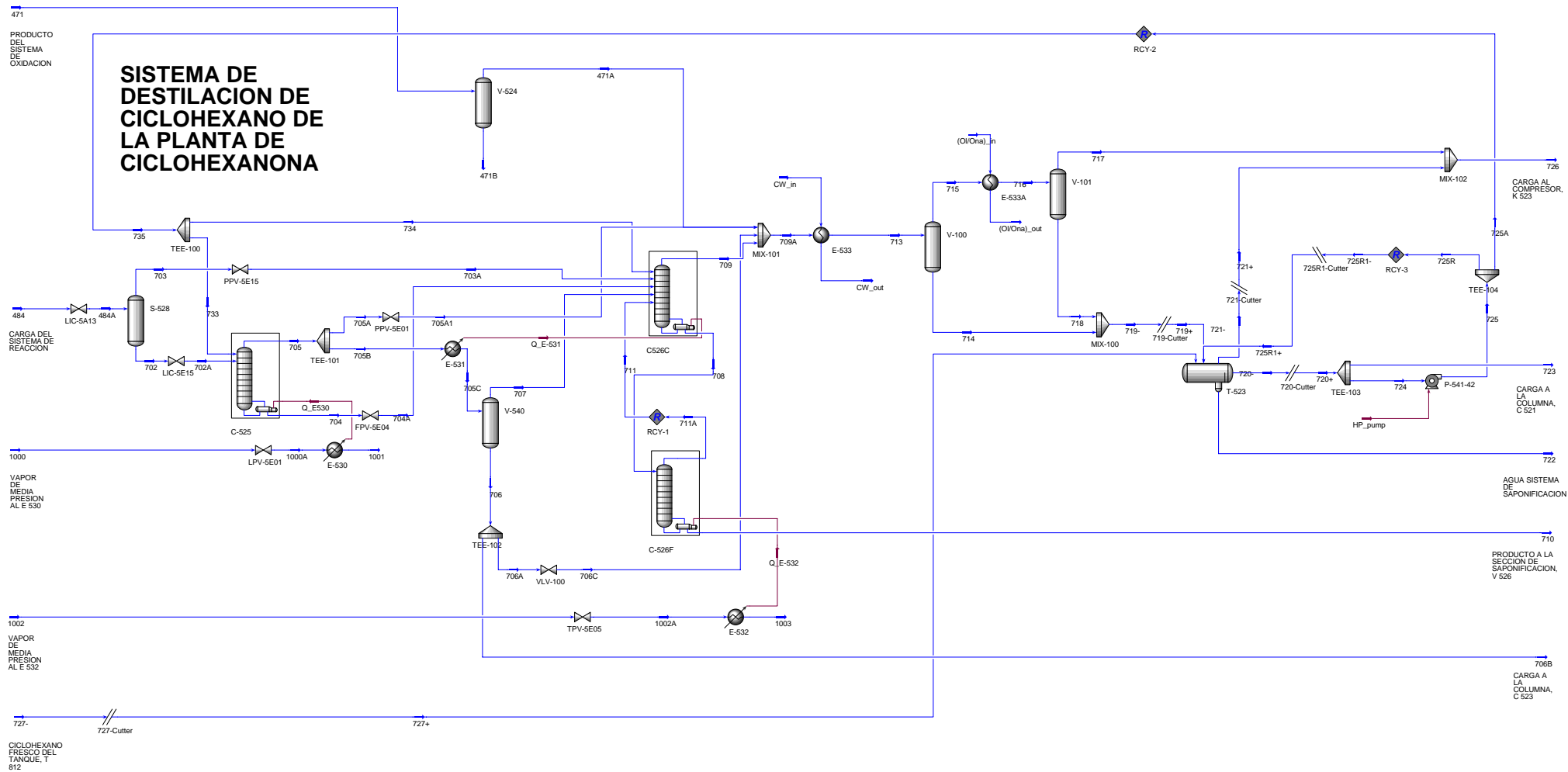


**ANEXO No. 3. Resultados arrojados por el modelo después del proceso de calibración**





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## Workbook: Case (Main)

### Streams

| Name                         | 484          | 703          | 703A       | 702        | 702A         |
|------------------------------|--------------|--------------|------------|------------|--------------|
| Vapour Fraction              | 0.0000       | 1.0000       | 1.0000     | 0.0000     | 0.0111       |
| Temperature (C)              | 141.7 *      | 140.6        | 140.6      | 140.6      | 139.2        |
| Pressure (kg/cm2_g)          | 11.80 *      | 4.600        | 0.4200     | 4.600      | 3.950        |
| Mass Flow (kg/h)             | 9.409e+004 * | 735.7        | 735.7      | 9.336e+004 | 9.336e+004   |
| Mass Density (kg/m3)         | 665.5        | 11.38        | 2.936      | 664.8      | 408.6        |
| Mass Enthalpy (kcal/kg)      | -434.2       | -339.9       | -339.9     | -434.9     | -434.9       |
| Molecular Weight             | 80.85        | 70.88        | 70.88      | 80.94      | 80.94        |
| Comp Mass Frac (Cyclohexane) | 0.9499 *     | 0.9016       | 0.9016     | 0.9503     | 0.9503       |
| Comp Mass Frac (cycHexanol)  | 0.0175 *     | 0.0116       | 0.0116     | 0.0175     | 0.0175       |
| Comp Mass Frac (CC6one)      | 0.0189 *     | 0.0051       | 0.0051     | 0.0191     | 0.0191       |
| Comp Mass Frac (H2O)         | 0.0121 *     | 0.0171       | 0.0171     | 0.0120     | 0.0120       |
| Comp Mass Frac (Oxygen)      | 0.0000 *     | 0.0023       | 0.0023     | 0.0000     | 0.0000       |
| Comp Mass Frac (Nitrogen)    | 0.0010 *     | 0.0610       | 0.0610     | 0.0006     | 0.0006       |
| Comp Mass Frac (CO)          | 0.0000 *     | 0.0007       | 0.0007     | 0.0000     | 0.0000       |
| Comp Mass Frac (1-Pentanol)  | 0.0005 *     | 0.0008       | 0.0008     | 0.0005     | 0.0005       |
| Comp Mass Frac (CC6Peroxide) | 0.0000 *     | 0.0000       | 0.0000     | 0.0000     | 0.0000       |
| Name                         | 484A         | 704          | 705        | 733        | 1000A        |
| Vapour Fraction              | 0.0089       | 0.0000       | 1.0000     | 0.0000     | 1.0000       |
| Temperature (C)              | 140.6        | 136.7        | 131.3      | 46.89      | 214.6        |
| Pressure (kg/cm2_g)          | 4.600        | 3.210 *      | 2.850 *    | 7.249      | 9.210        |
| Mass Flow (kg/h)             | 9.409e+004   | 5.512e+004   | 5.835e+004 | 2.011e+004 | 1.090e+004   |
