**Supporting Information**

**Product Design: Incorporating Make-or-Buy Analysis and Supplier Selection**

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Table S3.1: 20 Sets of Experimental Data for LDLD

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Mass fraction (%) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| LAS () | 5.18 | 6.15 | 6.88 | 6.99 | 5.2 | 6.1 | 6.1 | 4 | 5.36 | 7.97 |
| AEO | 1.11 | 0.56 | 0.28 | 0.14 | 1.32 | 0 | 0 | 3.5 | 1.75 | 0.88 |
| AEOS () | 4.44 | 5.38 | 5.67 | 7.12 | 3.68 | 2.45 | 2.03 | 1.58 | 2.16 | 2.66 |
| DEA () | 0.54 | 0.81 | 0.45 | 1.22 | 0.78 | 1.21 | 1.42 | 0.5 | 0.75 | 1.13 |
| TEA () | 0.85 | 0.56 | 0.65 | 0.67 | 0.28 | 0.14 | 0 | 0.5 | 0.25 | 0.46 |
| CDEA | 1.26 | 0.63 | 1.89 | 0.95 | 1.58 | 2.13 | 2.19 | 1.18 | 1.37 | 0.75 |
| NaOH | 0.25 | 0.38 | 0.57 | 0.3 | 0.32 | 0.3 | 0.25 | 0.2 | 0.36 | 0.54 |
| NaCl | 0.5 | 0.72 | 0.58 | 0.25 | 0.56 | 0.28 | 0.28 | 0.5 | 0.75 | 0.88 |
| Formalin | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 |
| Water | 85.67 | 84.58 | 82.83 | 82.16 | 86.08 | 87.19 | 87.53 | 87.84 | 87.05 | 84.53 |
| RMFH (cm) | 10.5 | 11.7 | 12.8 | 13.1 | 10.7 | 11.7 | 11.8 | 9.4 | 10 | 12.7 |
| VISC (cSt) | 94.5 | 260.3 | 740.5 | 38.4 | 300 | 190 | 274.6 | 80.7 | 526.6 | 1191.1 |
| SRC (%) | 99 | 98.5 | 130 | 121.9 | 100.9 | 103.5 | 102.5 | 87.7 | 106.7 | 112.6 |
| CLPT (°C) | 0.5 | 7 | 9.7 | 0.2 | 4.5 | 0.4 | -0.1 | 0.5 | 25.8 | 27.8 |
| pH | 7 | 6.9 | 6.9 | 7.3 | 7 | 6.8 | 6.7 | 6.9 | 6.6 | 7 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Mass fraction (%) | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| LAS () | 8.33 | 5.58 | 5.58 | 6.23 | 6.35 | 6.27 | 6.27 | 6.19 | 6.1 | 5.86 |
| AEO () | 0.44 | 1.29 | 0.77 | 0.22 | 0.11 | 0 | 0 | 0 | 0 | 0 |
| AEOS () | 2.89 | 1.7 | 1.28 | 1.48 | 1.18 | 0.94 | 0.94 | 1.49 | 0.94 | 0.94 |
| DEA () | 0.89 | 0.67 | 0.98 | 1.24 | 0.9 | 0.9 | 1.42 | 1.16 | 1.08 | 0.98 |
| TEA () | 0.13 | 0.38 | 0.29 | 0.29 | 0.3 | 0.3 | 0 | 0.1 | 0 | 0 |
| CDEA () | 0.38 | 1.72 | 2.28 | 1.8 | 2.16 | 2.46 | 2.29 | 2.31 | 2.28 | 2.46 |
| NaOH () | 0.79 | 0.38 | 0.27 | 0.27 | 0.41 | 0.39 | 0.28 | 0.34 | 0.39 | 0.39 |
| NaCl () | 0.56 | 0.38 | 0.29 | 0.41 | 0.3 | 0.3 | 0.24 | 0.26 | 0.24 | 0.24 |
| Formalin | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 |
| Water | 85.39 | 87.7 | 88.06 | 87.86 | 88.09 | 88.24 | 88.36 | 87.95 | 88.77 | 88.93 |
| RMFH (cm) | 12.7 | 10.5 | 9.7 | 11.6 | 11.3 | 11.5 | 11.6 | 11.8 | 11.5 | 10.9 |
| VISC (cSt) | 396.3 | 257.2 | 291 | 446.4 | 350.3 | 448.6 | 311.9 | 304.9 | 215.5 | 282.3 |
| SRC (%) | 110.6 | 102.8 | 108.6 | 102.1 | 100 | 103 | 100 | 102 | 102.2 | 98.9 |
| CLPT (°C) | 17.4 | 1.1 | 0.9 | 0.2 | 0.7 | 1.9 | 0.6 | 0.9 | 0.5 | 1.6 |
| pH | 6.9 | 6.8 | 6.7 | 6.8 | 6.8 | 6.7 | 6.6 | 6.7 | 7 | 6.8 |

