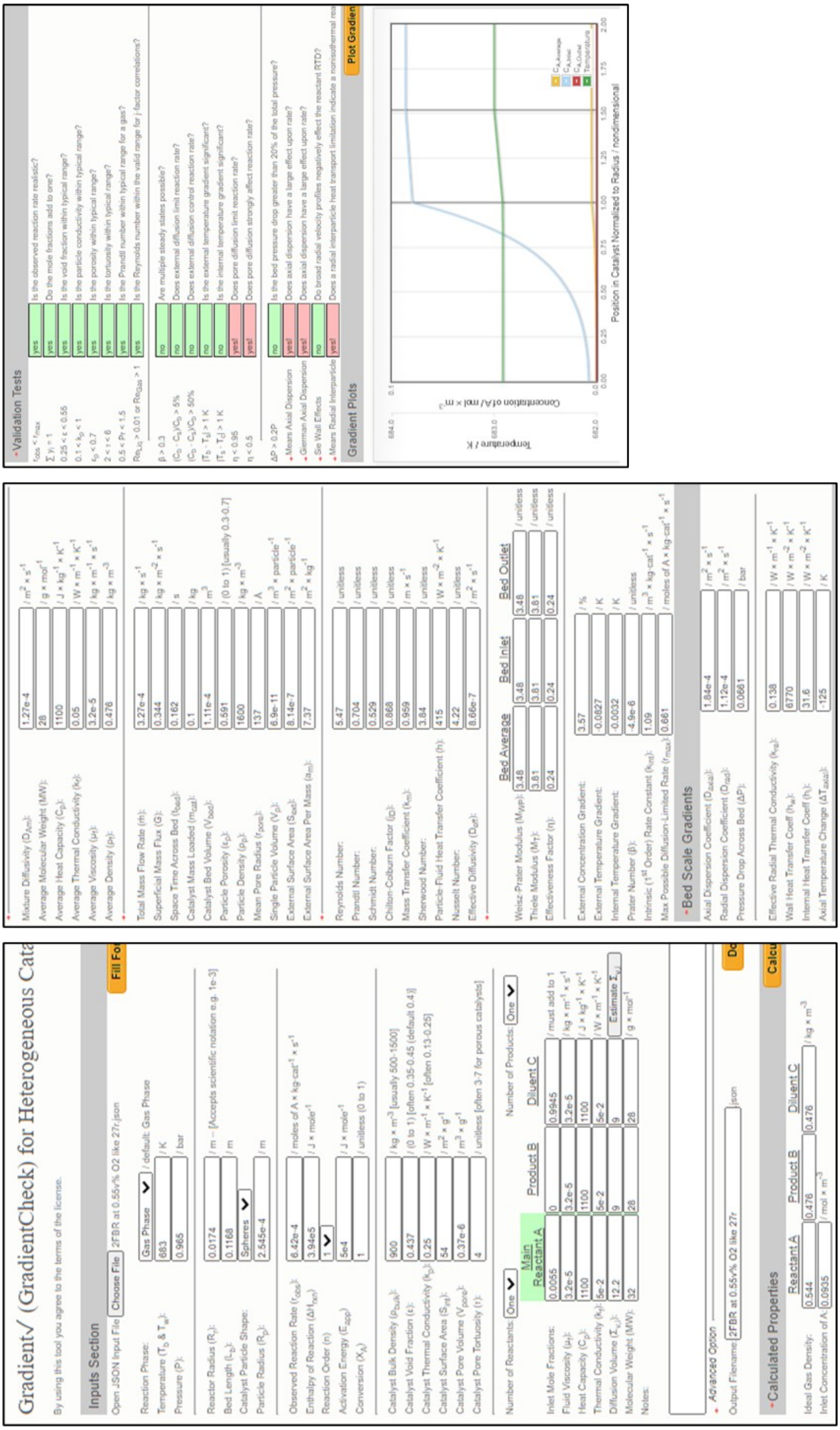
Table S1. Gradientcheck analysis of 2FBR-PBR catalyst bed and operating conditions



