Multi-Scale Modeling of a Direct Non-Oxidative Methane Dehydroaromatization Reactor with a Validated Model for Catalyst Deactivation

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Key Words

Non-oxidative methane dehydroaromatization (DHA), Fixed bed reactor, Data reconciliation, Dynamic parameter estimation, Catalyst deactivation

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APPENDIX A

Temperature profile for conducting the TGA experiment is shown in Figure A.1.

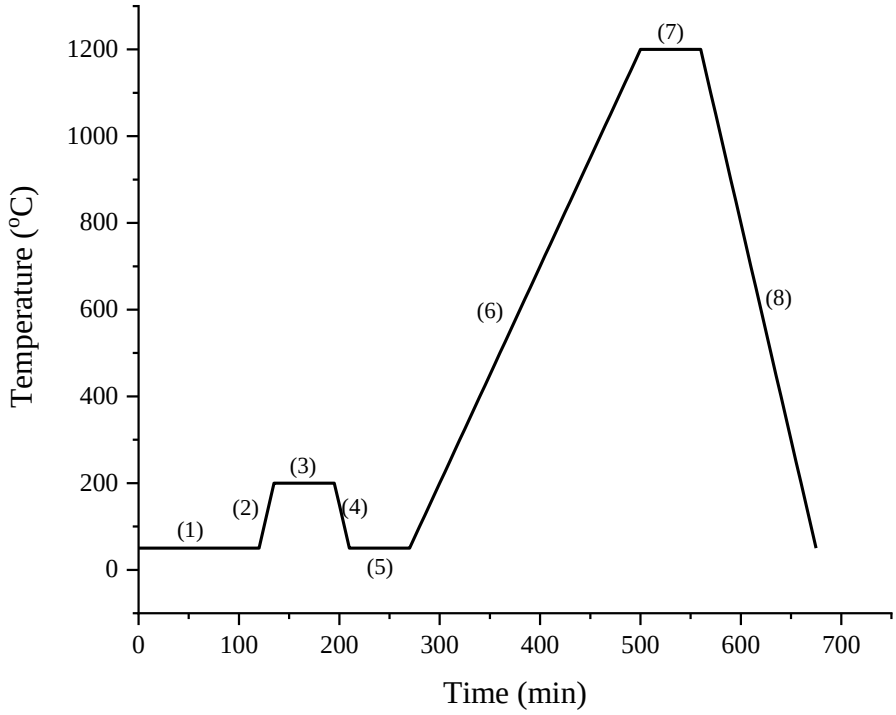

Figure A.1. Temperature profile of thermogravimetric analysis (TGA) experiments

The detail numerical reading for Figure 2 is shown in Table A.1.

Table A.1. Detailed numerical reading of Figure 2

Samples	Initial Weight	Weight at the End of Step 6	Weight at the End of Step 7	Total Weight Loss
			(mg)	
a	35.937	32.432	32.200	3.737
b	33.463	29.480	29.330	4.133
c	43.350	37.694	37.526	5.656
d	34.895	29.985	29.856	5.039

APPENDIX B

Data reconciliation for 725 ºC and 750 ºC temperature is shown in Figure B.1.

