Table A1. Description of subscripts, decision variables and parameters.

|  |  |  |
| --- | --- | --- |
| **Subscripts** |  |  |
|  | 1,2, …, | Biomass candidate harvest locations |
|  | 1,2, …, | Candidate distributed preprocessing facility locations |
|  | 1,2, …, | Candidate integrated facility locations |
|  | 1,2, …, | Natural gas candidate supplier locations |
|  | 1,2, …, | Allowed facility capacity levels |
|  | 1,2, …, | Project years |
|  | 1,2, …, | Co-products species |
|  | 1,2, …, | Chemicals species |
| **Decision Variables** |  |  |
|  | binary | Equal to one if a distributed preprocessing facility of capacity level exists in candidate facility location *j* |
|  | binary | Equal to one if an integrated facility of capacity level exists in candidate facility location *k* |
|  | metric ton/year | Amount of roadside chipped biomass transported from harvest location *i* to integrated preprocessing facility location *k* |
|  | metric ton/year | Amount of roadside chipped biomass transported from harvest location *i* to distributed preprocessing facility location *j* |
|  | metric ton/year | Amount of raw biomass transported from harvest location *i* to integrated preprocessing facility location *k* |
|  | metric ton/year | Amount of raw biomass transported from harvest location *i* to distributed preprocessing facility location *j* |
|  | metric ton/year | Amount of preprocessed biomass transported from distributed preprocessing facility location *j* to integrated biorefinery facility location *k* |
|  | metric ton/year | Amount of natural gas transported from natural gas supplier location *g* to integrated biorefinery facility location *k* |
|  | metric ton/year | Amount of chemical *m* transported from integrated biorefinery facility location *k* to fixed distribution center |
|  | metric ton/year | Amount of co-product *v*  in integrated biorefinery facility location *k* |
|  | metric ton/year | Total amount of transported biomass from harvest location *i* to other locations |
|  | metric ton/year | Total amount of transported biomass from harvest locations to the preprocessing facility location *j* |
|  | metric ton/year | Total amount of preprocessed biomass from the distributed preprocessing facility location *j* |
|  | metric ton/year | Total amount of raw biomass transported to integrated preprocessing facility location *k* |
|  | metric ton/year | Total amount of preprocessed biomass from the integrated preprocessing facility location *k* |
|  | metric ton/year | Total amount of preprocessed biomass for integrated biorefinery facility location *k* |
| **Parameter** |  |  |
|  | metric ton/year | Biomass availability in harvest location *i* |
|  | metric ton/year | Total collected biomass in harvest location *i* |
|  | metric ton/year | Capacity level *l* for the distributed preprocessing facility |
|  | metric ton/year | Capacity level *l* for the integrated facility |
|  | metric ton/year | Natural gas availability in supply location *n* |
|  | metric ton/year | The maximum products demand |
|  | $/metric ton | Unit collection cost for raw biomass in location *i* |
|  | $/metric ton | Unit collection cost for roadside chipped biomass in location *i* |
|  | $/(metric ton mile) | Unit transportation cost for raw biomass |
|  | $/(metric ton mile) | Unit transportation cost for roadside chipped biomass |
|  | $/(metric ton mile) | Unit transportation cost for preprocessed biomass |
|  | $/(metric ton mile) | Unit transportation cost for natural gas |
|  | $/(metric ton mile) | Unit transportation cost for chemicals |
|  | $/metric ton | Fixed transportation cost for unit biomass |
|  | mile | Distance from harvest location *i* to distributed preprocessing location *j* |
|  | mile | Distance from harvest location *i* to the integrated facility location *k* |
|  | mile | Distance from distributed preprocessed location *j* to the integrated facility location *k* |
|  | mile | Distance from natural gas supplier location *n* to the integrated facility location *k* |
|  | mile | Distance from integrated facility location *k* to the distribution center location |
|  | $/year | Fixed operating cost for distributed preprocessing facility at capacity level *l* |
|  | $/year | Fixed operating cost for the integrated facility at capacity level *l* |
|  | $ | Capital cost for distributed preprocessing facility at capacity level *l* |
|  | $ | Capital cost for integrated facility at capacity level *l* |
|  | $/metric ton | Variable operating cost for raw biomass preprocessing |
|  | $/metric ton | Variable operating cost for roadside chipped biomass preprocessing |
|  | $/metric ton | Variable operating cost for biorefinery facility |
|  | $/metric ton | Price of co-product *v* in year *t* |
|  | $/metric ton | Price of chemical *m* year *t* |
|  | kg CO2eq/metric ton | Emissions of unit raw biomass collection |
|  | kg CO2eq/metric ton | Emissions of unit roadside chipped biomass collection |
|  | kg CO2eq/(metric ton mile) | Emissions of unit raw biomass transportation |
|  | kg CO2eq/(metric ton mile) | Emissions of unit roadside chipped biomass transportation |
|  | kg CO2eq/(metric ton mile) | Emissions of unit preprocessed biomass transportation |
|  | kg CO2eq/(metric ton mile) | Emissions of unit natural gas transportation |
|  | kg CO2eq/(metric ton mile) | Emissions of unit chemicals transportation |
|  | kg CO2eq/metric ton | Emissions of converting unit raw biomass in preprocessing facility |
|  | kg CO2eq/metric ton | Emissions of converting unit roadside chipped biomass in preprocessing facility |
|  | kg CO2eq/metric ton | Emissions of converting unit biomass in integrated biorefinery facility |
|  |  | Discounted factor of year *t* |
|  |  | Interest rate |
|  |  | Biomass collection factor |
|  |  | Biomass loss factor |
|  |  | Preprocessed biomass conversion rate in preprocessing facility |
|  |  | Conversion rate of chemical *m* |
|  |  | Conversion rate of co-products *v* |
|  |  | Maximum number of the distributed preprocessing facilities |
|  |  | Maximum number of the integrated facilities |
|  |  | Natural gas demand rate based on preprocessed biomass |