| Mass Density (kg/m3)         | 458.8        | 670.5        | 9.041      | 755.6      | 4.462        |
| Mass Enthalpy (kcal/kg)      | -434.2       | -423.9       | -354.0     | -443.8     | -3119        |
| Molecular Weight             | 80.85        | 82.98        | 79.83      | 83.20      | 18.02        |
| Comp Mass Frac (Cyclohexane) | 0.9499       | 0.9369       | 0.9776     | 0.9927     | 0.0000 *     |
| Comp Mass Frac (cycHexanol)  | 0.0175       | 0.0244       | 0.0062     | 0.0036     | 0.0000 *     |
| Comp Mass Frac (CC6one)      | 0.0189       | 0.0323       | 0.0000     | 0.0000     | 0.0000 *     |
| Comp Mass Frac (H2O)         | 0.0121       | 0.0062       | 0.0145     | 0.0031     | 1.0000 *     |
| Comp Mass Frac (Oxygen)      | 0.0000       | 0.0000       | 0.0000     | 0.0000     | 0.0000 *     |
| Comp Mass Frac (Nitrogen)    | 0.0010       | 0.0000       | 0.0010     | 0.0004     | 0.0000 *     |
| Comp Mass Frac (CO)          | 0.0000       | 0.0000       | 0.0000     | 0.0000     | 0.0000 *     |
| Comp Mass Frac (1-Pentanol)  | 0.0005       | 0.0002       | 0.0007     | 0.0003     | 0.0000 *     |
| Comp Mass Frac (CC6Peroxide) | 0.0000       | 0.0000       | 0.0000     | 0.0000     | 0.0000 *     |
| Name                         | 1001         | 1000         | 704A       | 734        | 735          |
| Vapour Fraction              | 0.0000 *     | 1.0000       | 0.2809     | 0.0000     | 0.0000       |
| Temperature (C)              | 178.6        | 220.0 *      | 92.25      | 46.89      | 46.89 *      |
| Pressure (kg/cm2_g)          | 8.858        | 12.00 *      | 0.3515 *   | 7.249      | 7.249 *      |
| Mass Flow (kg/h)             | 1.090e+004   | 1.090e+004 * | 5.512e+004 | 2.030e+004 | 4.041e+004 * |
| Mass Density (kg/m3)         | 876.1        | 5.616        | 13.03      | 755.6      | 755.6        |
| Mass Enthalpy (kcal/kg)      | -3624        | -3119        | -423.9     | -443.8     | -443.8       |
| Molecular Weight             | 18.02        | 18.02        | 82.98      | 83.20      | 83.20        |
| Comp Mass Frac (Cyclohexane) | 0.0000       | 0.0000 *     | 0.9369     | 0.9927     | 0.9927 *     |
| Comp Mass Frac (cycHexanol)  | 0.0000       | 0.0000 *     | 0.0244     | 0.0036     | 0.0036 *     |
| Comp Mass Frac (CC6one)      | 0.0000       | 0.0000 *     | 0.0323     | 0.0000     | 0.0000 *     |
| Comp Mass Frac (H2O)         | 1.0000       | 1.0000 *     | 0.0062     | 0.0031     | 0.0031 *     |
| Comp Mass Frac (Oxygen)      | 0.0000       | 0.0000 *     | 0.0000     | 0.0000     | 0.0000 *     |
| Comp Mass Frac (Nitrogen)    | 0.0000       | 0.0000 *     | 0.0000     | 0.0004     | 0.0004 *     |
