****

**Fig. S1 - The technical route of this work**



Fig. S2 - The relation between Δ*T*min and total cost index target



Fig. S3 - Composite curves for syngas-to-methanol process



Fig. S4 - Grand composite curve for syngas-to-methanol process



Fig. S5 - The diagram of original HEN



Fig. S6 - The diagram of traditional optimal HEN

**Table S1 - The information of all blocks and streams**

|  |  |  |  |
| --- | --- | --- | --- |
| Block name | Stream in | Stream out | Usage |
| REACTOR2 | 3 | REA-OUT | Side reactions simulation |
| HP-SEP | 28 | 6&7 | Gas-liquid separation |
| FLASH | 7 | 8&CRUDE-ME | Decompression tank |
| FSP-1 | 6 | 12&15 | Gas splitter |
| GAS-MIX | FEED&CYC-GAS | 10 | Feed mixing |
| COMPR | 11 | CYC-GAS | Circulating gas compressor |
| CFQ-MIX | 12&8 | CF-GAS | Mixer |
| B11 | 15 | 11&18 | Buffer tank |
| LIQ-MIX | CRUDE-ME&H2O | 23 | Mixing crude methanol with water |
| PC | PCF-IN&PCD-IN | PCD-OUT&PCW-OUT | Removing light component impurities |
| S-1 | S1-IN | S1D-OUT&S1W-OUT | Gas-liquid separation |
| S-2 | S2-IN | FUEL-GAS&S2W-OUT | Gas-liquid separation |
| C-2 | PCD-OUT | S1-IN | Primary condensation |
| RL-MIX | S1W-OUT&S2W-OUT | PCD-IN | Reflux mixing |
| C-3 | S1D-OUT | S2-IN | Secondary condensation |
| P-1 | PCW-OUT | 21 | HP feed stream pressurization |
| H-2 | 21 | HCF-IN | HC feed stream preheating |
| H-1 | 23 | PCF-IN | PC feed stream preheating |
| HC | HCF-IN&HCD-IN | HCD-OUT&HCW-OUT | Refined methanol production |
| C-4 | 24 | 16 | Refined methanol cooling |
| C-5 | HCW-OUT | CCF-IN | CC feed stream cooling |
| CC | CCF-IN&CCW-IN | CCDCCF-IN-OUT&CCW-OUT | Refined methanol production and heavy component impurities removing |
| REACTOR1 | REA-IN | 3 | Main reactions simulation |
| C-6 | CCD-OUT | 31 | Refined methanol cooling |
| C-7 | 27 | W-WATER | Wastewater cooling |
| FSP-2 | 49 | 24&HCD-IN | Liquid splitter |
| FSP-3 | CCW-OUT | 27&52 | Liquid splitter |
| E-2 | HCD-OUT | 49&CCW-IN | Process streams heat exchanging |
| C-1 | 4 | 28 | Product cooling |
| E-1 | REA-OUT | 4&REA-IN | Process streams heat exchanger |
| PRO-MIX | 31&16 | S1 | Purified methanol mixing |

**Table S2 -** The main reactions and side reactions of methanol synthesis

|  |
| --- |
| **Main reactions** |
| (1) |  |
| (2) |  |
|  |
| **Side reactions** |
|  |

**Table S3 -** The compositions of syngas.

|  |  |
| --- | --- |
| **Composition** | **Volume fraction** |
| CO | 0.2686 |
| CO2 | 0.0415 |
| H2 | 0.6771 |
| N2 | 0.0082 |
| H2O | 0.0016 |
| CH4 | 0.0030 |

**Table S4 -** The compositions of crude methanol.

|  |  |
| --- | --- |
| **Composition** | **Volume fraction** |
| CO | 25.0 ppm |
| CO2 | 0.026017 |
| H2 | 2.47 ppm |
| N2 | 82.5 ppm |
| CH3OH | 0.930342 |
| H2O | 0.041034 |
| CH4 | 73.1 ppm |
| CH3CH2OH | 0.001185 |
| CH3OCH3 | 0.000325 |
| C4H9OH | 0.000273 |
| HCOOCH3 | 0.00064 |