

**SUPPORTING INFORMATION (SI)**

**Optimization of Energy Consumption in Formaldehyde Production Process  
Using Reboiled Absorption Process**

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Table S1. Heat and material balance for modified process

## HEAT AND MATERIAL BALANCE

|                                  | Unit        | Methanol     | Air      | 1        | 2            | 3           | 4           | 5           | 6           | 7           | 8           | 9            | 10          | 11          | 12          | 13          | 14           | 15           | Water2      |
|----------------------------------|-------------|--------------|----------|----------|--------------|-------------|-------------|-------------|-------------|-------------|-------------|--------------|-------------|-------------|-------------|-------------|--------------|--------------|-------------|
| <b>Total Phase Properties</b>    |             |              |          |          |              |             |             |             |             |             |             |              |             |             |             |             |              |              |             |
| Vapour Fraction                  |             | 0            | 1        | 1        | 1.27E-05     | 0           | 0.5600553   | 0.767308399 | 1           | 1           | 0           | 1            | 0           | 0.834996048 | 0.376142051 | 0           | 0            | 0            | 0           |
| Temperature                      | C           | 25           | 25       | 168,9168 | 38,36110962  | 38,45034274 | 40,584665   | 65          | 120         | 650         | 650         | 160          | 15,008529   | 131,6900909 | 126,6371238 | 110,0065897 | 15           | 15,00852896  | 25          |
| Pressure                         | bar         | 1,01324997   | 1,01325  | 3,03975  | 1,01324997   | 3,0397499   | 3,0397499   | 2,0397499   | 1,6397499   | 1,6397499   | 1,6397499   | 1,4397499    | 3,0397499   | 2,8397499   | 2,4397499   | 2,0397499   | 2,0397499    | 3,0397499    | 1,5         |
| Mol Weight                       |             | 31,90163263  | 28,85027 | 28,85027 | 28,44369644  | 28,44369644 | 28,65109712 | 28,65109712 | 28,65109712 | 25,77098615 | 36,0165166  | 25,77098615  | 18,01510048 | 18,01510048 | 18,01510048 | 18,01510048 | 18,01510048  | 18,01510048  | 18,01510048 |
| Molar Flow                       | kgmole/h    | 125,3854322  | 207,9703 | 207,9703 | 199,7203134  | 199,7203134 | 407,690635  | 407,690635  | 407,690635  | 453,2510886 | 0           | 453,2510886  | 223,0163438 | 223,0163438 | 223,0163438 | 223,0163438 | 223,0163438  | 223,0163438  | 145,0000001 |
| Mass Flow                        | kg/h        | 3999,999996  | 6000     | 6000     | 5680,783967  | 5680,783967 | 11680,78398 | 11680,78398 | 11680,78398 | 11680,72753 | 0           | 11680,72753  | 4017,661843 | 4017,661843 | 4017,661843 | 4017,661843 | 4017,661843  | 4017,661843  | 2612,189571 |
| Heat Flow                        | kJ/h        | -30078496,95 | 0        | 885831,4 | -46793594,96 | -46791626,9 | -45905795   | -42325799,1 | -38265800,1 | -38040717,4 | 0           | -47286246,46 | -63705869,2 | -54460340,1 | -58520339,1 | -62100335,4 | -63706397,01 | -63705869,16 | -41310806,3 |
| Std Gas Flow                     | STD. m3/h   | 2964,667882  | 4917,341 | 4917,341 | 4722,274254  | 4722,274254 | 9639,6153   | 9639,615305 | 9639,615305 | 10716,86655 | 0           | 10716,86655  | 5273,095766 | 5273,095766 | 5273,095766 | 5273,095766 | 5273,095766  | 5273,095766  | 3428,443285 |
| <b>Vapor Phase Properties</b>    |             |              |          |          |              |             |             |             |             |             |             |              |             |             |             |             |              |              |             |
| Mass Flow                        | kg/h        |              | 6000     | 6000     | 0,073258643  |             | 6621,16303  | 9113,870363 | 11680,78398 | 11680,72753 | 0           | 11680,72753  |             | 3354,731759 | 1511,211565 |             |              |              |             |
| Mol Weight                       |             |              | 28,85027 | 28,85027 | 28,86538045  |             | 28,9983065  | 29,13413709 | 28,65109712 | 25,77098615 | 25,77098615 | 25,77098615  |             | 18,01510048 | 18,01510048 |             |              |              |             |