| Comp Mass Frac (CO)          | 0.0000       | 0.0000 *     | 0.0000     | 0.0000     | 0.0000 *     |
| Comp Mass Frac (1-Pentanol)  | 0.0000       | 0.0000 *     | 0.0002     | 0.0003     | 0.0003 *     |
| Comp Mass Frac (CC6Peroxide) | 0.0000       | 0.0000 *     | 0.0000     | 0.0000     | 0.0000 *     |



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## Workbook: Case (Main) (continued)

### Streams (continued)

| Name                         | 705A     | 707        | 706        | 709        | 708     |
|------------------------------|----------|------------|------------|------------|---------|
| Vapour Fraction              | 1.0000   | 1.0000     | 0.0000     | 1.0000     | 0.0000  |
| Temperature (C)              | 131.3    | 118.0      | 118.0      | 92.18      | 103.3   |
| Pressure (kg/cm2_g)          | 2.850    | 2.830      | 2.830      | 0.4043 *   | 0.5709  |
| Mass Flow (kg/h)             | 6418     | 215.5      | 5.171e+004 | 7.296e+004 | 8908    |
| Mass Density (kg/m3)         | 9.041    | 7.645      | 687.0      | 3.822      | 758.2   |
| Mass Enthalpy (kcal/kg)      | -354.0   | -324.7     | -446.9     | -343.5     | -571.3  |
| Molecular Weight             | 79.83    | 65.63      | 79.90      | 82.35      | 83.72   |
| Comp Mass Frac (Cyclohexane) | 0.9776   | 0.8669     | 0.9780     | 0.9897     | 0.6098  |
| Comp Mass Frac (cycHexanol)  | 0.0062   | 0.0034     | 0.0062     | 0.0034     | 0.1497  |
| Comp Mass Frac (CC6one)      | 0.0000   | 0.0000     | 0.0000     | 0.0000     | 0.2236  |
| Comp Mass Frac (H2O)         | 0.0145   | 0.0155     | 0.0145     | 0.0055     | 0.0166  |
| Comp Mass Frac (Oxygen)      | 0.0000   | 0.0031     | 0.0000     | 0.0000     | 0.0000  |
| Comp Mass Frac (Nitrogen)    | 0.0010   | 0.1091     | 0.0006     | 0.0011     | 0.0000  |
| Comp Mass Frac (CO)          | 0.0000   | 0.0012     | 0.0000     | 0.0000     | 0.0000  |
| Comp Mass Frac (1-Pentanol)  | 0.0007   | 0.0009     | 0.0007     | 0.0002     | 0.0003  |
| Comp Mass Frac (CC6Peroxide) | 0.0000   | 0.0000     | 0.0000     | 0.0000     | 0.0000  |
| Name                         | 711A     | 710        | 711        | 1002       | 1002A   |
| Vapour Fraction              | 1.0000   | 0.0000     | 1.0000     | 1.0000     | 1.0000  |
| Temperature (C)              | 103.4    | 133.4      | 103.4 *    | 220.0 *    | 210.9   |
| Pressure (kg/cm2_g)          | 0.5709   | 0.6039 *   | 0.5709 *   | 12.00 *    | 7.340 * |
| Mass Flow (kg/h)             | 5517     | 3391       | 5504 *     | 1132 *     | 1132    |