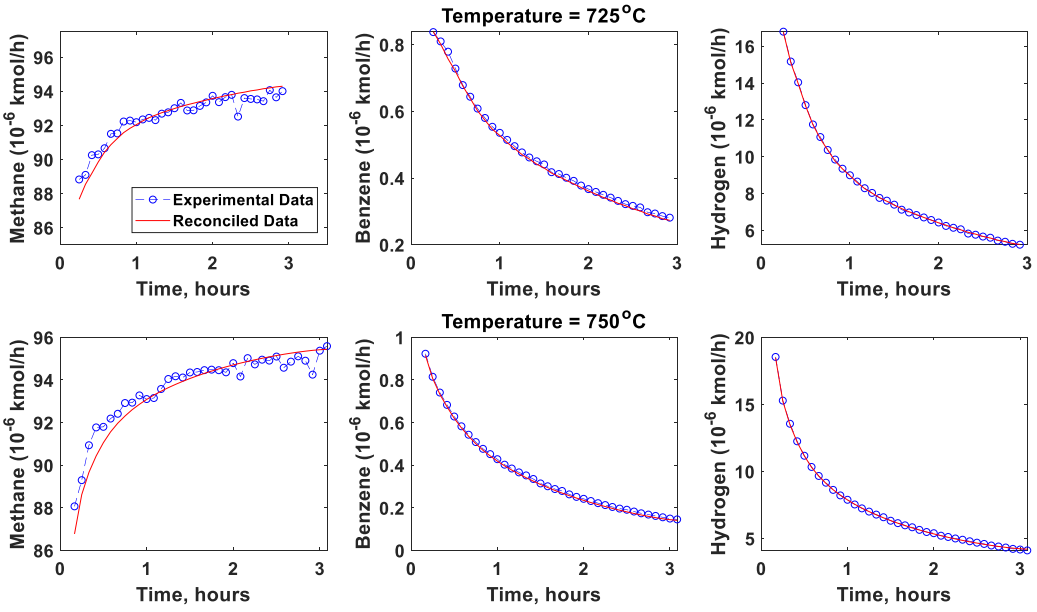

Figure B.1. Data reconciliation plots for 725 ºC and 750 ºC temperature

APPENDIX C

The comparison of parameter estimation model result with experimental data for 800 ºC is shown in Figure C.1.

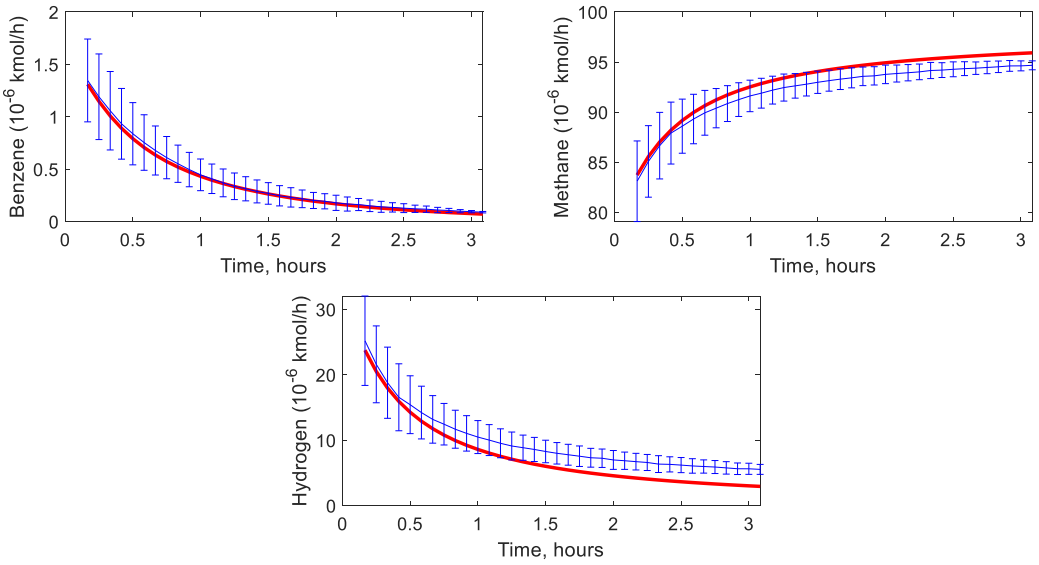

Figure C.1. Comparison of parameter estimation model with experimental data for 800 ºC

APPENDIX D

Sample Gantt chart for 2 parallel reactor cyclic operation is shown in Figure D.1. The blue color indicates reactor undergoing methane DHA reaction, black color indicates catalyst regeneration, and green color indicates cooling/preparation time. It should be noted that this is not an optimized Gantt chart. Figure D.1 shows the Gantt chart for 2 parallel reactor cyclic operation. Here, the total number of reactors required is 4 for continuous operation, and at any given time 2 reactors are undergoing methane DHA reaction.

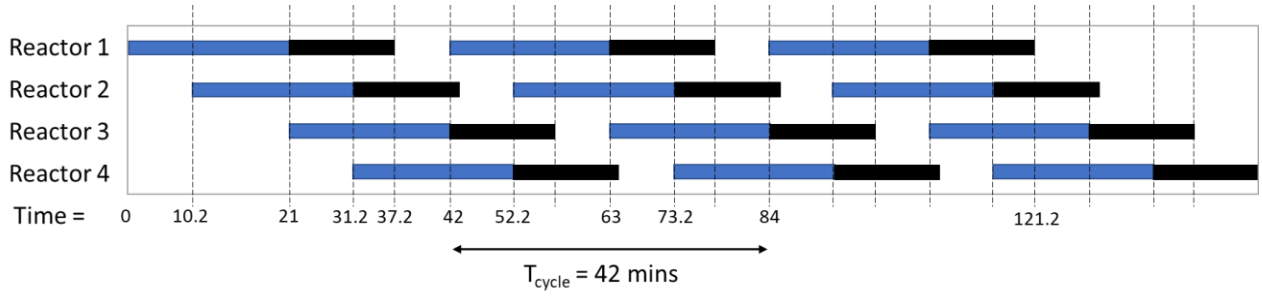

Figure D.1. Gantt chat for 2 parallel reactor cyclic operation