| Mass Density                     | kg/m3       |              | 1,179247 | 2,386015 | 1,129257287  |             | 3,37925683  | 2,113698079 | 1,437255087 | 0,550566321 | 0,55056632  | 1,030274712  |             | 1,519870314 | 1,322289227 |             |              |              |             |
| Actual Gas Vol Flow              | m3/h        |              | 5087,991 | 2514,653 | 0,064873297  |             | 1959,35478  | 4311,812767 | 8127,147427 | 21215,84102 | 0           | 11337,48833  |             | 2207,24869  | 1142,875201 |             |              |              |             |
| Compressibility Factor           |             |              | 1        | 1        | 1,000001632  |             | 1,00000001  | 1           | 1           | 1           | 1           | 1            |             | 1           | 1           |             |              |              |             |
| Cp/Cv                            |             |              | 1,399162 | 1,382646 | 1,33785528   |             | 1,37466765  | 1,319741644 | 1,285108301 | 1,218221987 | 1,21822199  | 1,297410667  |             | 1,239122338 | 1,245058887 |             |              |              |             |
| Viscosity                        | cP          |              | 0,018829 | 0,025036 | 0,01466637   |             | 0,01814472  | 0,014684593 | 0,014683349 | 0,031345997 | 0,031346    | 0,015952462  |             | 0,013230234 | 0,01304301  |             |              |              |             |
| Heat Capacity                    | kJ/kgmole-C | 115,0871494  | 29,14405 | 30,0431  | 32,91429326  | 103,1407126 | 30,5058128  | 34,31790719 | 37,47666572 | 46,41506953 | 46,4150695  | 36,27037131  | 75,4369977  | 43,08490262 | 42,24258773 | 75,81443585 | 75,44124632  | 75,43699956  | 75,69799524 |
| Thermal Conductivity             | W/m-K       |              | 0,025916 | 0,035667 | 0,024191199  |             | 0,02603282  | 0,024806608 | 0,027203353 | 0,075126942 | 0,07512694  | 0,034201523  |             | 0,027038086 | 0,026609851 |             |              |              |             |
| <b>Liquid Phase Properties</b>   |             |              |          |          |              |             |             |             |             |             |             |              |             |             |             |             |              |              |             |
| Mass Flow                        | kg/h        | 3999,999996  |          |          | 5680,710709  | 5680,783967 | 5059,62095  | 2566,913617 |             | 0           | 0           |              |             |             |             |             |              |              |             |
| Mol Weight                       |             | 31,90163263  |          |          | 28,44369109  | 28,44369644 | 28,2090951  | 27,05825654 |             | 36,01651657 | 36,0165166  |              |             |             |             |             |              |              |             |
| Mass Density                     | kg/m3       | 787,0014591  |          |          | 786,9278858  | 786,949376  | 785,836351  | 764,2349601 |             | 2000,917587 | 2000,91759  |              |             |             |             |             |              |              |             |
| Actual Liq Vol Flow              | m3/h        | 5,082582694  |          |          | 7,21884535   | 7,218741308 | 6,43851731  | 3,358801613 |             | 0           | 0           |              |             |             |             |             |              |              |             |
| Viscosity                        | cP          | 0,546944242  |          |          | 0,408470075  | 0,408012787 | 0,39327298  | 0,274400896 |             | 0,1619735   | 0,1619735   |              |             |             |             |             |              |              |             |
| Heat Capacity                    | kJ/kgmole-C |              |          |          | 103,1344434  |             | 102,460373  | 100,9453633 |             | 43,84267544 | 43,8426754  |              |             | 76,73000517 | 76,49061398 |             |              |              |             |
