



## Supplementary Tables

# Application of teaching-learning-based optimization algorithm in designing 100 kW power plant using pyrolysis of oil palm empty fruit bunches

Chayangkul Janta-in<sup>a,†</sup>, Kitti Wiriyalapsakul<sup>b,†</sup>, Thongchai Rohitathisa Srinophakun<sup>c,\*</sup>

<sup>a</sup> Interdisciplinary of Sustainable Energy and Resources Engineering, Faculty of Engineering, Kasetsart University, Bangkok 10900, Thailand

<sup>b</sup> Chemical Engineering Practice School, Faculty of Engineering, King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand

<sup>c</sup> Department of Chemical Engineering, Faculty of Engineering, Kasetsart University, Bangkok 10900, Thailand

**Table S1** Process operating conditions

| Equipment | Temperature (°C) | Pressure (bar abs) |
|-----------|------------------|--------------------|
| Blower    | 40               | 1.2                |
| HX-Air    | -                | 1.2                |
| Dryer     | 100              | 1.1                |
| Mixer     | 100              | 1.1                |
| Milling   | 100              | 1.1                |
| Screen    | 100              | 1.1                |
| Reactor   | 450–550          | 1.1                |
| Gas Sep1  | 550              | 1.1                |
| HX-Quench | 100              | 1.1                |
| Quench 2  | 45               | 1                  |
| Pump-Liq  | 50               | 1.2                |
| Gas Com1  | 50               | 1.2                |
| Gas Com2  | 50               | 1.5                |
| Comb      | 730              | 1.5                |
| Gas Sep2  | 730              | 1.5                |
| HX-Comb3  | -                | 1.5                |
| Turbine   | 200              | 1.5                |
| Pumpbo    | 50               | 87                 |
| H2-Comp   | 50               | 87                 |
| HX1-Cold  | -                | 87                 |
| HDT       | 390              | 87                 |
| HX1-Hot   | -                | 20                 |
| HX2-Hot   | -                | 20                 |
| Flash-HDT | 50               | 20                 |
| Decantor  | 50               | 20                 |
| PSACOL    | 50               | 20                 |
| HX2-Cold  | -                | 20                 |
| Gasolcol  | 70               | 1.5                |

<sup>†</sup> Equal contribution.

\* Corresponding author.

E-mail address: [fengtcs@hotmail.com](mailto:fengtcs@hotmail.com) (T.R. Srinophakun)

**Table S1** Continued

| Equipment  | Temperature (°C) | Pressure (bar abs) |
|------------|------------------|--------------------|
| Deieselcol | 250              | 1.2                |
| Bot pump   | 250              | 20                 |
| H2-Comp2   | 250              | 90                 |
| HX3-Cold   | 680              | 90                 |
| HCK        | 680              | 90                 |
| HX3-Hot    | -                | 20                 |
| Cool-HCK   | 50               | 20                 |
| HCK-Gas    | 50               | 20                 |

## Reaction information

### Primary cellulose decomposition

- CELLULOS --> CELL-ACT  $k=8e13, E=52900\text{kcal/kmol}$
- CELL-ACT --> .95 GLYCOALD + .25 GLYOXAL + .2 ACETALDY + .25 HDRMTFUR + .16 CO<sub>2</sub> + .23 CO + .9 WATER + .1 CH<sub>4</sub> + .61 C + .2 ACETONE  $k=1e9, E=30000\text{kcal/kmol}$
- CELL-ACT --> LEVOGLUC  $k=4, n=1, E=10000\text{kcal/kmol}$
- CELLULOS --> 5 WATER + 6 C  $k=8e7, E=36800\text{kcal/kmol}$
- HEMICELL --> .4 HEMCELL1 + .6 HEMCELL2  $k=1e10, E=31000\text{kcal/kmol}$
- HEMICELL1 --> 1.25 H<sub>2</sub> + .5 CO<sub>2</sub> + CO + .5 FORMALDY + .25 METHANOL + .125 ETHANOL + 1.125 WATER + 2.3 C + .075 ETHENE + .05 CH<sub>4</sub>.  $k=3e9, E=2700\text{kcal/kmol}$
- HEMICELL1 --> XYLOSE  $k=3, n=1, E=11000\text{kcal/kmol}$
- HEMICELL2 --> .75 CO<sub>2</sub> + .3 CH<sub>4</sub> + .5 CO + .2 H<sub>2</sub> + .3 FORMALDY + .25 METHANOL + .125 ETHANOL + 1.525 WATER + 1.35 C + .05 ETHENE + .2 ETYLDIOL + .4 ACETALDY  $k=1e10, E=3300\text{kcal/kmol}$
- HEMICELL2 --> ACETICAC + 1.2 WATER + .22 1PC10CHR + .2 FORMALDY + .15 FORMICAC + .15 PROPNCAC  $k=8e9, E=33000\text{kcal/kmol}$

