**Process Design and Economic Assessment of Large-scale production of Molybdenum Disulfide Nanomaterials**

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**Supporting information**

**Table S.1.** Interaction parameters used in the simulation with Aspen Plus.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  Component i |  Component j | Source | Aij | Aji | Bij | Bji | Cij | Dij | Eij | Eji | Fij | Fji | Temprature min | Temperature max |
| H2O | NH3 | APV110 ENRTL-RK | -0.5441 | -0.1642 | 1678.469 | -1027.53 | 0.2 | 0 | 0 | 0 | 0 | 0 | 0 | 200 |
| Ethylenediamine | H2O | APV110 VLE-LIT | 0 | 0 | -558.731 | 1118.546 | 0.7907 | 0 | 0 | 0 | 0 | 0 | 100 | 120 |
| N2H4 | H2O | APV110 VLE-LIT | 0 | 0 | -863.982 | 507.1204 | 0.2989 | 0 | 0 | 0 | 0 | 0 | 100 | 115 |
| H2O | Acetone | APV110 VLE-LIT | 0 | 0 | 602.5584 | 317.5539 | 0.5343 | 0 | 0 | 0 | 0 | 0 | 55 | 80 |
| LIOH | H2O | NISTV110 NIST-IG | -2.89201 | 6.63495 | -6.93428 | 2.04823 | 0.1 | 0 | 0 | 0 | 0 | 0 | 113.865 | 153.041 |
| N2H4 | NH3 | NISTV110 NIST-IG | -3.29307 | 3.67466 | 311.804 | -44.9196 | 0.1 | 0 | 0 | 0 | 0 | 0 | 4.969 | 40.06 |
| Ethylenediamine | N2 | R-PCES | 0 | 0 | 999.2772 | -607.218 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| Ethylenediamine | NH3 | R-PCES | 0 | 0 | 1518.832 | -777.476 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| Ethylenediamine | Acetone | R-PCES | 0 | 0 | 199.7579 | -173.921 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| Ethylenediamine | N2H4 | R-PCES | 0 | 0 | -143.427 | 355.1045 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| N2H4 | N2 | R-PCES | 0 | 0 | 188.3481 | -167.277 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| N2H4 | Acetone | R-PCES | 0 | 0 | 315.8567 | -36.7079 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| H2O | N2 | R-PCES | 0 | 0 | -35.8278 | 142.4195 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| N2 | NH3 | R-PCES | 0 | 0 | 109.5506 | -102.389 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| N2 | Acetone | R-PCES | 0 | 0 | -725.818 | 1320.705 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |
| NH3 | Acetone | R-PCES | 0 | 0 | -858.087 | 1808.126 | 0.3 | 0 | 0 | 0 | 0 | 0 | 25 | 25 |

NRTL (Non Random Two-Liquids) model is able to calculate activity coefficients for different property methods. It is recommended for highly non-ideal chemical systems, and can be used for both vapor-liquid and liquid-liquid equilibrium applications. The equation for NRTL model is :

Where aij, bij, eij, and fij are unsymmetrical. Which means that aij may not be equal to aji , but cij and dij are equal to cji and dji and:

**Table S.2.** Description of the major units of the developed Processes in Aspen Plus

|  |  |
| --- | --- |
| Block | Description |
| ACTCFUGE | Third centrifuge for the acetone washing of the Solid cake containing the MoS2 |
| B3 | Mixer of Fresh and Recycled Reactants |
| B7 | Solid liquid separator of remaining impurities |
| B8 | Mixer of Acetone and solid cake prior to second washing round |
| CFUGE | Second centrifuge for the water washing of the Solid cake containing the MoS2 |
| CFUGESEP | First centrifuge for liquid-solid separation of the reactor output stream |
| COOLER | Cooling down the Reactor effluent to 35 C |
| DRYER | Vaccum dryer to remove the remaining liquids |
| MIXWTR | Mixer of Water and solid cake prior to washing step |
| REACTOR | The heated autoclave reactor  |
| SPLITTER | Split the recycle stream into purge and recyclable streams  |
| B2 | Design specification block to control the make-up feed to prevent accumulation  |