Table A2. Total capital costs and fixed operating costs for various levels of facilities.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Level** | | **Capacity**  **(dry metric ton/day)** | | | **Total Capital Cost**  **($million)** | | | |
|  | | |  | Distributed Preprocessing Facility | | | | Integrated Facility |
| L1 | | | 100 | 6.6 | | 37.3 | | |
| L2 | | | 200 | 10 | | 56.5 | | |
| L3 | | | 500 | 17.3 | | 97.9 | | |
| L4 | | | 1000 | 26.2 | | 148.3 | | |
| L5 | | | 2000 | 39.7 | | 224.9 | | |
| **Level** | **Capacity**  **(dry metric ton/day)** | | | **Fixed Operating Cost**  **($million)** | | | | |
|  |  | | | Distributed Preprocessing Facility | | | | Integrated Facility |
| L1 | 100 | | | 2 | | | 3.2 | |
| L2 | 200 | | | 2.2 | | | 3.9 | |
| L3 | 500 | | | 2.5 | | | 5.3 | |
| L4 | 1000 | | | 2.8 | | | 7.1 | |
| L5 | 2000 | | | 3.3 | | | 9.8 | |

Table A3. Variable unit operating cost and emissions.

|  |  |
| --- | --- |
| **Preprocessing Facility** | **$/metric ton** |
| Electricity for chopping | 0.83 |
| Electricity for grinding | 2.025 |
| Electricity for compressor | 6.425 |
| **Total** | **9.28** |
|  |  |
| **Integrated Biorefinery Facility** | **$/metric ton** |
| Solid disposal | 0.1 |
| Natural gas | 5.58 |
| Process water | 0.18 |
| Electricity | 15.96 |
| Catalyst | 7.17 |
| **Total** | **28.99** |
|  |  |
| **Emissions** | **kg CO2eq/(metric ton mile)** |
| Raw biomass collection  **(kg CO2eq/metric ton)** | 4.76 |
| Road chipped biomass collection  **(kg CO2eq/metric ton)** | 14.2 |
| Raw biomass transportation | 0.55 |
| Road chipped biomass transportation | 0.26 |
| Preprocessed biomass transportation | 0.13 |
| Natural gas transportation | 0.23 |
| Chemicals transportation | 0.26 |
| Raw biomass preprocessing  **(kg CO2eq/metric ton)** | 149.77 |
| Roadside chipped biomass preprocessing  **(kg CO2eq/metric ton)** | 133.4 |
| Biorefinery facility production  **(kg CO2eq/metric ton)** | 215.35 |

Table A4. Chemical yields and calculated prices for the next 20 years

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Yield** | **Chemicals Price ( $/metric ton)** | | | | | | | | | |
| **% of preprocessed biomass** | | **y1** | **y2** | **y3** | **y4** | **y5** | **y6** | **y7** | **y8** | **y9** | **y10** |
| Benzene | 0.859 | 1280 | 1322 | 1355 | 1330 | 1350 | 1361 | 1370 | 1378 | 1387 | 1398 |
| Toluene | 1.587 | 1068 | 1102 | 1128 | 1109 | 1124 | 1133 | 1140 | 1147 | 1154 | 1162 |
| Xylenes | 0.616 | 1105 | 1139 | 1164 | 1145 | 1161 | 1169 | 1176 | 1183 | 1189 | 1198 |
| Ethylene | 2.582 | 1297 | 1336 | 1367 | 1344 | 1363 | 1373 | 1381 | 1389 | 1397 | 1407 |
| Propylene | 4.342 | 1514 | 1570 | 1613 | 1581 | 1607 | 1621 | 1633 | 1644 | 1656 | 1670 |
| Butylene | 1.146 | 750 | 750 | 750 | 750 | 750 | 750 | 750 | 750 | 750 | 750 |
| Ethylbenzene | 0.075 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| Styrene | 0.046 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 |
| Indene | 0.016 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 |
| Naphthalene | 0.016 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 |
|  | | **y11** | **y12** | **y13** | **y14** | **y15** | **y16** | **y17** | **y18** | **y19** | **y20** |
| Benzene | 0.859 | 1409 | 1420 | 1431 | 1442 | 1453 | 1463 | 1473 | 1484 | 1498 | 1509 |
| Toluene | 1.587 | 1172 | 1181 | 1189 | 1198 | 1207 | 1215 | 1223 | 1232 | 1242 | 1252 |
| Xylenes | 0.616 | 1207 | 1215 | 1224 | 1232 | 1241 | 1248 | 1256 | 1265 | 1275 | 1284 |
| Ethylene | 2.582 | 1418 | 1429 | 1439 | 1450 | 1460 | 1469 | 1479 | 1489 | 1502 | 1513 |
| Propylene | 4.342 | 1686 | 1701 | 1716 | 1730 | 1745 | 1758 | 1771 | 1787 | 1805 | 1821 |
| Butylene | 1.146 | 750 | 750 | 750 | 750 | 750 | 750 | 750 | 750 | 750 | 750 |
| Ethylbenzene | 0.075 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| Styrene | 0.046 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 |
| Indene | 0.016 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 |
| Naphthalene | 0.016 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 | 850 |

\*y1-y20 indicates the year 1 to year 20 (2010-2030)

\*Butylene, ethylbenzene, styrene, indene and naphthalene are assumed to have fixed prices.