### Cellulose secondary reactions

- LEVOGLUC --> HDRMTFUR + 2 WATER  $k=1.25e12, E=60000\text{kcal/kmol}$
- HDRMTFUR --> FURFURAL + FORMALDY  $k=5e12, E=59000\text{kcal/kmol}$
- PROPANOL --> ETHANE + FORMALDY  $k=1e13, E=59000\text{kcal/kmol}$
- GLYCOALD --> 2 FORMALDY  $k=5e12, E=60000\text{kcal/kmol}$
- GLYCOALD --> 1PCH<sub>2</sub>OH + 1PCHO  $k=3e16, E=82000\text{kcal/kmol}$
- PROPANOL --> PROPENE + WATER  $k=1e12, E=59000\text{kcal/kmol}$
- ACETICAC --> 2 FORMALDE  $k=5e12, E=60000\text{kcal/kmol}$
- ETYLDIOL --> FORMALDY + METHANOL  $k=1e13, E=59000\text{kcal/kmol}$
- ETYLDIOL --> WATER + ACETALDY  $k=5e12, E=59000\text{kcal/kmol}$
- FORMALDY --> 1RH + H<sub>2</sub> + CO<sub>2</sub>  $k=1e13, E=10000\text{kcal/kmol}$

### Lignin decomposition and secondary reactions

#### Initial decomposition reactions

- 1LIGH --> PROPENE + 1ROH + 1RLIGM2A  $k=1e13, E=163245\text{ kJ/kmol}$
- LIGNIN-H --> 1PRLIGH + 1RH  $k=1e13, E=163245\text{ kJ/kmol}$
- 1LIGM2 --> 1RPHOXM2 + 1RADIOM2  $k=1e13, E=163245\text{ kJ/kmol}$
- LIGN-OH --> 1PRLGM2A + 1RH  $k=1e13, E=163245\text{ kJ/kmol}$
- LIGN-OH + 1RH --> 1RPHOXM2 + 1RADIOM2  $k=1e13, E=163245\text{ kJ/kmol}$
- 1LIG --> 1RPHENOX + 1RADIO  $k=1e13, E=184184\text{ kJ/kmol}$
- LIGNIN-C --> 1PRLIG-A + 1RH  $k=1e13, E=184184\text{ kJ/kmol}$
- LIGNIN-C --> 1RPHENOX + 1PRADIO  $k=1e13, E=188370\text{ kJ/kmol}$
- 1PADIOM2 --> 1RADIOM2  $k=1e13, E=171626\text{ kJ/kmol}$
- 1PADIO --> 1PRADIO + 1RH  $k=1e13, E=179998\text{ kJ/kmol}$
- 1PKETM2 --> 1PRKETM2 + 1RH  $k=1e13, E=167440\text{ kJ/kmol}$
- 1PLIGC --> LIGNIN-C + KETEN-01  $k=1e8, E=121394\text{ kJ/kmol}$
- LIGNIN-O --> LIGN-OH + CO<sub>2</sub>  $k=1e9, E=108836\text{ kJ/kmol}$