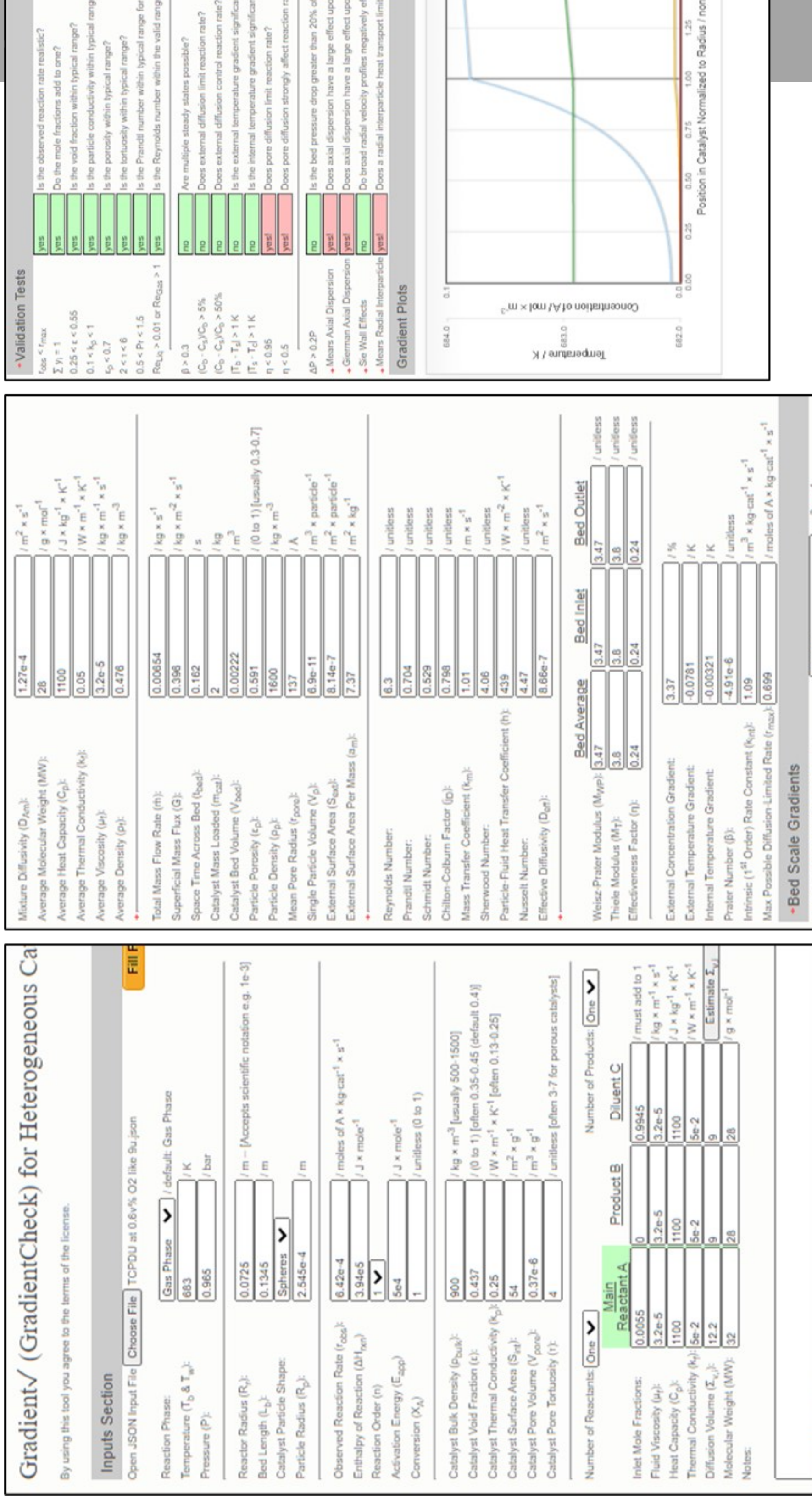


Table S2. Gradientcheck analysis of conceptual TCPDU-PBR catalyst bed (with no cooling tubes) and operating conditions