| Mass Density (kg/m3)         | 3.922    | 809.6      | 3.920      | 5.616      | 3.675   |
| Mass Enthalpy (kcal/kg)      | -408.6   | -664.2     | -408.9     | -3119      | -3119   |
| Molecular Weight             | 78.05    | 94.95      | 78.03      | 18.02      | 18.02   |
| Comp Mass Frac (Cyclohexane) | 0.9098   | 0.1216     | 0.9096 *   | 0.0000 *   | 0.0000  |
| Comp Mass Frac (cycHexanol)  | 0.0279   | 0.3477     | 0.0279 *   | 0.0000 *   | 0.0000  |
| Comp Mass Frac (CC6one)      | 0.0381   | 0.5254     | 0.0382 *   | 0.0000 *   | 0.0000  |
| Comp Mass Frac (H2O)         | 0.0240   | 0.0046     | 0.0241 *   | 1.0000 *   | 1.0000  |
| Comp Mass Frac (Oxygen)      | 0.0000   | 0.0000     | 0.0000 *   | 0.0000 *   | 0.0000  |
| Comp Mass Frac (Nitrogen)    | 0.0000   | 0.0000     | 0.0000 *   | 0.0000 *   | 0.0000  |
| Comp Mass Frac (CO)          | 0.0000   | 0.0000     | 0.0000 *   | 0.0000 *   | 0.0000  |
| Comp Mass Frac (1-Pentanol)  | 0.0001   | 0.0006     | 0.0001 *   | 0.0000 *   | 0.0000  |
| Comp Mass Frac (CC6Peroxide) | 0.0000   | 0.0000     | 0.0000 *   | 0.0000 *   | 0.0000  |
| Name                         | 1003     | CW_in      | CW_out     | 713        | 715     |
| Vapour Fraction              | 0.0000 * | 0.0000     | 0.0000     | 0.0039     | 1.0000  |
| Temperature (C)              | 169.7    | 31.90 *    | 44.97      | 46.78      | 46.78   |
| Pressure (kg/cm2_g)          | 6.988    | 4.500 *    | 3.500 *    | 0.4037     | 0.4037  |
| Mass Flow (kg/h)             | 1132     | 6.687e+005 | 6.687e+005 | 8.177e+004 | 158.2   |
| Mass Density (kg/m3)         | 884.9    | 1002       | 992.3      | 449.9      | 2.145   |
| Mass Enthalpy (kcal/kg)      | -3633    | -3773      | -3760      | -454.8     | -170.7  |
| Molecular Weight             | 18.02    | 18.02      | 18.02      | 82.01      | 40.49   |
| Comp Mass Frac (Cyclohexane) | 0.0000   | 0.0000 *   | 0.0000     | 0.9880     | 0.4588  |
| Comp Mass Frac (cycHexanol)  | 0.0000   | 0.0000 *   | 0.0000     | 0.0037     | 0.0003  |
| Comp Mass Frac (CC6one)      | 0.0000   | 0.0000 *   | 0.0000     | 0.0000     | 0.0000  |
| Comp Mass Frac (H2O)         | 1.0000   | 1.0000 *   | 1.0000     | 0.0065     | 0.0014  |
| Comp Mass Frac (Oxygen)      | 0.0000   | 0.0000 *   | 0.0000     | 0.0000     | 0.0197  |
| Comp Mass Frac (Nitrogen)    | 0.0000   | 0.0000 *   | 0.0000     | 0.0014     | 0.5075  |
| Comp Mass Frac (CO)          | 0.0000   | 0.0000 *   | 0.0000     | 0.0000     | 0.0122  |
| Comp Mass Frac (1-Pentanol)  | 0.0000   | 0.0000 *   | 0.0000     | 0.0003     | 0.0001  |
| Comp Mass Frac (CC6Peroxide) | 0.0000   | 0.0000 *   | 0.0000     | 0.0000     | 0.0000  |