*Secondary decomposition reactions*

|                                                 |                          |
|-------------------------------------------------|--------------------------|
| • 1RPHOXM2 --> CO + .5 1C10H2M4 + 0.5 H2        | k=4e10, E=209300 kJ/kmol |
| • 1RPHEXOX --> .5 1C10H2 + CO + 1.5 H2          | k=4e10, E=209300 kJ/kmol |
| • 1PRKETM2 + 1RH --> 1KETDM2 + 1ROH             | k=1e13, E=121394 kJ/kmol |
| • 1PRLIGH --> 1PRLGM2A + ACETONE                | k=1e13, E=133952 kJ/kmol |
| • 1RADIOM2 --> 1RGUAI + PROPNCAC                | k=1e13, E=133952 kJ/kmol |
| • 1RLIGM2A --> 1KETM2 + 1RPHOXM2                | k=5e12, E=133952 kJ/kmol |
| • 1PRLGM2A --> 1PKETM2 + 1RPHOXM2               | k=5e12, E=133952 kJ/kmol |
| • 1RLIGM2A --> 1RGUAI + 1PFET3M                 | k=1e13, E=163254 kJ/kmol |
| • 1PRFETM2 --> 1RPHOXM2 + PROPDIAL              | k=1e13, E=133952 kJ/kmol |
| • 1RADIO --> 1RPHEXOL + PROPNCAC                | k=1e13, E=153254 kJ/kmol |
| • 1RLIG-A --> 1KET + 1RPHEXOX                   | k=1e13, E=138138 kJ/kmol |
| • 1RLIG-A --> 1RPHEXOL + 1PFET3                 | k=1e13, E=163254 kJ/kmol |
| • 1PRFET3 --> 1RPHEXOX + PROPDIAL               | k=1e13, E=138138 kJ/kmol |
| • 1RADIOM2 --> 1ROH + SINPYALC                  | k=3e11, E=104650 kJ/kmol |
| • 1RKETM2 --> 1ROH + 1KETDM2                    | k=3e11, E=104650 kJ/kmol |
| • 1RADIO --> 1ROH + CMRYLALC                    | k=3e11, E=104650 kJ/kmol |
| • 1RKET --> 1ROH + 1KETD                        | k=3e11, E=113022 kJ/kmol |
| • 1RC3H7O2 --> 1RMETNOL + ACETALDY              | =1e13, E=129766 kJ/kmol  |
| • 0.5 1C10H2M4 --> 1RMETNOL + 1RPHEXOX          | k=1e13, E=196742 kJ/kmol |
| • 1C10H2M2 --> 1RMETNOL + 0.5 1C10H2 + 1RPHEXOX | k=1e13, E=196742 kJ/kmol |

*H- abstraction reactions*

|                                                  |                          |
|--------------------------------------------------|--------------------------|
| • 0.5 1C10H2 + 1RPHEXOL --> PHENOL + .5 1PC10CHR | k=1e8, E= 54418 kJ/kmol  |
| • 1RGUAI + 1KETM2 --> 1MGUAIAC + 1RKETM2         | k=1e12, E= 54418 kJ/kmol |
| • 1RGUAI + 1RH --> 1MGUAIAC                      | k=1e12, E= 60000 kJ/kmol |

*Substitutive addition reactions*

|                                                                                               |                          |