| Thermal Conductivity             | W/m-K       | 0,182456232  |          |          | 0,245971888  | 0,245939946 | 0,2505027   | 0,268468106 |             | 0,042834543 | 0,04283454  |              |             |             |             |             |              |              |             |
| Surface Tension                  | dyne/cm     | 30,01652658  |          |          | 36,16360841  | 36,14806215 | 36,3440262  | 34,71251707 |             | 0           |             |              |             |             |             |             |              |              |             |
| <b>Mass Fraction Composition</b> |             |              |          |          |              |             |             |             |             |             |             |              |             |             |             |             |              |              |             |
| Methanol                         |             | 0,994352922  | 0        | 0        | 0,701075533  | 0,701075533 | 0,34095816  | 0,340958163 | 0,340958163 | 0,153295531 | 0,00278704  | 0,153295531  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| Formaldehyde                     |             | 0            | 0        | 0        | 0,149264305  | 0,149264305 | 0,072592582 | 0,072592582 | 0,072592582 | 0,22547673  | 0,0118225   | 0,22547673   | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| H2O                              |             | 0,005647078  | 0        | 0        | 0,149607516  | 0,149607516 | 0,0727595   | 0,072759498 | 0,072759498 | 0,15921645  | 0,00420151  | 0,15921645   | 1           | 1           | 1           | 1           | 1            | 1            | 1           |
| Nitrogen                         |             | 0            | 0,767073 | 0,767073 | 1,46E-05     | 1,46E-05    | 0,39402511  | 0,394025108 | 0,394025108 | 0,394027012 | 0,3492777   | 0,394027012  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| Oxygen                           |             | 0            | 0,232927 | 0,232927 | 1,40E-06     | 1,40E-06    | 0,11964681  | 0,119646806 | 0,119646806 | 0,032560943 | 0,00800603  | 0,032560943  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| CO                               |             | 0            | 0        | 0        | 1,41E-07     | 1,41E-07    | 6,84E-08    | 6,84E-08    | 6,84E-08    | 0,003398017 | 0,003398665 | 0,003398017  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| CO2                              |             | 0            | 0        | 0        | 3,64E-05     | 3,64E-05    | 1,77E-05    | 1,77E-05    | 1,77E-05    | 0,028350471 | 0,61974702  | 0,028350471  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| Hydrogen                         |             | 0            | 0        | 0        | 1,09E-07     | 1,09E-07    | 5,28E-08    | 5,28E-08    | 5,28E-08    | 0,003674845 | 0,00022155  | 0,003674845  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| <b>Mole Fraction Composition</b> |             |              |          |          |              |             |             |             |             |             |             |              |             |             |             |             |              |              |             |
| Methanol                         |             | 0,99         | 0        | 0        | 0,622346966  | 0,622346966 | 0,30487659  | 0,304876591 | 0,304876591 | 0,123294091 | 0,00313276  | 0,123294091  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| Formaldehyde                     |             | 0            | 0        | 0        | 0,141399346  | 0,141399346 | 0,069269    | 0,069268998 | 0,069268998 | 0,193525487 | 0,01418131  | 0,193525487  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| H2O                              |             | 0,01         | 0        | 0        | 0,236212436  | 0,236212436 | 0,11571623  | 0,115716226 | 0,115716226 | 0,227762533 | 0,00839982  | 0,227762533  | 1           | 1           | 1           | 1           | 1            | 1            | 1           |