Table S3.2. Experimental Data Regression Results

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Spec. |  |  |  |  |  |  |  |  |  | MAPE |
| RMFH (cm) | 4.14 | 0.86 | 0.06 | 0.28 | 0.60 | -0.17 | 0.40 | / | / | 1.91% |
| GSTT (%) | -17.25 | 12.46 | 9.56 | 4.99 | -1.06 | -1.27 | 16.59 | / | / | 2.43% |
| VISC (cSt) | -3168.22 | -330.75 | 178.34 | -15.56 | 1934.38 | 1558.93 | 579.38 | 4301.57 | 1362.40 | 9.85% |
| CLPT (°C) | -55.43 | 41.73 | 4.72 | 0.57 | -99.27 | -83.03 | 1.48 | -251.773 | 36.54 | 0.73% |
| pH | 6.56 | -4.42 | / | / | 12.46 | 9.38 | 0.70 | 31.17 | / | 1.07% |

Table S3.3. Supplier Information for LAB, Oleum, AEO, AEOS, DEA, TEA, CDEA, NaCl, NaOH, and Formalin (MPC: maximum production capacity; MOQ: minimum order quantity)

|  |  |  |  |
| --- | --- | --- | --- |
| LAB | | | |
| Supplier | 1 | 2 | 3 |
| Purity | 99% | 98% | 99% |
| Plant location | (-400, 200) | (-340, 170) | (400, -370) |
| MPC (ton/m) | 1200 | 1800 | 1500 |
| MOQ (ton) | 10 | 15 | 15 |
| Price ($/ton) | < 40 t, 3375  ≥ 40 t, 3100 | < 60 t, 3250  ≥ 60 t, 3075 | < 45 t, 3400  ≥ 45 t, 3150 |
| Oleum | | | |
| Supplier | 1 | 2 | 3 |
| Purity | 99% | 98% | 98% |
| Plant location | (-340, 270) | (-1040, 170) | (-200, -170) |
| MPC (ton/m) | 2000 | 3000 | 3500 |
| MOQ (ton) | 10 | 15 | 10 |
| Price ($/ton) | < 20 t, 375  ≥ 20 t, 325 | < 25 t, 425  ≥ 25 t, 375 | < 20 t, 375  ≥ 20 t, 350 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| AEO | | | | |
| Supplier | 1 | 2 | 3 | 4 |
| Purity | 98% | 98% | 99% | 98% |
| Plant location | (-115, 972) | (337, 447) | (-172, 229) | (377, 447) |
| MPC (ton/m) | 800 | 800 | 100 | 1200 |
| MOQ (ton) | 5 | 1 | 1 | 0.5 |
| Price ($/ton) | < 80 t, 4500  ≥ 80 t, 3750 | < 60 t, 4250  ≥ 60 t, 4000 | < 30 t, 5000  ≥ 30 t, 4500 | < 100 t, 4000  ≥ 100 t, 3600 |