|-----------------------------------------------------------------------------------------------|--------------------------|
| • 1ADIOM2 + 1RPHOXM2 --> 1C10H2M4 + .5 H2 + 2 1PH2 + 2 1PCOH + 1RC3H7O2                       | k=1e9, E=121394 kJ/kmol  |
| • 1KETM2 + 1RPHOXM2 --> 1C10H2M4 + .5 H2 + 2 1PH2 + 2 1PCOH + 1RPRPACD                        | k=1e9, E= 121394 kJ/kmol |
| • 1KETDM2 + 1RPHOXM2 --> 1C10H2M4 + .5 H2 + 2 1PH2 + 2 1PCOH + 1RC3H3O                        | k=1e9, E= 121394 kJ/kmol |
| • SINPYALC + 1RPHOXM2 --> 1C10H2M4 + H2 + 3 1PH2 + 2 1PCOH + 1RC3H3O                          | k=1e9, E= 121394 kJ/kmol |
| • 1ADIOM2 + 1RPHEXOX --> .5 1C10H2M4 + .5 1C10H2 + 1.5 H2 + 2 1PH2 + 1PCOS + 1PCOH + 1RC3H7O2 | k=1e9, E= 121394 kJ/kmol |
| • 1KETM2 + 1RPHEXOX --> .5 1C10H2M4 + .5 1C10H2 + .5 H2 + 4 1PH2 + 2 1PCOS + 1RPRPACD         | k=1e9, E= 121394 /kmol   |
| • 1KETDM2 + 1RPHEXOX --> .5 1C10H2M4 + .5 1C10H2 + .5 H2 + 2 1PH2 + 1PCOS + 1PCOH + 1RC3H3O   | k=1e9, E= 121394 kJ/kmol |
| • SINPYALC + 1RPHOXM2 --> 1C10H2M4 + H2 + 3 1PH2 + 2 1PCOH + 1RC3H3O                          | k=1e9, E= 121394 kJ/kmol |
| • 1ADIO + 1RPHEXOX --> 1C10H2 + 1.5 H2 + 4 1PH2 + 2 1PCOS + 1RC3H7O2                          | k=1e9, E= 121394 kJ/kmol |
| • 1KET + 1RPHEXOX --> 1C10H2 + 1.5 H2 + 4 1PH2 + 2 1PCOS + 1RPRPACD                           | k=1e9, E= 121394 kJ/kmol |
| • 1KETD + 1RPHEXOX --> 1C10H2 + 1.5 H2 + 4 1PH2 + 2 1PCOS + 1RC3H3O                           | k=1e9, E= 121394 kJ/kmol |
| • CMRYLALC + 1RPHEXOX --> 1C10H2 + 2.5 H2 + 4 1PH2 + 2 1PCOS + 1RC3H3O                        | k=1e9, E= 121394 kJ/kmol |
| • 1ADIO + 1RPHOXM2 --> .5 1C10H2M4 + .5 1C10H2 + 1.5 H2 + 2PH2 + 1PCOS + 1PCOH + 1RC3H7O2     | k=1e9, E= 108836 kJ/kmol |
| • 1KET + 1RPHOXM2 --> .5 1C10H2M4 + .5 1C10H2 + 1.5 H2 + 2PH2 + 1PCOS + 1PCOH + 1RPRPACD      | k=1e9, E= 108836 kJ/kmol |
| • 1KETD + 1RPHOXM2 --> .5 1C10H2M4 + .5 1C10H2 + 1.5 H2 + 2PH2 + 1PCOS + 1PCOH + 1RC3H3O      | k=1e9, E= 108836 kJ/kmol |
| • CMRYLALC + 1RPHOXM2 --> .5 1C10H2M4 + .5 1C10H2 + 1.5 H2 + 4 1PH2 + 1PCOS + 1PCOH + 1RC3H3O | k=1e9, E= 115115 kJ/kmol |
| • 1RPHOXM2 + .5 1C10H2M4 --> 1C10H2M2 + 1PCHO + 1.5 H2 + 1RMETNOL + 1PCOH                     | k=1e9, E= 115115 kJ/kmol |