**Table S.3**. Description of the streams

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Stream | ACTNMIX | CAKESTRW | COLDSTRE | DRYERVEN | MOS2 | PURGE | FRESHFEED | RECY |
| From | B8 | CFUGE | COOLER | DRYER | DRYER | SPLITTER |   | SPLITTER |
| To | ACTCFUGE | B8 | CFUGESEP |   |   |   | B3 | B3 |
| Description | Input stream of acetone washing centrifuge | Output of acetone washing centrifuge  | Output of cooler , it contains same composition as reactor output | Output Vent gas stream of Dryer | Pure MoS2 stream | Stream of purged split of recycled stream | Reactant’s Make-up feed stream | Recycled stream after purging |
|  |  |  |  |  |  |  |  |  |
| Stream | ROUTPUT | R-INPUT | SLOVHYDR | SOLIDD | SOLIDPHA | WAHED | WASHACET | WATERCLN |
| From | REACTOR | B3 | CFUGESEP | B7 | CFUGESEP | ACTCFUGE |   |   |
| To | COOLER | REACTOR | SPLITTER | DRYER | MIXWTR | B7 | B8 | MIXWTR |
| Description | Reactor’s output  | Reactor input stream  | Liquid output stream of 1st centrifugation |   |   |   |   | Water feed for washing |

**Table S.4.** Mass Balance Results computed by Aspen Plus (Base Case)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Components** | **Units** | ACTNMIX | CAKESTRW | COLDSTRE | DRYERVEN | MOS2 | R-INPUT | ROUTPUT | SLOVYDR |
| MoS2 | tonne/year | 99.855832 | 99.855832 | 99.855832 | 0 | 99.855832 | 0 | 99.85583201 | 0 |
| LiOH | tonne/year | 1150 | 1150 | 1150 | 0 | 0 | 1150 | 1150 | 0 |
| S | tonne/year | 11.2932892 | 11.2932892 | 11.2932892 | 0 | 0 | 51.3 | 11.29328916 | 0 |
| (NH4)6Mo7O24 | tonne/year | 31.064 | 31.064 | 31.064 | 0 | 0 | 141.2 | 31.064 | 0 |
| Ethylenediamine | tonne/year | 133.046433 | 133.046433 | 129600 | 0 | 0 | 129600 | 129600 | 129465.0433 |
| N2H4 | tonne/year | 8.41807611 | 8.41807611 | 8200.01439 | 0 | 0 | 8230 | 8200.014393 | 8191.47545 |
| H2O | tonne/year | 9858.49923 | 9858.49923 | 44.9530405 | 491.583985 | 0 | 0 | 44.95304046 | 44.9062294 |
| N2 | tonne/year | 0.02691006 | 0.02691006 | 26.2129793 | 0 | 0 | 0 | 26.21297934 | 26.18568291 |
| NH3 | tonne/year | 0.00934842 | 0.00934842 | 9.10626328 | 0 | 0 | 0 | 9.10626328 | 9.096780631 |
| ACETONE | tonne/year | 15000 | 0 | 0 | 747.959663 | 0 | 0 | 0 | 0 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Components** | **Units** | SOLIDD | SOLIDPHA | WAHED | WASHACET | WATERCLN | WATERMIX | WST | WSTACTON | WSTWR |
| MoS2 | tonne/year | 99.85583201 | 99.85583201 | 99.85583201 | 0 | 0 | 99.85583201 | 0 | 0 | 0 |
| LiOH | tonne/year | 0 | 1150 | 1150 | 0 | 0 | 1150 | 1150 | 0 | 0 |
| S | tonne/year | 0 | 11.29328916 | 11.29328916 | 0 | 0 | 11.29328916 | 11.29328916 | 0 | 0 |
| (NH4)6Mo7O24 | tonne/year | 0 | 31.064 | 31.064 | 0 | 0 | 31.064 | 31.064 | 0 | 0 |
| Ethylenediamine | tonne/year | 0 | 134.9567033 | 132.6844868 | 0 | 0 | 134.9567033 | 132.6844868 | 0.361945992 | 1.910270514 |
| N2H4 | tonne/year | 0 | 8.538942205 | 8.395175167 | 0 | 0 | 8.538942205 | 8.395175167 | 0.022900944 | 0.120866093 |
| H2O | tonne/year | 491.5839846 | 0.046811066 | 9831.679691 | 0 | 10000 | 10000.04681 | 9340.095707 | 26.81954119 | 141.5475785 |
| N2 | tonne/year | 0 | 0.02729643 | 0.02683685 | 0 | 0 | 0.02729643 | 0.02683685 | 7.32E-05 | 0.000386373 |
| NH3 | tonne/year | 0 | 0.009482649 | 0.009322993 | 0 | 0 | 0.009482649 | 0.009322993 | 2.54E-05 | 0.000134224 |
| ACETONE | tonne/year | 747.9596635 | 0 | 14959.19327 | 15000 | 0 | 0 | 14211.23361 | 40.80673014 | 0 |