| Nitrogen                         |             | 0            | 0,79     | 0,79     | 1,48E-05     | 1,48E-05    | 0,40300044  | 0,403000444 | 0,403000444 | 0,362491147 | 0,44906885  | 0,362491147  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| Oxygen                           |             | 0            | 0,21     | 0,21     | 1,24E-06     | 1,24E-06    | 0,10712538  | 0,107125383 | 0,107125383 | 0,026222738 | 0,00901092  | 0,026222738  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| CO                               |             | 0            | 0        | 0        | 1,43E-07     | 1,43E-07    | 7,00E-08    | 7,00E-08    | 7,00E-08    | 0,003126292 | 0,00506176  | 0,003126292  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| CO2                              |             | 0            | 0        | 0        | 2,36E-05     | 2,36E-05    | 1,15E-05    | 1,15E-05    | 1,15E-05    | 0,016601331 | 0,50718656  | 0,016601331  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |
| Hydrogen                         |             | 0            | 0        | 0        | 1,53E-06     | 1,53E-06    | 7,51E-07    | 7,51E-07    | 7,51E-07    | 0,046976382 | 0,00395801  | 0,046976382  | 0           | 0           | 0           | 0           | 0            | 0            | 0           |

Table S1. Heat and material balance for modified process (continued)

|                                  | Unit        | Off gas     | 16          | 17           | 18          | 19          | Off gas 2 | 20          | 21           | 22           | 23           | 24       | Formaldehyde | Formaldehyde 37% | Water        |
|----------------------------------|-------------|-------------|-------------|--------------|-------------|-------------|-----------|-------------|--------------|--------------|--------------|----------|--------------|------------------|--------------|
| <b>Total Phase Properties</b>    |             |             |             |              |             |             |           |             |              |              |              |          |              |                  |              |
| Vapour Fraction                  |             | 1           | 0           | 0            | 1           | 0,000139348 | 1         | 0           | 0            | 0            | 0            | 0        | 5,00E-09     | 0                | 0            |
| Temperature                      | C           | 83,5809081  | 87,84137915 | 70,0034106   | 106,0733325 | 70          | 70        | 70          | 70,00341147  | 70,00341147  | 70,00341147  | 70,00341 | 109,0003729  | 92,79769391      | 25           |
| Pressure                         | bar         | 1,4         | 1,4         | 1,2          | 1,2         | 1,1         | 1,1       | 1,1         | 1,2          | 1,2          | 1,2          | 1,2      | 1,3          | 1,01             | 1,01         |
| Mol Weight                       |             | 24,12395578 | 23,3417694  | 22,60811387  | 22,61061878 | 22,61061878 | 26,28909  | 22,61010612 | 22,61010612  | 22,61010612  | 22,61010612  | 22,61097 | 23,86787286  | 22,45905956      | 18,01510048  |
| Molar Flow                       | kgmole/h    | 420,2043777 | 178,046711  | 19,46203924  | 94,00523747 | 94,00523747 | 0,013099  | 93,99213806 | 93,99213806  | 19,46032438  | 74,53181368  | 74,33488 | 103,5035127  | 136,3159492      | 32,81243641  |
| Mass Flow                        | kg/h        | 10136,99183 | 4155,925271 | 439,9999992  | 2125,516587 | 2125,516587 | 0,344372  | 2125,172216 | 2125,172216  | 439,9999992  | 1685,172216  | 1680,784 | 2470,408683  | 3061,528022      | 591,119339   |
| Heat Flow                        | kJ/h        | -50484892,6 | -38111922,2 | -4376964,181 | -17915770,2 | -21137673,9 | -1194,4   | -21136479,5 | -21136443,77 | -4376132,519 | -16760311,25 | -1,7E+07 | -21249403,09 | -30597762,42     | -9348359,335 |
| Std Gas Flow                     | STD_m3/h    | 9935,495699 | 4209,81414  | 460,1689496  | 2222,700862 | 2222,700862 | 0,309728  | 2222,391134 | 2222,391134  | 460,1284027  | 1762,262731  | 1757,606 | 2447,282228  | 3223,113795      | 775,831567   |
| <b>Vapor Phase Properties</b>    |             |             |             |              |             |             |           |             |              |              |              |          |              |                  |              |
| Mass Flow                        | kg/h        | 10136,99183 |             |              | 2125,516587 | 0,344371597 | 0,344372  | 0           |              |              |              |          | 1,20E-05     |                  |              |