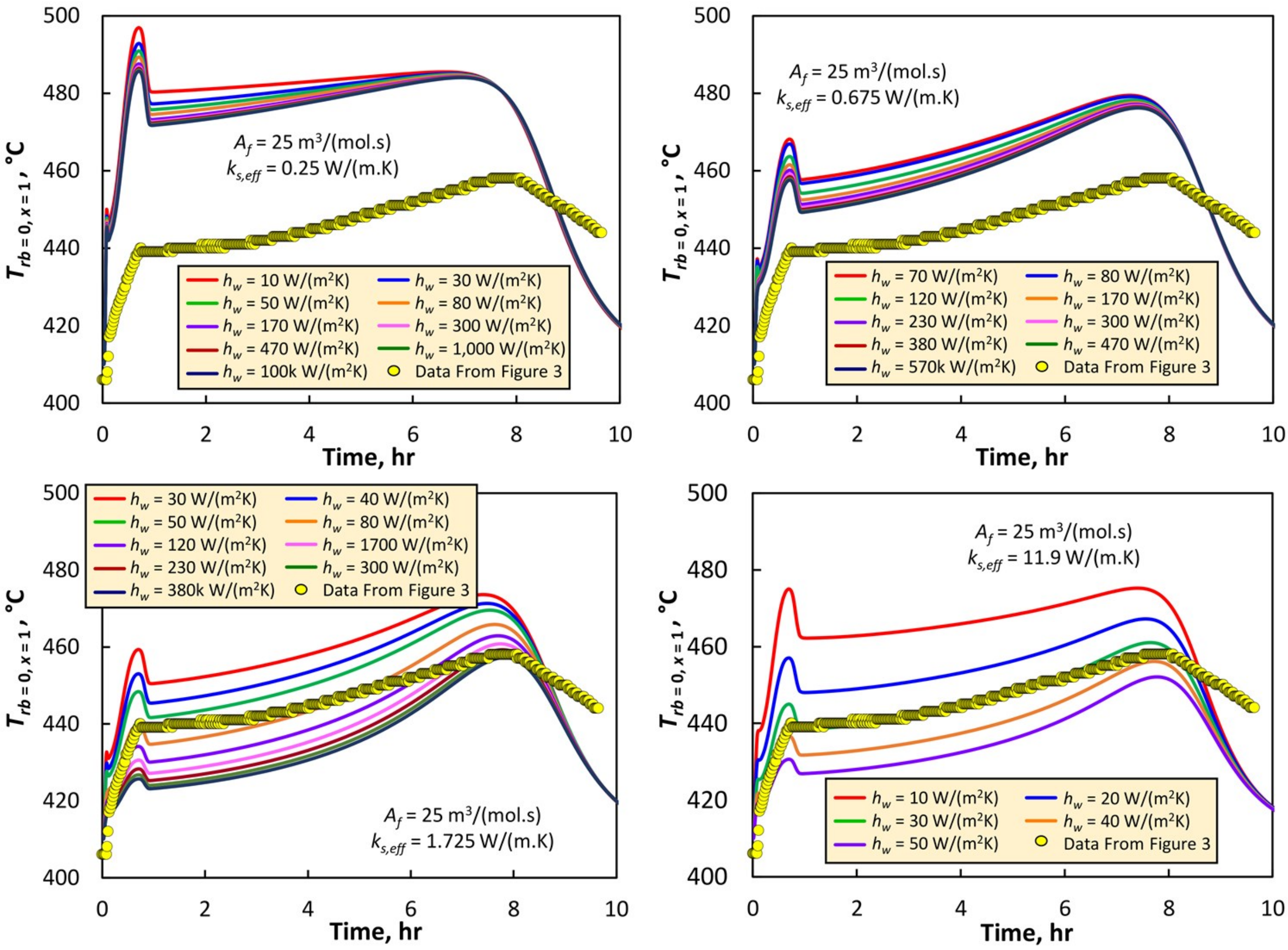


Figure S1. 2FBR modelled temperature profiles at center point of outlet (r_b = 0, x = 1) compared to data from Figure 3.

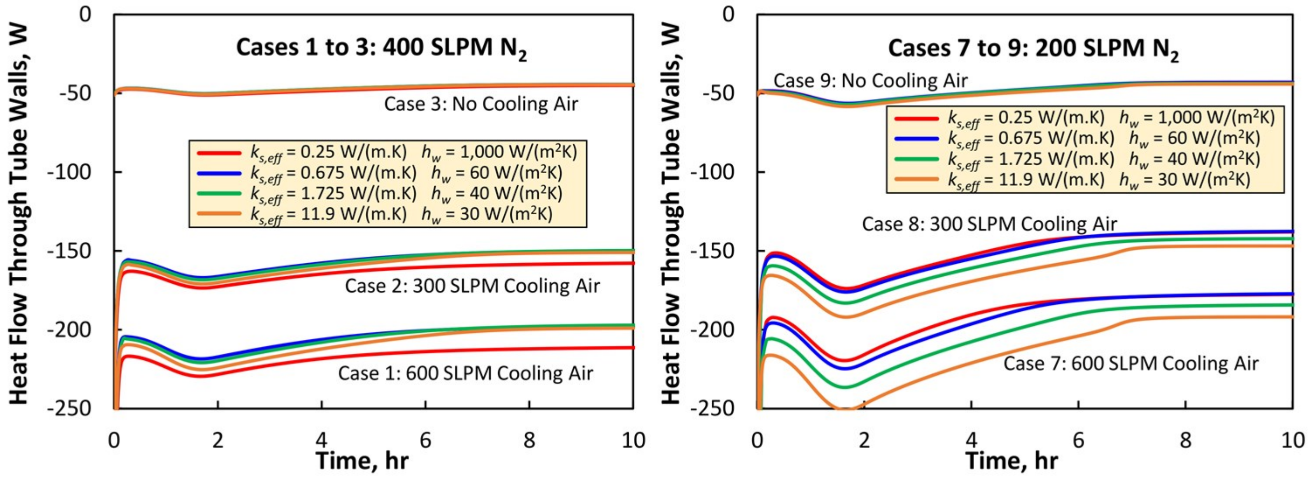


Figure S2. Tube wall heat flow profiles for TCPDU model, for process N2 flows of 400 SLPM (left) and 200 SLPM (right).