 **Table S.5.**Mass Balance Results computed by Aspen Plus (Recycle Case )

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  **Components** | **Units** | ACTNMIX | CAKESTRW | COLDSTRE | DRYERVEN | MOS2 | R-INPUT | RECY | ROUTPUT |
| MoS2 | tonne/year | 99.855832 | 99.855832 | 99.855832 | 0 | 99.855832 | 0 | 0 | 0 |
| LiOH | tonne/year | 1150 | 1150 | 1150 | 0 | 0 | 0 | 1150 | 0 |
| S | tonne/year | 11.29328916 | 11.29328916 | 11.29328916 | 0 | 0 | 0 | 51.3 | 0 |
| (NH4)6Mo7O24 | tonne/year | 31.064 | 31.064 | 31.064 | 0 | 0 | 0 | 141.2 | 0 |
| Ethylenediamine | tonne/year | 132.7753747 | 132.7753747 | 130112.1839 | 0 | 0 | 19496.62533 | 19631.277 | 110480.8768 |
| N2H4 | tonne/year | 8.228968953 | 8.228968953 | 8063.913389 | 0 | 0 | 1208.33494 | 1246.64668 | 6847.231329 |
| H2O | tonne/year | 9858.756928 | 9858.756928 | 297.7497625 | 491.5968343 | 0 | 44.61623336 | 0 | 252.8253224 |
| N2 | tonne/year | 0.177177393 | 0.177177393 | 173.6235924 | 0 | 0 | 26.01658066 | 0 | 147.4272904 |
| NH3 | tonne/year | 0.061550576 | 0.061550576 | 60.31600312 | 0 | 0 | 9.038035321 | 0 | 51.21553349 |
| ACETONE | tonne/year | 15000 | 0 | 0 | 747.9596635 | 0 | 0 | 0 | 0 |

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Components** | **Units** | SLOVYDR | SOLIDD | SOLIDPHA | WAHED | WASHACET | WATERCLN | WATERMIX | WST | WSTACTON | WSTWR |
| MoS2 | tonne/year | 0 | 99.855832 | 99.855832 | 99.855832 | 0 | 0 | 99.855832 | 0 | 0 | 0 |
| LiOH | tonne/year | 0 | 0 | 1150 | 1150 | 0 | 0 | 1150 | 1150 | 0 | 0 |
| S | tonne/year | 0 | 0 | 11.29328916 | 11.29328916 | 0 | 0 | 11.29328916 | 11.29328916 | 0 | 0 |
| (NH4)6Mo7O24 | tonne/year | 0 | 0 | 31.064 | 31.064 | 0 | 0 | 31.064 | 31.064 | 0 | 0 |
| Ethylenediamine | tonne/year | 129977.5022 | 0 | 134.6817534 | 132.4141661 | 0 | 0 | 134.6817534 | 132.4141661 | 0.361208592 | 129977.5022 |
| N2H4 | tonne/year | 8055.566269 | 0 | 8.347119861 | 8.206582466 | 0 | 0 | 8.347119861 | 8.206582466 | 0.022386488 | 8055.566269 |
| H2O | tonne/year | 297.4415557 | 491.5968343 | 0.308206802 | 9831.936686 | 0 | 10000 | 10000.30821 | 9340.339852 | 26.82024223 | 297.4415557 |
| N2 | tonne/year | 173.4438711 | 0 | 0.179721292 | 0.176695391 | 0 | 0 | 0.179721292 | 0.176695391 | 0.000482002 | 173.4438711 |
| NH3 | tonne/year | 60.25356881 | 0 | 0.062434315 | 0.061383131 | 0 | 0 | 0.062434315 | 0.061383131 | 0.000167445 | 60.25356881 |
| ACETONE | tonne/year | 0 | 747.9596635 | 0 | 14959.19327 | 15000 | 0 | 0 | 14211.23361 | 40.80673014 | 0 |