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## Workbook: Case (Main) (continued)

### Streams (continued)

| Name                         | 714        | 716        | (OI/Ona)_in  | (OI/Ona)_out | 717        |
|------------------------------|------------|------------|--------------|--------------|------------|
| Vapour Fraction              | 0.0000     | 0.8528     | 0.0000       | 0.0000       | 1.0000     |
| Temperature (C)              | 46.78      | 24.70      | 12.00 *      | 22.31        | 24.70      |
| Pressure (kg/cm2_g)          | 0.4037     | 0.3992     | 12.00 *      | 12.00        | 0.3992     |
| Mass Flow (kg/h)             | 8.162e+004 | 158.2      | 1200 *       | 1200         | 110.6      |
| Mass Density (kg/m3)         | 756.0      | 2.690      | 918.6        | 908.9        | 1.881      |
| Mass Enthalpy (kcal/kg)      | -455.4     | -205.2     | -688.2       | -683.6       | -97.24     |
| Molecular Weight             | 82.17      | 40.49      | 95.58        | 95.58        | 33.17      |
| Comp Mass Frac (Cyclohexane) | 0.9890     | 0.4588     | 0.2000 *     | 0.2000       | 0.2279     |
| Comp Mass Frac (cycHexanol)  | 0.0037     | 0.0003     | 0.3200 *     | 0.3200       | 0.0000     |
| Comp Mass Frac (CC6one)      | 0.0000     | 0.0000     | 0.4800 *     | 0.4800       | 0.0000     |
| Comp Mass Frac (H2O)         | 0.0065     | 0.0014     | 0.0000 *     | 0.0000       | 0.0003     |
| Comp Mass Frac (Oxygen)      | 0.0000     | 0.0197     | 0.0000 *     | 0.0000       | 0.0282     |
| Comp Mass Frac (Nitrogen)    | 0.0005     | 0.5075     | 0.0000 *     | 0.0000       | 0.7261     |
| Comp Mass Frac (CO)          | 0.0000     | 0.0122     | 0.0000 *     | 0.0000       | 0.0175     |
| Comp Mass Frac (1-Pentanol)  | 0.0003     | 0.0001     | 0.0000 *     | 0.0000       | 0.0000     |
| Comp Mass Frac (CC6Peroxide) | 0.0000     | 0.0000     | 0.0000 *     | 0.0000       | 0.0000     |
| Name                         | 718        | 719-       | 705C         | 705B         | 709A       |
| Vapour Fraction              | 0.0000     | 0.0000     | 0.0050       | 1.0000       | 0.9894     |
| Temperature (C)              | 24.70      | 46.76      | 118.0        | 131.3        | 92.16      |
| Pressure (kg/cm2_g)          | 0.3992     | 0.3992     | 2.830        | 2.850        | 0.4043     |
| Mass Flow (kg/h)             | 47.68      | 8.166e+004 | 5.193e+004   | 5.193e+004   | 8.177e+004 |
| Mass Density (kg/m3)         | 775.2      | 755.1      | 501.9        | 9.041        | 3.847      |
