Supplementary material to “A Novel Cost-Efficient Tributyl Citrate Production Process”

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Kinetic model Simultaneous Acidification-Esterification for the production of Tributyl Citrate

The mass balance of each species involved was represented in molality, which is defined as the number of moles of a compound per kilogram of liquid ()

Prefix and corresponds to each esterification reaction step, and and 2 represents the solid-solid-liquid reactions. Thus, the expression for each reaction rate involved can be expressed as follows:

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The kinetic parameters used for modeling the simultaneous acidification-esterification are condensed in Table S1.

Table S1: Kinetic parameter for acidification-esterification reaction system

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| --- | --- | --- | --- | --- | --- |
| **Parameter** | **Units** | **Value** | **Parameter** | **Units** | Value |
|  | kg2/ (mol·molcat · s) | 7.238e5 |  | J/mol | 59459.9 |
|  | 5.1870e5 |  | J/mol | 60358.10 |
|  | 4.3102e5 |  | J/mol | 62506.40 |
|  | kg/ (mol \* s) | 4907 |  | J/mol | 32173 |
|  | 0.5605 |  | - | 3.56 |
|  | - | 8.68 |  | - | 1.4 |

Table S2. Conditions and operational parameters for the production of TBC through the SAE process

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| --- | --- | --- |
| **Acidification-Esterification** | | |
| **Variable** | **Value** | **Feedback** |
| Dissolution Time (Hours) | 6 | Total Dissolution Time |
| Butanol mass (kg) | 16000 | Time (t) of addition:  **t(0 h):** 16000 kg |
| Mass of calcium acid citrate (kg) | 9583 | **t(0 h):** Addition speed: 4126 kg/h  Adding time: 2h  t(6 h): Adding speed: 4126 kg/h  Adding time: 0.32 h |
| Mass of H2SO4 (kg) |  | **t(2 h):** Addition speed 2334.05 kg/h  Adding time: 1.75h. |
| Temperature (K) | T0 = 298 K | Hold T0 to t = 2h  **t(2 h):** Heating from 298 K to 376 K  Heating speed: 20 K/h  Temperature of 333 K for t > h |
| Pressure (bar) | 1 | - |
| **Esterification** | | |
| **Variable** | **Value** | **Feedback** |
| Reaction Time (Hours) | 22 | Total esterification reaction time |
| Mass of MSDs (kg) | 40 | Addition Time: h. Add the mass required in 1 minute. Purity 70% P. |
| Temperature (K) | T0 = 333 K | **t(0 h):** Heating from 333 K to 376 K  Heating speed: 20 K/h  **t(2 h):** Maintain 376 K to t = 4 h  **t(4 h):** Heating from 376 K to 403 K  Heating rate: 2.7 K/h  **t (10h):** Hold 403 K |
| Pressure (bar) | 1 | **-** |
| **Purification** | | |
| Purification Time (Hours) | 8 | Purification Time |
| Purification Time (Hours) | 8 | Total Purification Time |

Table S3. Conditions and operational parameters for the production of TBC through the conventional process

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| **Dissolution** | | |
| **Variable** | **Value** | **Feedback** |
| Dissolution Time (Hours) | 14 | Total Dissolution Time |
| Butanol mass (kg) | 16000 | Addition times (t):  **t(0 h):** 6000 kg  **t(6 h):** 6000 kg  **t(10 h):** 4000 kg |
| Citric acid mass (kg) | 8000 | Add 1000 kg every hour until the total quantity is completed. First point of addition **t = 1h** |
| Mass of MSDs (kg) | 40 | Adding time: 10h. Add the mass required in 1 min. Purity 70%p |
| Temperature (K) | T0 = 313 K | Heating ramp 1K/h and maintain temperature of 333 K for t > 10 h |
| Pressure (bar) | 1 | - |
| **Esterification** | | |
| **Variable** | **Value** | **Feedback** |
| Reaction Time (Hours) | 24 | Total esterification reaction time |
| Temperature (K) | T0 = 333 K | **t(0 h):** Heating from 333 K to 376 K  Heating speed: 20 K/h  **t(2 h):** Maintain 376 K to t = 4 h  **t(4 h):** Heating from 376 K to 403 K  Heating rate: 2.7 K/h  **t (10h):** Hold 403 K |
| Pressure (bar) | 1 | **-** |
| **Purification** | | |
| Purification Time (Hours) | 8 | Purification Time |
| Purification Time (Hours) | 8 | Total Purification Time |
| Temperature (K) | T0 = 403 K | Constant Temperature |
| Pressure (bar) | 0.1 | Constant Pressure |
| **Total time:** 46 hours | | |