**Table S.6.** Operating costs calculation (without depreciation)

|  |  |
| --- | --- |
|  | Definition |
| Variable costs |  |
|  Raw materials (RM) | Calculated |
|  Utilities (U) | Calculated |
| Fixed costs |  |
|  Operating labor (OL) | Calculated |
|  Operating supervision (S) | 15% of OL  |
|  Laboratory charges  | 15% of OL  |
|  Maintenance (M) | 4% of FCI |
|  Operating supplies  | 15% of M |
|  Plant overheads  | 60% of (OL+S+M) |
|  Taxes and insurance  | 3% of FCI |
|  Water Treatment | 1.3% of FCI |
|  Process waste disposal | 1.5 % of FCI |
| General expenses  | 5% of Variable + Fixed |
| Total operating cost | Variable + Fixed + General expenses |
| Operating cost/kg MoS2 |  |

**Calculation of Profitability Indicators**

The profitability indicators are return on investment (ROI), pay-back period (PBP) and net present value (NPV) are done based on Peters et al.(1) as described below.

**Return on investment (ROI):** ROI is calculated as an average over the whole project life time with the formula:

**Net profit** is the profit after taxes and is calculated as:

Net profit = (Revenues – Total operating costs (without depreciation) – Depreciation)

**Pay-back Period (PBP):** is calculated as an average over the whole project life time with the formula:

**Net Cash Flow**: Is calculated by adding Depreciation to the net profit to make up the cash flow:

Net Cash flow = Depreciation + Net profit.

**Net Present Value (NPV):** NPV is the sum of the present values of the future cash flows and is calculated with:

where

cash flow in year n;

 project life in years which is 20 year in our case;

 interest rate

**Table** **S.7.** Annual Cash Flow Table for base case

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Year | Revenues | Taxes rate | Fixed Capital Investment | Working capital | Operating costs | Depreciation | Annual Cash flow | NPV(year n) | Net Profit |
| 0 | 0 | 0 | 12300000 | 2000000 | 0 | 0 | 0 | 0 | 0 |
| 1 | 25960800.3 | 0 | 0 | 0 | 166871492.9 | 1205400 | -140910692.6 | -128100629.6 | -142116092.6 |
| 2 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -200117978.8 | -243348154.4 |
| 3 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -181925435.3 | -243348154.4 |
| 4 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -165386759.4 | -243348154.4 |
| 5 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -150351599.4 | -243348154.4 |
| 6 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -136683272.2 | -243348154.4 |
| 7 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -124257520.2 | -243348154.4 |
| 8 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -112961382 | -243348154.4 |
| 9 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -102692165.4 | -243348154.4 |
| 10 | 51921600.6 | 0 | 0 | 0 | 294064355 | 1205400 | -242142754.4 | -93356514.04 | -243348154.4 |
| 11 | 51921600.6 | 0 | 0 | 0 | 294064355 | 0 | -242142754.4 | -84869558.22 | -242142754.4 |
| 12 | 51921600.6 | 0 | 0 | 0 | 294064355 | 0 | -242142754.4 | -77154143.84 | -242142754.4 |
| 13 | 51921600.6 | 0 | 0 | 0 | 294064355 | 0 | -242142754.4 | -70140130.76 | -242142754.4 |
| 14 | 51921600.6 | 0 | 0 | 0 | 294064355 | 0 | -242142754.4 | -63763755.24 | -242142754.4 |
| 15 | 51921600.6 | 0 | 0 | 0 | 294064355 | 0 | -242142754.4 | -57967050.22 | -242142754.4 |
| 16 | 51921600.6 | 0.0875 | 0 | 0 | 294064355 | 0 | -220955263.4 | -48086303.02 | -220955263.4 |
| 17 | 51921600.6 | 0.0875 | 0 | 0 | 294064355 | 0 | -220955263.4 | -43714820.93 | -220955263.4 |
| 18 | 51921600.6 | 0.0875 | 0 | 0 | 294064355 | 0 | -220955263.4 | -39740746.3 | -220955263.4 |
| 19 | 51921600.6 | 0.0875 | 0 | 0 | 294064355 | 0 | -220955263.4 | -36127951.18 | -220955263.4 |
| 20 | 51921600.6 | 0.0875 | 0 | -2000000 | 294064355 | 0 | -220955263.4 | -32843591.98 | -220955263.4 |