|  |  |  |
| --- | --- | --- |
| AEOS | | |
| Supplier | 1 | 2 |
| Purity | 98% | 99% |
| Plant location | (-115, 972) | (-200, 694) |
| MPC (ton/m) | 1800 | 1000 |
| MOQ (ton) | 5 | 5 |
| Price ($/ton) | < 100 t, 2900  ≥ 100 t, 2400 | < 100 t, 3100  ≥ 100 t, 2600 |
|  |  |  |

|  |  |  |  |
| --- | --- | --- | --- |
| DEA | | | |
| Supplier | 1 | 2 | 3 |
| Purity | 99% | 98% | 98% |
| Plant location | (-255, -643) | (-100, 294) | (-242, 190) |
| MPC (ton/m) | 3000 | 1000 | 500 |
| MOQ (ton) | 1 | 1 | 1 |
| Price ($/ton) | < 100 t, 4500  ≥ 100 t, 4250 | < 80 t, 4000  ≥ 80 t, 3600 | < 50 t, 4250  ≥ 50 t, 3750 |

|  |  |  |  |
| --- | --- | --- | --- |
| TEA | | | |
| Supplier | 1 | 2 | 3 |
| Purity | 99% | 98% | 98% |
| Plant location | (294, 787) | (-622, 945) | (-672, 929) |
| MPC (ton/m) | 100 | 150 | 300 |
| MOQ (ton) | 1 | 10 | 15 |
| Price ($/ton) | < 20 t, 4500  ≥ 20 t, 4250 | < 30 t, 4000  ≥ 30 t, 3750 | < 60 t, 3750  ≥ 60 t, 3500 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| CDEA | | | | |
| Supplier | 1 | 2 | 3 | 4 |
| Purity | 98% | 98% | 98% | 99% |
| Plant location | (486, 415) | (400, 150) | (-400, 694) | (-75, 1000) |
| MPC (ton/m) | 500 | 300 | 500 | 200 |
| MOQ (ton) | 10 | 1 | 20 | 5 |
| Price ($/ton) | < 60 t, 3750  ≥ 60 t, 3500 | < 100 t, 4000  ≥ 100 t, 3375 | < 50 t, 4100  ≥ 50 t, 3750 | < 20 t, 5200  ≥ 20 t, 4375 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| NaOH | | | | |
| Supplier | 1 | 2 | 3 | 4 |
| Purity | 98% | 98% | 98% | 99% |
| Plant location | (-200, 694) | (558, 316) | (100, 1163) | (181, 1190) |
| MPC (ton/m) | 8000 | 3000 | 6000 | 5000 |
| MOQ (ton) | 25 | 20 | 25 | 20 |
| Price ($/ton) | < 200 t, 950  ≥ 200 t, 850 | < 100 t, 1250  ≥ 100 t, 1150 | < 150 t, 1200  ≥ 150 t, 1050 | < 150 t, 1000  ≥ 150 t, 900 |
|  |  |  |  |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| NaCl | | | | |
| Supplier | 1 | 2 | 3 | 4 |
| Purity | 98% | 98% | 98% | 99% |
| Plant location | (306, 388) | (320, 912) | (454, 827) | (294, 934) |
| MPC (ton/m) | 10000 | 5000 | 12000 | 8000 |
| MOQ (ton) | 5 | 10 | 10 | 10 |
| Price ($/ton) | < 200 t, 200  ≥ 200 t, 160 | < 100 t, 250  ≥ 100 t, 130 | < 200 t, 300  ≥ 200 t, 140 | < 100 t, 200  ≥ 100 t, 125 |

|  |  |  |  |
| --- | --- | --- | --- |
| Formalin | | | |
| Supplier | 1 | 2 | 3 |
| Purity | 98% | 99% | 98% |
| Plant location | (-115, 972) | (35, 229) | (337, 447) |
| MPC (ton/m) | 2000 | 1000 | 3000 |
| MOQ (ton) | 5 | 1 | 5 |
| Price ($/ton) | < 50 t, 1000  ≥ 50 t, 875 | < 20 t, 1350  ≥ 20 t, 1150 | < 80 t, 1000  ≥ 80 t, 750 |