- 0.5 1C10H2M2 + 1RPHOXM2 --> .5 1C10H2 + .5 H2 + 1RMETNOL + .5 1C10H2M4 + 1PCOH  
k=1e9, E= 115115 kJ/kmol
- 0.5 1C10H2M2 + 1RPHEXOX --> 1C10H2 + 1.5 H2 + 1RMETNOL + 1PCOS  
k=1e9, E= 117208 kJ/kmol
- 0.5 1C10H2M4 + 1RPHEXOX --> .5 1C10H2 + 1.5 H2 + 1RMETNOL + 1PCOS + .5 1C10H2M2  
k=1e9, E= 117208 kJ/kmol

### Recomposition reactions

- 1RMETNOL + 1RPHEXOX --> CO2 + .5 1C10H2 + 1.5 H2 + 1RCH3  
k=1e8, E= 54418 kJ/kmol
- 1RMETNOL + 1RPHOXM2 --> 1RCH3 + CO2 + .5 1C10H2M4 + .5 H2  
k=1e8, E= 54418 kJ/kmol
- 1RPHEXOX --> 1PCOH + .5 1C10H2 + 3 1PH2  
k=1e8, E= 48139 kJ/kmol
- 1RPHOXM2 --> 1PCOH + .5 1C10H2M4 + 1PH2  
k=1e8, E= 48139 kJ/kmol
- 1RMETNOL + 1RCH3 --> ETHANOL  
k=1e8, E= 12558 kJ/kmol
- 1RMETNOL --> ACETALDY + WATER  
k=1e8, E= 12558 kJ/kmol
- 1RMETNOL + 1PRADIOM + 1PH2 --> 1PCH2OH + 1PADIOM2  
k=1e8, E= 52325 kJ/kmol
- 1RMETNOL + 1PRKETM2 + 1PH2 --> 1PCH2OH + 1PKETM2  
k=1e8, E= 52325 kJ/kmol
- 1RADIOM2 --> 2 1PCH2OH + 2 1PCH2 + 2 1PCHOHP + 2 1PH2 + 1C10H2M4 + 2 1PCOH  
k=3.16e7, E=83720 kJ/kmol
- 2 1RLIGM2A --> .2 1PC10CHR + 2 1PCH2OH + 6 1PH2 + 2 1C10H2M4 + 4 1PCOH + 2 1PCHOHP  
k=3.16e7, E=83720 kJ/kmol
- 2 1RLIGM2A --> 2 1PCHO + 2 WATER + 6 1PH2 + 2 1C10H2M4 + 4 1PCOH + 2 1PC2H2  
k=3.16e7, E=83720 kJ/kmol
- 2 1RGUAI --> 4 1PH2 + 1C10H2M4 + 2 1PCOH  
k=3.16e7, E=83720 kJ/kmol
- 2 1RKETM2 --> 2 1PCH2OH + 2 1PH2 + 1C10H2M4 + 4 1PCOH + 2 1PCH2  
k=3.16e7, E=83720 kJ/kmol
- 2 1PRFETM2 --> 2 1PCHO + 2 1PH2 + 1C10H2M4 + 3 1PCOH + 2 1PCH2 + 1PCHOHP  
k=3.16e7, E=83720 kJ/kmol
- 2 1RC3H7O2 --> 2 WATER + 2 1PC2H2 + 2 1PCHOHP + 2 1PH2  
k=1e8, E= 12558 kJ/kmol
- 2 1RPRACD --> 2 WATER + 2 1PC2H2 + 2 1PCOH + 2 1PH2  
k=1e8, E= 12558 kJ/kmol
- 2 1RC3H3O --> 2 1PCOH + 2 1PC2H2 + 2 1PH2  
k=1e8, E= 12558 kJ/kmol
- 1ROH + 1RCH3 --> METHANOL  
k=1e8, E= 12558 kJ/kmol
- 2 1RCH3 --> ETHANE  
k=1e8, E= 12558 kJ/kmol
- 2 1PRADIO --> 1PCOS + 1PCOH + 1C10H2 + H2 + 2 1PCH2 + 2 1PCH2OH + 2 1PCHOHP + 2 1PH2  
k=6.2e7, E= 92092 kJ/kmol
- 1PRADIOM + 1RH --> 1PADIOM2  
k=1e8, E= 48139 kJ/kmol
- 1RGUAI + 1RH --> 1MGUAIAC  
k=1e8, E= 48139 kJ/kmol
- 1PRKETM2 + 1RH --> 1RKETM2  
k=1e8, E= 48139 kJ/kmol
- 2 1RADIO --> 1PCOS + 2 1PCHOHP + 2 1PCH2 + 1C10H2 + 4 1PH2 + H2 + 1PCOH + 2 1PCH2OH  
k=3.16e7, E=92092kJ/kmol
- 1RPHEXOX + 1RLIG-A --> 3 1PCOS + 1PCHOHP + WATER + 1PC2H2 + 1.5 1C10H2 + 6 1PH2 + 1.5 H2  
k=3.16e7, E=83720 kJ/kmol
- 1LIG + 1RLIG-A --> 4 1PCOS + .2 1PC10CHR + 2 1PCH2OH + 2 1PCHOHP + 2 1C10H2 + 10 1PH2 + 2.5 H2  
k=3.16e7, E=83720 kJ/kmol
- 2 1PRLIG-A --> 2 1PCHOHP + 2 WATER + 2 1PC2H2 + 2 1C10H2 + 4 1PCOS + 6 1PH2 + 2 H2  
k=1e8, E= 54418 kJ/kmol
- 2 1PRFET3 --> 2 1PCOH + 2 1PCH2 + 2 1PCH2OH + 2 1PCOS + 1C10H2 + H2 + 2 1PH2  
k=3.16e7, E=83720 kJ/kmol
- 2 1RKET --> 3 1PCOH + 2 1PCH2 + 2 1PCH2OH + 1PCOS + 1C10H2 + H2 + 4 1PH2  
k=3.16e7, E=83720 kJ/kmol
- 2 1PRLIGH --> 2 1PCHOHP + 3 WATER + 3 1PC2H2 + 5 1PCOH + 2 1C10H2M4 + H2 + 2 1RCH3 + 1PCH2  
k=3.16e7, E=83720 kJ/kmol
- 1RPHEXOX + 1RPHEXOL --> 2 1PCOS + 1C10H2 + 1.5 H2 + 4 1PH2  
k=5e7, E= 83720 kJ/kmol
- 1RPHEXOX + 1RC3H3O --> 1PCOS + .5 1C10H2 + H2 + 2 1PH2 + 1PC2H2 + 1PCOH  
k=1e8, E= 48139 kJ/kmol
- 1RPHEXOX --> 1PCOS + .5 1C10H2 + 1.5 H2  
k=3e7, E= 104650 kJ/kmol
- 1RPHOXM2 --> 1PCOS + .5 1C10H2M4 + .5 H2  
k=3e7, E= 104650 kJ/kmol