| Mass Enthalpy (kcal/kg)      | -455.5     | -455.4     | -446.4       | -354.0       | -347.1     |
| Molecular Weight             | 82.89      | 82.17      | 79.83        | 79.83        | 82.01      |
| Comp Mass Frac (Cyclohexane) | 0.9943     | 0.9890     | 0.9776       | 0.9776       | 0.9880     |
| Comp Mass Frac (cycHexanol)  | 0.0011     | 0.0037     | 0.0062       | 0.0062       | 0.0037     |
| Comp Mass Frac (CC6one)      | 0.0000     | 0.0000     | 0.0000       | 0.0000       | 0.0000     |
| Comp Mass Frac (H2O)         | 0.0039     | 0.0065     | 0.0145       | 0.0145       | 0.0065     |
| Comp Mass Frac (Oxygen)      | 0.0000     | 0.0000     | 0.0000       | 0.0000       | 0.0000     |
| Comp Mass Frac (Nitrogen)    | 0.0005     | 0.0005     | 0.0010       | 0.0010       | 0.0014     |
| Comp Mass Frac (CO)          | 0.0000     | 0.0000     | 0.0000       | 0.0000       | 0.0000     |
| Comp Mass Frac (1-Pentanol)  | 0.0002     | 0.0003     | 0.0007       | 0.0007       | 0.0003     |
| Comp Mass Frac (CC6Peroxide) | 0.0000     | 0.0000     | 0.0000       | 0.0000       | 0.0000     |
| Name                         | 706A       | 706B       | 471          | 471A         | 471B       |
| Vapour Fraction              | 0.0000     | 0.0000     | 0.0011       | 1.0000       | 0.0000     |
| Temperature (C)              | 118.0      | 118.0 *    | 61.50 *      | 61.48        | 61.48      |
| Pressure (kg/cm2_g)          | 2.830      | 2.830      | 1.500 *      | 1.300        | 1.300      |
| Mass Flow (kg/h)             | 2327       | 4.939e+004 | 9.409e+004 * | 66.46        | 9.403e+004 |
| Mass Density (kg/m3)         | 687.0      | 687.0      | 673.1        | 3.382        | 746.7      |
| Mass Enthalpy (kcal/kg)      | -446.9     | -446.9     | -435.6       | -178.2       | -435.8     |
| Molecular Weight             | 79.90      | 79.90      | 84.80        | 41.12        | 84.86      |
| Comp Mass Frac (Cyclohexane) | 0.9780     | 0.9780     | 0.9537 *     | 0.4732       | 0.9540     |
| Comp Mass Frac (cycHexanol)  | 0.0062     | 0.0062     | 0.0079 *     | 0.0008       | 0.0079     |
| Comp Mass Frac (CC6one)      | 0.0000     | 0.0000     | 0.0034 *     | 0.0002       | 0.0034     |
| Comp Mass Frac (H2O)         | 0.0145     | 0.0145     | 0.0003 *     | 0.0001       | 0.0003     |
| Comp Mass Frac (Oxygen)      | 0.0000     | 0.0000     | 0.0000 *     | 0.0190       | 0.0000     |
| Comp Mass Frac (Nitrogen)    | 0.0006     | 0.0006     | 0.0010 *     | 0.4833       | 0.0007     |
| Comp Mass Frac (CO)          | 0.0000     | 0.0000     | 0.0000 *     | 0.0233       | 0.0000     |