Table S3.4. Input Parameters in CRG Herbicide Example

|  |  |  |
| --- | --- | --- |
| Parameters | Symbol | Value |
| Material Constant | *C* | 6 |
| Binder surface tension |  | 0.035 N/m |
| Binder contact angle |  | 61° |
| Binder dynamic viscosity |  | 0.001-0.03 Pa∙s |
| Importance of layering on the granule growth |  | 0.6 |
| Coefficient of restitution |  | 0.5 |
| Ratio of asperities over liquid layer |  | 5 |
| Yield stress |  | 3000 Pa |
| Critical Stokes’ number for deformation |  | 0.2 |
| Liquid layer thickness before consolidation |  | 100 μm |
| Density of AIs: 24D, MCPA, and metolachlor |  | 1420, 1560, 1120 kg/m3 |
| Density of fillers: starch, lignin, cellulose, and PCL |  | 1500, 1300, 1500, 1145 kg/m3 |
| Density of binder |  | 1200 kg/m3 |
| Mass of AI: 24D, MCPA, and metolachlor for treating 1 hectare land |  | 1.25, 1.5, 1 kg |
| Dissolution rate constant of cellulose and PCL |  | 0.0864, 0.0089 kg/m2/day |
| Diffusion coefficient of starch and lignin |  | 1.728×10-6, 8.64 ×10-10 m2/day |
| Pricing parameter |  | 0.7 |
| Pricing parameter |  | 0.6 |
| Price of the competitors’ products | , | 25, 20 |
| Quality score of competitor’s product | , | 0.8, 0.75 |
| Capital cost of a reference mixer for granule production |  | $250k |
| Production capacity of a reference mixer for granule production |  | 5400 ton/quarter |
| Capital cost of a reference granulator for granule production |  | $5M |
| Production capacity of a reference granulator for granule production |  | 3600 ton/quarter |
| Capital cost of a reference facility for metolachlor production |  | $21M |
| Production capacity of a reference facility for metolachlor production |  | 120 ton/quarter |
| Scaling factor for capital cost |  | 0.6 |
| Operating cost of producing one ton granule |  | $600 |
| Operating cost for producing 1 ton metholachlor |  | $3500 |
| Cost of storing 1 ton ingredient for 1 quarter |  | $90 |
| Safety stock coefficient |  | 0.33 |
| Maximum storage capacity of intermediate ingredient inventory |  | 1000 ton |
| Maximum storage capacity of intermediate ingredient inventory |  | 3000 ton |
| Cost of storing one ton granule for 1 month |  | $7.5 |
| Cost of distributing 1 ton granule to consumer |  | $50 |
| Cost of transporting 1 ton ingredient by 1 km |  | $0.25/ton/km |
| Advertisement cost in one quarter |  | $0.2 M |
| Time for product design and facility construction |  | 1 quarter |
| Time for product life |  | 3 years |
| Tax rate |  | 0.4 |
| Discount rate |  | 0.07 |
| Percentage of annual capital depreciation |  | 33.3% |

Table S3.5. Supplier Information for 24D, MCPA, Metolachlor, MEA, CAC, Starch, Lignin, Cellulose, PCL, and PVP

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 24D | | | | | | |
| Supplier | 1 | | 2 | | 3 | |
| Purity | 97% | | 95% | | 95% | |
| Plant location | (-185, -700) | | (540, 700) | | (540, 700) | |
| MPC (ton/q) | 300 | | 1500 | | 1500 | |
| MOQ (ton) | 2 | | 1 | | 2 | |
| Price ($/ton) | < 30 t, 21000  ≥ 30 t, 19000 | | < 60 t, 19000  ≥ 60 t, 17000 | | < 45 t, 19500  ≥ 45 t, 17500 | |
| MCPA | | | | | | | |
| Supplier | | 1 | | 2 | | 3 | |
| Purity | | 95% | | 98% | | 98% | |
| Plant location | | (-105, 1035) | | (540, 300) | | (540, 300) | |
| MPC (ton/q) | | 900 | | 1500 | | 1500 | |
| MOQ (ton) | | 1 | | 1 | | 1 | |
| Price ($/ton) | | < 15 t, 18000  ≥ 15 t, 18500 | | < 30 t, 20000  ≥ 30 t, 18000 | | < 15 t, 20500  ≥ 15 t, 18500 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metolachlor | | | | |
| Supplier | | 1 | | In-house |
| Purity | 99% | | 99% | |
| Plant location | (540, 300) | | (0, 0) | |
| MPC (ton/quarter) | 300 | | Up to 300 | |
| MOQ (ton) | 1 | | / | |
| Price ($/ton) | < 15 t, 31000  ≥ 15 t, 29000 | | around 20000 | |