### Primary char devolatilization reactions

- 1PCOS --> CO  
k=2e8, E= 199300 kJ/kmol
- 1PCOH --> CO  
k=2e8, E= 138138 kJ/kmol
- 1PH2 --> H2  
k=2e8, E= 209300 kJ/kmol
- 1PC2H2 --> H2 + .2 1PC10CHR  
k=5e8, E= 205114 kJ/kmol

- $1\text{PCH}_2\text{OH} \rightarrow 1\text{ROH} + 1\text{PCH}_2$   $k=2e8, E=0 \text{ kJ/kmol}$
- $1\text{PCHOHP} \rightarrow 1\text{ROH} + .5 \text{ } 1\text{PC}_2\text{H}_2$   $k=2e8, E=0 \text{ kJ/kmol}$
- $1\text{PCHO} \rightarrow 1\text{ROH} + .1 \text{ } 1\text{PC}_{10}\text{CHR}$   $k=2e8, E=0 \text{ kJ/kmol}$
- $1\text{PCH}_2 \rightarrow \text{H}_2 + .1 \text{ } 1\text{PC}_{10}\text{CHR}$   $k=2.5e9, E=209300 \text{ kJ/kmol}$
- $1\text{PCH}_2\text{OH} \rightarrow .5 \text{ CH}_4 + .5 \text{ CO}_2 + .5 \text{ H}_2$   $k=3e8, E=0 \text{ kJ/kmol}$
- $1\text{PCHOHP} \rightarrow .5 \text{ CH}_4 + .5 \text{ CO}_2$   $k=3e8, E=0 \text{ kJ/kmol}$
- $1\text{PCHO} \rightarrow .25 \text{ CO}_2 + .25 \text{ CH}_4 + .5 \text{ CO}$   $k=3e8, E=0 \text{ kJ/kmol}$

#### Reactions with estimated kinetics, with stoichiometry from literature

For the following equations, the reaction stoichiometry was taken from various sources in the literature, while the kinetic factors were derived from an independent bibliography or were adjusted manually to reproduce the published reaction behavior (such as temperature of the start of decomposition, percentage decomposed after the given time). As every reaction was based on individual sources, the corresponding references are given with each one.