| Comp Mass Frac (1-Pentanol)  | 0.0007     | 0.0007     | 0.0000 *     | 0.0000       | 0.0000     |
| Comp Mass Frac (CC6Peroxide) | 0.0000     | 0.0000     | 0.0336 *     | 0.0000       | 0.0336     |



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## Workbook: Case (Main) (continued)

### Streams (continued)

| Name                         | 705A1      | 720-       | 721-       | 722      | 723        |
|------------------------------|------------|------------|------------|----------|------------|
| Vapour Fraction              | 1.0000     | 0.0000     | 1.0000     | 0.0000   | 0.0000     |
| Temperature (C)              | 131.3      | 46.28      | 46.28      | 46.28    | 46.28      |
| Pressure (kg/cm2_g)          | 0.4043 *   | 0.3992     | 0.3992     | 0.3992   | 0.3992     |
| Mass Flow (kg/h)             | 6418       | 8.771e+004 | 0.0000     | 271.1    | 4.471e+004 |
| Mass Density (kg/m3)         | 3.347      | 755.2      | 3.584      | 991.1    | 755.2      |
| Mass Enthalpy (kcal/kg)      | -354.0     | -444.1     | -530.8     | -3756    | -444.1     |
| Molecular Weight             | 79.83      | 83.20      | 67.76      | 18.03    | 83.20      |
| Comp Mass Frac (Cyclohexane) | 0.9776     | 0.9927     | 0.9336     | 0.0000   | 0.9927     |
| Comp Mass Frac (cycHexanol)  | 0.0062     | 0.0036     | 0.0005     | 0.0009   | 0.0036     |
| Comp Mass Frac (CC6one)      | 0.0000     | 0.0000     | 0.0000     | 0.0000   | 0.0000     |
| Comp Mass Frac (H2O)         | 0.0145     | 0.0031     | 0.0659     | 0.9991   | 0.0031     |
| Comp Mass Frac (Oxygen)      | 0.0000     | 0.0000     | 0.0000     | 0.0000   | 0.0000     |
| Comp Mass Frac (Nitrogen)    | 0.0010     | 0.0004     | 0.0000     | 0.0000   | 0.0004     |
| Comp Mass Frac (CO)          | 0.0000     | 0.0000     | 0.0000     | 0.0000   | 0.0000     |
| Comp Mass Frac (1-Pentanol)  | 0.0007     | 0.0003     | 0.0000     | 0.0000   | 0.0003     |
| Comp Mass Frac (CC6Peroxide) | 0.0000     | *** *      | *** *      | *** *    | 0.0000     |
| Name                         | 724        | 725        | 726        | 727-     | 706C       |
| Vapour Fraction              | 0.0000     | 0.0000     | 1.0000     | 0.0000   | 0.1560     |
| Temperature (C)              | 46.28      | 46.90      | 24.70      | 35.00 *  | 92.03      |
| Pressure (kg/cm2_g)          | 0.3992     | 7.249      | 0.3992     | 2.000 *  | 0.4043 *   |
| Mass Flow (kg/h)             | 4.300e+004 | 4.300e+004 | 110.6      | 3735 *   | 2327       |
| Mass Density (kg/m3)         | 755.2      | 755.6      | 1.881      | 764.5    | 23.14      |