| Mol Weight                       |             | 24,12395578 |             |              | 22,61061878 | 26,28909354 | 26,28909  | 26,28909354 |              |              |              |          | 23,24125074  |                  |              |
| Mass Density                     | kg/m3       | 1,138693907 |             |              | 0,860541613 | 1,013578893 | 1,013579  | 1,013578893 |              |              |              |          | 0,950915293  |                  |              |
| Actual Gas Vol Flow              | m3/h        | 8902,297416 |             |              | 2469,975367 | 0,339758059 | 0,339758  | 0           |              |              |              |          | 1,26E-05     |                  |              |
| Compressibility Factor           |             | 1,000004807 |             |              | 1,000000073 | 1           | 1         | 1           |              |              |              |          | 0,999999984  |                  |              |
| Cp/Cv                            |             | 1,316306467 |             |              | 1,287714872 | 1,334755149 | 1,334755  | 1,334755149 |              |              |              |          | 1,287197945  |                  |              |
| Viscosity                        | cP          | 0,013006129 |             |              | 0,009736665 | 0,014303614 | 0,014304  | 0,014303614 |              |              |              |          | 0,009868197  |                  |              |
| Heat Capacity                    | kJ/kgmole-C | 34,60031037 | 91,33953118 | 84,66479892  | 37,21246809 | 33,15167051 | 33,15167  | 33,15167051 | 84,66855409  | 84,66855409  | 84,66855409  | 84,67024 | 37,26448195  | 90,50133955      | 75,7004081   |
| Thermal Conductivity             | W/m-K       | 0,029107022 |             |              | 0,02332418  | 0,028669672 | 0,02867   | 0,028669672 |              |              |              |          | 0,023416066  |                  |              |
| <b>Liquid Phase Properties</b>   |             |             |             |              |             |             |           |             |              |              |              |          |              |                  |              |
| Mass Flow                        | kg/h        |             |             | 427,6792946  |             | 2064,822798 | 0         | 2064,822798 | 2064,83499   | 427,5076567  | 1637,327334  | 1633,62  |              |                  |              |
| Mol Weight                       |             |             |             | 22,60749653  |             | 22,6094748  | 22,60947  | 22,6094748  | 22,60947525  | 22,60947525  | 22,60947525  | 22,61035 |              |                  |              |
| Mass Density                     | kg/m3       |             |             | 793,4446175  |             | 793,3868143 | 793,3868  | 793,3868143 | 793,3829743  | 793,3829743  | 793,3829743  | 793,3554 |              |                  |              |
| Actual Liq Vol Flow              | m3/h        |             |             | 0,539015938  |             | 2,602542367 | 0         | 2,602542367 | 2,602570331  | 0,538841481  | 2,063728851  | 2,059128 |              |                  |              |
| Viscosity                        | cP          |             |             | 0,197974964  |             | 0,197922663 | 0,197923  | 0,197922663 | 0,197914024  | 0,197914024  | 0,197914024  | 0,197887 |              |                  |              |
| Heat Capacity                    | kJ/kgmole-C |             |             | 85,3716768   |             | 84,66816658 | 84,66817  | 84,66816658 | 85,37676922  | 85,37676922  | 85,37676922  | 85,37904 | 107,5871165  |                  |              |
| Thermal Conductivity             | W/m-K       |             |             | 0,394465861  |             | 0,394370241 | 0,39437   | 0,394370241 | 0,394369085  | 0,394369085  | 0,394369085  | 0,394326 |              |                  |              |
| Surface Tension                  | dyne/cm     |             |             | 44,10803876  |             | 44,0999809  | 44,09998  | 44,0999809  | 44,09933662  | 44,09933662  | 44,09933662  | 44,09548 |              |                  |              |
| <b>Mass Fraction Composition</b> |             |             |             |              |             |             |           |             |              |              |              |          |              |                  |              |