**Table S.8.** Annual Cash Flow Table for recycle case

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Year | Revenues | Taxes rate | Fixed Capital Investment | Working capital | Operating costs | Depreciation | Annual Cash flow | NPV(year n) | Net Profit |
| 0 | 0 | 0 | 15000000 | 2400000 | 0 | 0 | 0 | 0 | 0 |
| 1 | 25960980.03 | 0 | 0 | 0 | 29267425.5 | 1470000 | -3306445.47 | -3005859.518 | -4776445.47 |
| 2 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 1435118.231 | 266493.06 |
| 3 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 1304652.938 | 266493.06 |
| 4 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 1186048.125 | 266493.06 |
| 5 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 1078225.568 | 266493.06 |
| 6 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 980205.0621 | 266493.06 |
| 7 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 891095.511 | 266493.06 |
| 8 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 810086.8282 | 266493.06 |
| 9 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 736442.5711 | 266493.06 |
| 10 | 51921960.06 | 0 | 0 | 0 | 50185467 | 1470000 | 1736493.06 | 669493.2464 | 266493.06 |
| 11 | 51921960.06 | 0 | 0 | 0 | 50185467 | 0 | 1736493.06 | 608630.224 | 1736493.06 |
| 12 | 51921960.06 | 0 | 0 | 0 | 50185467 | 0 | 1736493.06 | 553300.2037 | 1736493.06 |
| 13 | 51921960.06 | 0 | 0 | 0 | 50185467 | 0 | 1736493.06 | 503000.1851 | 1736493.06 |
| 14 | 51921960.06 | 0 | 0 | 0 | 50185467 | 0 | 1736493.06 | 457272.8956 | 1736493.06 |
| 15 | 51921960.06 | 0 | 0 | 0 | 50185467 | 0 | 1736493.06 | 415702.6323 | 1736493.06 |
| 16 | 51921960.06 | 0.0875 | 0 | 0 | 50185467 | 0 | 1584549.917 | 344844.2291 | 1584549.917 |
| 17 | 51921960.06 | 0.0875 | 0 | 0 | 50185467 | 0 | 1584549.917 | 313494.7537 | 1584549.917 |
| 18 | 51921960.06 | 0.0875 | 0 | 0 | 50185467 | 0 | 1584549.917 | 284995.2307 | 1584549.917 |
| 19 | 51921960.06 | 0.0875 | 0 | 0 | 50185467 | 0 | 1584549.917 | 259086.5733 | 1584549.917 |
| 20 | 51921960.06 | 0.0875 | 0 | -2400000 | 50185467 | 0 | 1584549.917 | 235533.2485 | 1584549.917 |

**Reference**

1. Peters MS, Timmerhaus K, West R. Plant Design and Economics for Chemical Engineers. Columbus: McGraw-Hill; 2004.