- $\text{FURAN} \rightarrow \text{WATER} + .125 \text{ CH}_4 + .125 \text{ ETHENE} + .08333333 \text{ BENZENE} + .0625 \text{ NAPHTLEN} + .25 \text{ } 1\text{PC}_{10}\text{CHR}$ ; Assumptions:  $\text{CH}_4$ , ethane, benzene and naphthalene in equal mole C conversion fractions, each pathway independent, producing char.  $k=7.5e8, E=142000 \text{ kJ} \cdot \text{kmol}^{-1}$
- $\text{PROPDIAL} \rightarrow 2 \text{ WATER} + .3 \text{ } 1\text{PC}_{10}\text{CHR}$  -  $k=2e6, E=175000 \text{ kJ/kmol}$   $k=7.5e8, E=142000 \text{ kJ/kmol}$
- $\text{LEVOGLUC} \rightarrow .27 \text{ } 1\text{PC}_{10}\text{CHR} + 2.7 \text{ WATER} + .7 \text{ ACETALDY} + .7 \text{ CO} + .3 \text{ ACETONE} + .3 \text{ CO}_2$   $k=250000, E=95000 \text{ kJ/kmol}$
- $1\text{KETM}_2 \rightarrow 1\text{RMGUA} + 1 \text{ RC}_3\text{H}_3\text{O}$   $k=1.5e4, E=90000 \text{ kJ/kmol}$
- $\text{XYLOSE} \rightarrow \text{FORMICAC} + \text{WATER} + 2 \text{ C} + \text{CO}_2 + \text{CH}_4 + \text{H}_2$   $k=1e4, E=90000 \text{ kJ/kmol}$
- $1\text{KETDM}_2 \rightarrow 1\text{MGUA} + \text{WATER} + .3 \text{ } 1\text{PC}_{10}\text{CHR}$   $k=1.2e4, E=95000 \text{ kJ/kmol}$
- $\text{SINPYALC} \rightarrow 1\text{MGUA} + \text{METHANOL} + .2 \text{ } 1\text{PC}_{10}\text{CHR}$   $k=1e4, E=95000 \text{ kJ/kmol}$
- $\text{CMRYLALC} \rightarrow \text{PHENOL} + \text{METHANOL} + .2 \text{ } 1\text{PC}_{10}\text{CHR}$   $k=1e4, E=95000 \text{ kJ/kmol}$
- $\text{FURFURAL} \rightarrow .5 \text{ CH}_4 + .4 \text{ } 1\text{PC}_{10}\text{CHR} + .5 \text{ CO}_2 + \text{WATER}$   $k=9.5e4, E=105000 \text{ kJ} \cdot \text{kmol}^{-1}$
- $\text{ACETICAC} \rightarrow \text{CO}_2 + \text{CH}_4$   $k=5.75e5, E=43500 \text{ kcal/kmol}$
- $\text{ACETICAC} \rightarrow \text{KETEN-01} + \text{WATER}$   $k: 5.25e12, E=70.51 \text{ kcal/kmol}$
- $\text{PROPDIAL} \rightarrow \text{ACETALDY} + \text{CO}$ ; Assumptions: decarboxylation by CO production.  $k=8e8$  and  $E=130000 \text{ kJ/kmol}$
- $\text{FORMALDY} \rightarrow \text{H}_2 + \text{CO}$   $k=2.8e6, E=33500 \text{ kcal/kmol}$
- $\text{METHANOL} \rightarrow \text{CO} + 2 \text{ H}_2$   $k=8000, E=195000 \text{ kJ/kmol}$
- $\text{FURFURAL} \rightarrow \text{FURAN} + \text{CO}$   $k=2.5e8, E=155000 \text{ kJ/kmol}$
- $\text{XYLOSE} \rightarrow \text{FURFURAL} + 3\text{WATER}$ ; fast route assumed.  $k=1.3e7, E=149000 \text{ kJ/kmol}$
- $\text{XYLOSE} \rightarrow \text{CO}_2 + \text{ACETONE} + \text{FORMALDY} + 3 \text{ WATER} + .75 \text{ GLYCOALD} + .175 \text{ } 1\text{PC}_{10}\text{CHR} + .25 \text{ ACETALDY} + .25 \text{ CO} + 1\text{PCHOHP}$ ; slow route assumed.  $k=2.6e5, E=102500 \text{ kJ/kmol}$
- $\text{LEVOGLUC} \rightarrow .8 \text{ GLYCOALD} + .7 \text{ ACETOL} + .45 \text{ CO}_2 + .3 \text{ CO} + .055 \text{ } 1\text{PC}_{10}\text{CHR} + .3 \text{ ETYLDIOL} + .2 \text{ ACETALDY}$ .  $k=5e9, E=165000 \text{ kJ/kmol}$
- $\text{KETEN-01} \rightarrow \text{CO} + .085 \text{ ETHENE} + .0415 \text{ } 1\text{PC}_{10}\text{CHR} + .415 \text{ CH}_4$ ; Assumptions: basis: CO 65%, ethene 5%, CH<sub>4</sub> 30%, H<sub>2</sub> 3% + carbon-like mass.  $k=9.5e9, E=55500 \text{ kcal/kmol}$
- $\text{PROPNCAC} \rightarrow .55 \text{ CO}_2 + .4 \text{ ETHANE} + .6 \text{ WATER} + .3 \text{ PROPENE} + .45 \text{ CO} + .15 \text{ CH}_4 + .15 \text{ ETHENE}$ ; Assumptions: integrated the given reaction mechanisms into one single reaction, as intermediate product is no compound of the simulation.  $k=1e8, E=49000 \text{ kcal/kmol}$
- $\text{ACETONE} \rightarrow \text{KETENE} + \text{CH}_4$ ; Assumptions: at 580°C, 15% mol conversion after 2,5min residence time.  $k=2e7, E=145000 \text{ kJ/kmol}$
- $\text{ACETALDY} \rightarrow .8 \text{ CO} + .7 \text{ CH}_4 + .1 \text{ H}_2 + .1 \text{ ETHENE} + .1 \text{ ETHANE} + .1 \text{ CO}_2$   $k=50000, E=98000 \text{ kJ/kmol}$
- $1\text{PRADIO} + 1\text{RCH}_3 \rightarrow \text{CMRYLALC} + 1\text{PCH}_2\text{OH}$   $k=1e8, E=48139 \text{ kJ/kmol}$
- $1\text{PRKETM}_2 + 1 \text{ PRKETM}_2 \rightarrow 2 \text{ } 1\text{PCH}_2\text{OH} + 1\text{C}_{10}\text{H}_2\text{M}_4 + 4 \text{ PCOH} + 2 \text{ } 1\text{PCH}_2$   $k=3.16e7, E=83720 \text{ kJ/kmol}$