| Mass Enthalpy (kcal/kg)      | -444.1     | -443.8     | -97.24     | -437.6   | -446.9     |
| Molecular Weight             | 83.20      | 83.20      | 33.17      | 84.16    | 79.90      |
| Comp Mass Frac (Cyclohexane) | 0.9927     | 0.9927     | 0.2279     | 1.0000 * | 0.9780     |
| Comp Mass Frac (cycHexanol)  | 0.0036     | 0.0036     | 0.0000     | 0.0000 * | 0.0062     |
| Comp Mass Frac (CC6one)      | 0.0000     | 0.0000     | 0.0000     | 0.0000 * | 0.0000     |
| Comp Mass Frac (H2O)         | 0.0031     | 0.0031     | 0.0003     | 0.0000 * | 0.0145     |
| Comp Mass Frac (Oxygen)      | 0.0000     | 0.0000     | 0.0282     | 0.0000 * | 0.0000     |
| Comp Mass Frac (Nitrogen)    | 0.0004     | 0.0004     | 0.7261     | 0.0000 * | 0.0006     |
| Comp Mass Frac (CO)          | 0.0000     | 0.0000     | 0.0175     | 0.0000 * | 0.0000     |
| Comp Mass Frac (1-Pentanol)  | 0.0003     | 0.0003     | 0.0000     | 0.0000 * | 0.0007     |
| Comp Mass Frac (CC6Peroxide) | 0.0000     | 0.0000     | 0.0000     | 0.0000 * | 0.0000     |
| Name                         | 720+       | 721+       | 719+       | 725R1-   | 725R1+     |
| Vapour Fraction              | 0.0000     | 0.0000     | 0.0000     | 0.0000   | 0.0000     |
| Temperature (C)              | 46.28      | 46.28      | 46.76      | 46.89 *  | 46.89      |
| Pressure (kg/cm2_g)          | 0.3992     | 0.3992     | 0.3992     | 7.249 *  | 7.249      |
| Mass Flow (kg/h)             | 8.771e+004 | 0.0000     | 8.166e+004 | 2579     | 2579       |
| Mass Density (kg/m3)         | 755.2      | 777.5      | 755.4      | 755.6    | 755.6      |
| Mass Enthalpy (kcal/kg)      | -444.1     | -652.1     | -455.4     | -443.8   | -443.8     |
| Molecular Weight             | 83.20      | 67.76      | 82.17      | 83.20    | 83.20      |
| Comp Mass Frac (Cyclohexane) | 0.9927     | 0.9336     | 0.9890     | 0.9927 * | 0.9927     |
| Comp Mass Frac (cycHexanol)  | 0.0036     | 0.0005     | 0.0037     | 0.0036 * | 0.0036     |
| Comp Mass Frac (CC6one)      | 0.0000     | 0.0000     | 0.0000     | 0.0000 * | 0.0000     |
| Comp Mass Frac (H2O)         | 0.0031     | 0.0659     | 0.0065     | 0.0031 * | 0.0031     |
| Comp Mass Frac (Oxygen)      | 0.0000     | 0.0000     | 0.0000     | 0.0000 * | 0.0000     |
| Comp Mass Frac (Nitrogen)    | 0.0004     | 0.0000     | 0.0005     | 0.0004 * | 0.0004     |
| Comp Mass Frac (CO)          | 0.0000     | 0.0000     | 0.0000     | 0.0000 * | 0.0000     |
| Comp Mass Frac (1-Pentanol)  | 0.0003     | 0.0000     | 0.0003     | 0.0003 * | 0.0003     |
| Comp Mass Frac (CC6Peroxide) | 0.0000     | 0.0000     | *** *      | 0.0000 * | *** *      |