| Methanol                         |             | 0,176113968 | 0,001284306 | 0,003124359  | 0,003157913 | 0,003157913 | 0,108811  | 0,003140792 | 0,003140792  | 0,003140792  | 0,003140792  | 0,003122 | 7,53E-19     | 0                | 0            |
| Formaldehyde                     |             | 0,026558269 | 0,568949425 | 0,504236326  | 0,504332425 | 0,504332425 | 0,135623  | 0,504392172 | 0,504392172  | 0,504392172  | 0,504392172  | 0,50449  | 0,613019357  | 0,494657678      | 0            |
| H2O                              |             | 0,265009191 | 0,429641395 | 0,492462285  | 0,492228856 | 0,492228856 | 0,121921  | 0,492288862 | 0,492288862  | 0,492288862  | 0,492288862  | 0,492211 | 0,386980643  | 0,505342322      | 1            |
| Nitrogen                         |             | 0,454006918 | 6,20E-05    | 4,92E-05     | 0,000131449 | 0,000131449 | 0,507802  | 4,92E-05    | 4,92E-05     | 4,92E-05     | 4,92E-05     | 4,92E-05 | 4,82E-33     | 0                | 0            |
| Oxygen                           |             | 0,037517336 | 5,43E-06    | 4,71E-06     | 1,16E-05    | 1,16E-05    | 0,042448  | 4,72E-06    | 4,72E-06     | 4,72E-06     | 4,72E-06     | 4,72E-06 | 1,10E-30     | 0                | 0            |
| CO                               |             | 0,003915259 | 5,69E-07    | 4,75E-07     | 1,21E-06    | 1,21E-06    | 0,004545  | 4,75E-07    | 4,75E-07     | 4,75E-07     | 4,75E-07     | 4,75E-07 | 9,48E-35     | 0                | 0            |
| CO2                              |             | 0,032644782 | 5,64E-05    | 0,00012228   | 0,000135518 | 0,000135518 | 0,074729  | 0,000123431 | 0,000123431  | 0,000123431  | 0,000123431  | 0,000123 | 5,04E-25     | 0                | 0            |
| Hydrogen                         |             | 0,004234277 | 4,90E-07    | 3,67E-07     | 1,03E-06    | 1,03E-06    | 0,004121  | 3,67E-07    | 3,67E-07     | 3,67E-07     | 3,67E-07     | 3,67E-07 | 6,35E-36     | 0                | 0            |
| <b>Mole Fraction Composition</b> |             |             |             |              |             |             |           |             |              |              |              |          |              |                  |              |
| Methanol                         |             | 0,132594056 | 0,000935586 | 0,002204484  | 0,002228406 | 0,002228406 | 0,089275  | 0,002216275 | 0,002216275  | 0,002216275  | 0,002216275  | 0,002203 | 5,61E-19     | 0                | 0            |
| Formaldehyde                     |             | 0,021337999 | 0,442295825 | 0,379667886  | 0,379782318 | 0,379782318 | 0,118745  | 0,379818698 | 0,379818698  | 0,379818698  | 0,379818698  | 0,379907 | 0,487296516  | 0,37             | 0            |
| H2O                              |             | 0,354872848 | 0,556676905 | 0,618017281  | 0,61779278  | 0,61779278  | 0,177918  | 0,617854084 | 0,617854084  | 0,617854084  | 0,617854084  | 0,61778  | 0,512703484  | 0,63             | 1            |
| Nitrogen                         |             | 0,39097714  | 5,17E-05    | 3,97E-05     | 0,000106099 | 0,000106099 | 0,476552  | 3,97E-05    | 3,97E-05     | 3,97E-05     | 3,97E-05     | 3,97E-05 | 4,10E-33     | 0                | 0            |
| Oxygen                           |             | 0,02828333  | 3,96E-06    | 3,33E-06     | 8,19E-06    | 8,19E-06    | 0,034873  | 3,33E-06    | 3,33E-06     | 3,33E-06     | 3,33E-06     | 3,33E-06 | 8,24E-31     | 0                | 0            |
| CO                               |             | 0,003371956 | 4,74E-07    | 3,84E-07     | 9,78E-07    | 9,78E-07    | 0,004265  | 3,83E-07    | 3,83E-07     | 3,83E-07     | 3,83E-07     | 3,84E-07 | 8,08E-35     | 0                | 0            |
| CO2                              |             | 0,017894266 | 2,99E-05    | 6,28E-05     | 6,96E-05    | 6,96E-05    | 0,044639  | 6,34E-05    | 6,34E-05     | 6,34E-05     | 6,34E-05     | 6,33E-05 | 2,73E-25     | 0                | 0            |
| Hydrogen                         |             | 0,050668405 | 5,68E-06    | 4,12E-06     | 1,16E-05    | 1,16E-05    | 0,053733  | 4,12E-06    | 4,12E-06     | 4,12E-06     | 4,12E-06     | 4,12E-06 | 7,52E-35     | 0                | 0            |