#### Reactions for nitrogen containing compounds

- $\text{GLUTACID} \rightarrow \text{AMMONIA} + \text{CO}_2 + \text{ACETICAC} + \text{PROPNCAC} + \text{WATER} + .3 \text{ } 1\text{PC}_{10}\text{CHR} + \text{CHAR-N} + 1\text{PCHO}$  acc. to  $k=1e6, E=90000 \text{ kJ/kmol}$
- $\text{GLUTACID} \rightarrow \text{PYRROLID} + \text{CO}_2 + \text{WATER}$   $k=9e8, E=117000 \text{ kJ/kmol}$

- PYRROLE --> .15 NAPHTLEN + .5 HCN + .15 ETHENE + .0975 1PC10CHR + .2 PROPENE + .05 ETHANE + .025 CH<sub>4</sub> + .4 CHAR-N + .1 AMMONIA , Assumptions: reaction mechanism by regression based on given product components, Naphthalene representing PCHs, ethane / propene representing propyne); Assumptions: propyne and HCN as main products; k=2,25e13, E=49500 kcal/kmol
- PYRROLID --> HCN + .5 ACETONE + .3 CO + .2 ETHANE + .2 ETHENE + .075 H<sub>2</sub> + .2 WATER + .075 CH<sub>4</sub> + .025 1PC10CHR + .025 PROPENE , with acetone introduced as intermediate product (acetone instead of propanal). k= 1e6, E= 120000 kJ/kmol
- GLUTACID --> PYRROLE + CO<sub>2</sub> + 2 WATER k= 4,5e8, E= 117000 kJ/kmol
- PYRROLE --> HCN + .66666666 PROPENE + .1 1PC10CHR ; Assumptions: HCN and propene + C (instead of propyne) as primary decomposition products. k=9e13, E=62.500kcal/kmol

**Table S2** Detail of equipment costs in each section from Aspen Process Evaluation Analysis

| Section              | Equipment                 | Equipment cost (USD) |
|----------------------|---------------------------|----------------------|
| Pretreatment         | Compressor (BLOWER)       | 540,500              |
|                      | Heat Exchanger (HX-AIR)   | 10,900               |
|                      | Dryer (DRYER)             | 83,600               |
|                      | Crusher (MILLING)         | 67,200               |
|                      | Screenner (SCREEN)        | 18,300               |
| Pyrolysis            | Pyrolysis reactor (PYR)   | 451,700              |
| Separation           | Cyclone (GS-SEP1)         | 28,300               |
|                      | Heat Exchanger (QUENCH)   | 10,700               |
|                      | Flash Vessel (QUENCH2)    | 19,100               |
|                      | Pump (PUMPLIQ)            | 19,900               |
|                      | Compressor (GAS-COM1)     | 560,100              |
| Combustion           | Heat Exchanger (HX-GAS)   | 12,000               |
|                      | Compressor (GAS-COM2)     | 671,900              |
|                      | Combustion chamber (COMB) | 63,500               |
|                      | Cyclone (GS-SEP2)         | 503,200              |
|                      | Heat Exchanger (HX-COMB3) | 21,100               |
| Hydrotreating        | Turbine (TURBINE)         | 99,700               |
|                      | Pump (PUMPBO)             | 66,600               |
|                      | Compressor (H2-COMP1)     | 1,900,100            |
|                      | Heat Exchanger (HX1-COLD) | 122,700              |
| Distillation         | Reactor (HDT)             | 127,610              |
|                      | Heat Exchanger (HX1-HOT)  | 12,000               |
|                      | Heat Exchanger (HX2-HOT)  | 10,900               |
|                      | Flash (FLSH-HDT)          | 23,000               |
|                      | Flash (PSACOL)            | 29,500               |
|                      | Decanter (DECANTER)       | 83,600               |
|                      | Heat Exchanger (HX2-COLD) | 11,000               |
|                      | Distillation (GASOLCOL)   | 226,245              |
|                      | Distillation (DIESLCOL)   | 315,797              |
|                      | Pump (BOTPUMP)            | 83,600               |
| Hydrocracking        | Heat Exchanger (COOL-HCK) | 19,500               |
|                      | Flash (FLSH-HCK)          | 19,200               |
|                      | Compressor (H2-COMP2)     | 1,502,400            |
|                      | Heat Exchanger (HX3-COLD) | 25,800               |
|                      | Reactor (HCK)             | 61,200               |
|                      | Heat Exchanger (HX3-HOT)  | 11,300               |
|                      | Diesel generator          | 22,000               |
| Total equipment cost |                           | 7,855,752            |