|  |  |  |
| --- | --- | --- |
| 2-methyl-6-ethyl-N-1'-methyl-2'-methoxyethylaniline (MEA) | | |
| Supplier | 1 | 2 |
| Purity | 98% | 95% |
| Plant location | (600, 1150) | (-150, 200) |
| MPC (ton/quarter) | 3000 | 1200 |
| MOQ (ton) | 1 | 1 |
| Price ($/ton) | < 45 t, 19100  ≥ 45 t, 18800 | < 30 t, 19000  ≥ 30 t, 18600 |

|  |  |  |
| --- | --- | --- |
| Chloroacetyl chloride (CAC) | | |
| Supplier | 1 | 2 |
| Purity | 98% | 96% |
| Plant location | (540, 300) | (160, 1200) |
| MPC (ton/quarter) | 300 | 900 |
| MOQ (ton) | 2 | 2 |
| Price ($/ton) | < 45 t, 7500  ≥ 45 t, 6200 | < 30 t, 7500  ≥ 30 t, 6900 |

|  |  |  |
| --- | --- | --- |
| Starch | | |
| Supplier | 1 | 2 |
| Purity | 90% | 95% |
| Plant location | (1050, 150) | (15, 100) |
| MPC (ton/quarter) | 90000 | 9000 |
| MOQ (ton) | 3 | 1 |
| Price ($/ton) | < 300 t, 520  ≥ 300 t, 500 | < 150 t, 640  ≥ 150 t, 570 |

|  |  |  |
| --- | --- | --- |
| Lignin | | |
| Supplier | 1 | 2 |
| Purity | 95% | 90% |
| Plant location | (540, 300) | (-200, 660) |
| MPC (ton/quarter) | 3000 | 9000 |
| MOQ (ton) | 1 | 1 |
| Price ($/ton) | < 90 t, 300  ≥ 90 t, 200 | < 150 t, 250  ≥ 150 t, 180 |

|  |  |  |
| --- | --- | --- |
| Cellulose | | |
| Supplier | 1 | 2 |
| Purity | 95% | 98% |
| Plant location | (130, 1040) | (510, 150) |
| MPC (ton/quarter) | 5400 | 6000 |
| MOQ (ton) | 2 | 2 |
| Price ($/ton) | < 300 t, 3700  ≥ 300 t, 3500 | < 300 t, 4500  ≥ 300 t, 4000 |

|  |  |  |
| --- | --- | --- |
| PCL | | |
| Supplier | 1 | 2 |
| Purity | 98% | 98% |
| Plant location | (-200, 660) | (-150, 200) |
| MPC (ton/quarter) | 3600 | 4500 |
| MOQ (ton) | 1 | 1 |
| Price ($/ton) | < 30 t, 7150  ≥ 30 t, 6800 | < 45 t, 7000  ≥ 45 t, 6500 |

|  |  |  |
| --- | --- | --- |
| PVP | | |
| Supplier | 1 | 2 |
| Purity | 99% | 96% |
| Plant location | (540, 340) | (600, 1150) |
| MPC (ton/quarter) | 15000 | 19500 |
| MOQ (ton) | 1 | 1 |
| Price ($/ton) | < 50 t, 6000  ≥ 50 t, 4500 | < 50 t, 5500  ≥ 50 t, 4000 |