

Příloha A.4 - Aspen report - model PFR reaktoru s Ni katalyzátorem

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+
+ + ASPEN PLUS CALCULATION REPORT + +
+
+ +

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ASPEN TECHNOLOGY, INC.
781/221-6400

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PLATFORM: WINDOWS
VERSION: 36.0 Build 249
INSTALLATION:

JUNE 21, 2020
SUNDAY
4:52:18 P.M.

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RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO CZECH TECHNICAL UNIVERSI

TYPE OF RUN: EDIT

INPUT FILE NAME: _4032zom.inm

INPUT PROBLEM DATA FILE NAME : _4032zom
OUTPUT PROBLEM DATA FILE NAME: _4744dir
LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:

NUMBER OF FILE RECORDS (PSIZE) = 0
NUMBER OF IN-CORE RECORDS = 256
PSIZE NEEDED FOR SIMULATION = 1

CALLING PROGRAM NAME:

apmain

LOCATED IN: C:\Program Files (x86)\AspenTech\Aspen Plus V10.0\Engine\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

| STREAM IN | SOURCE ---- | DEST PFREAC | STREAM OUT | SOURCE PFREAC | DEST ---- |
|--------------|----------------|----------------|---------------|------------------|--------------|
|--------------|----------------|----------------|---------------|------------------|--------------|

FLOWSHEET CONNECTIVITY BY BLOCKS

| BLOCK PFREAC | INLETS IN | OUTLETS OUT |
|-----------------|--------------|----------------|
|-----------------|--------------|----------------|

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
PFREAC

OVERALL FLOWSHEET BALANCE

| *** MASS AND ENERGY BALANCE *** | | | | |
|---------------------------------------|----------|--------------|------------|----------------|
| | IN | OUT | GENERATION | RELATIVE DIFF. |
| CONVENTIONAL COMPONENTS (KMOL/HR) | | | | |
| METHA-01 | 0.00000 | 0.199664 | 0.199664 | 0.00000 |
| CARBO-01 | 0.199718 | 0.547167E-04 | -0.199664 | -0.276522E-16 |
| WATER | 0.00000 | 0.399327 | 0.399327 | 0.00000 |
| HYDRO-01 | 0.798874 | 0.218867E-03 | -0.798655 | 0.138193E-15 |
| CARBO-02 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| TOTAL BALANCE | | | | |
| MOLE (KMOL/HR) | 0.998592 | 0.599265 | -0.399327 | 0.111179E-15 |
| MASS (KG/HR) | 10.4000 | 10.4000 | | 0.170804E-15 |
| ENTHALPY (CAL/SEC) | -4633.97 | -6991.67 | | 0.337216 |

| *** CO2 EQUIVALENT SUMMARY *** | | | |
|--------------------------------|---------|-------|--|
| FEED STREAMS CO2E | 8.78957 | KG/HR | |
| PRODUCT STREAMS CO2E | 80.0813 | KG/HR | |
| NET STREAMS CO2E PRODUCTION | 71.2918 | KG/HR | |
| UTILITIES CO2E PRODUCTION | 0.00000 | KG/HR | |
| TOTAL CO2E PRODUCTION | 71.2918 | KG/HR | |

PHYSICAL PROPERTIES SECTION

COMPONENTS

| ID | TYPE | ALIAS | NAME |
|----------|------|-------|-----------------|
| METHA-01 | C | CH4 | METHANE |
| CARBO-01 | C | CO2 | CARBON-DIOXIDE |
| WATER | C | H2O | WATER |
| HYDRO-01 | C | H2 | HYDROGEN |
| CARBO-02 | C | CO | CARBON-MONOXIDE |

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REACTION SECTION

REACTION: R-1 TYPE: GENERAL

Unit operations referencing this reaction model:

Reactor Name: PFREAC Block Type: RPLUG

U-O-S BLOCK SECTION

BLOCK: PFREAC MODEL: RPLUG

INLET STREAM: IN
OUTLET STREAM: OUT
PROPERTY OPTION SET: RKSMHV2 RKS-MHV2 EQUATION OF STATE

| | *** MASS AND ENERGY BALANCE *** | | | |
|---------------------|---------------------------------|----------|------------|----------------|
| | IN | OUT | GENERATION | RELATIVE DIFF. |
| TOTAL BALANCE | | | | |
| MOLE (KMOL/HR) | 0.998592 | 0.599265 | -0.399327 | 0.111179E-15 |
| MASS (KG/HR) | 10.4000 | 10.4000 | | 0.170804E-15 |
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| TOTAL CO2E PRODUCTION | 71.2918 | KG/HR |

*** INPUT DATA ***

REACTOR TYPE:

SPECIFIED TEMPERATURE

TWO-PHASE

| | | |
|----------------------------|-------|-------------|
| REACTOR TUBE LENGTH | METER | 1.0000 |
| REACTOR DIAMETER | METER | 0.30000 |
| REACTOR RISE | METER | 0.0000 |
| NUMBER OF REACTOR TUBES | | 1 |
| REACTOR VOLUME | L | 70.686 |
| PRESSURE DROP OPTION: | | SPECIFIED |
| HOLDUP OPTION: | | NO-SLIP |
| ERROR TOLERANCE | | 0.10000E-03 |
| INTEGRATION METHOD | | GEAR |
| CORRECTOR METHOD | | NEWTON |
| INITIAL STEP SIZE FACTOR | | 0.10000E-01 |
| CORRECTOR TOLERANCE FACTOR | | 0.10000 |
| MAXIMUM NUMBER OF STEPS | | 1000 |

CONSTANT REACTOR TEMPERATURE SET TO THE (MIXED)
INLET PROCESS STREAM TEMPERATURE OF 299.90 C

REACTION PARAGRAPH ID: R-1 TYPE: GENERAL

GLOBAL BASES:

| | |
|--------|------------|
| KBASIS | MOLE-GAMMA |
| CBASIS | MOLARITY |
| SBASIS | GLOBAL |

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U-O-S BLOCK SECTION

BLOCK: PFREAC MODEL: RPLUG (CONTINUED)
STOICHIOMETRY:

| | | | | | | | |
|------------------|---------|----------|---------|----------|---------|----------|---|
| REACTION NUMBER: | 1 | | | | | | |
| SUBSTREAM: MIXED | | | | | | | |
| METHA-01 | 1.0000 | CARBO-01 | -1.0000 | WATER | 2.0000 | HYDRO-01 | - |
| 4.0000 | | | | | | | |
| REACTION NUMBER: | 2 | | | | | | |
| SUBSTREAM: MIXED | | | | | | | |
| CARBO-01 | -1.0000 | WATER | 1.0000 | HYDRO-01 | -1.0000 | CARBO-02 | |
| 1.0000 | | | | | | | |
| REACTION NUMBER: | 3 | | | | | | |
| SUBSTREAM: MIXED | | | | | | | |
| METHA-01 | 1.0000 | WATER | 1.0000 | HYDRO-01 | -3.0000 | CARBO-02 | - |
| 1.0000 | | | | | | | |

REAC-DATA ENTRIES:

| REACTION NO | TYPE | PHASE | DELT C | BASIS |
|-------------|---------|-------|-----------|----------|
| 1 | KINETIC | V | 0.0000 | MOLARITY |
| 2 | KINETIC | V | 900.00 | MOLARITY |
| 3 | KINETIC | V | 0.0000 | MOLARITY |

*** RESULTS ***

| | | |
|-------------------------------|---------|-------------|
| REACTOR DUTY | CAL/SEC | -2357.7 |
| RESIDENCE TIME | HR | 0.12384E-01 |
| REACTOR MINIMUM TEMPERATURE C | | 299.90 |
| REACTOR MAXIMUM TEMPERATURE C | | 299.90 |

*** RESULTS PROFILE (PROCESS STREAM) ***

| LENGTH METER | PRESSURE BAR | TEMPERATURE C | VAPOR FRAC | RES-TIME HR |
|-----------------|-----------------|------------------|------------|----------------|
| 0.0000 | 5.0000 | 299.90 | 1.0000 | 0.0000 |
| 0.10000 | 5.0000 | 299.90 | 1.0000 | 0.11724E-02 |
| 0.20000 | 5.0000 | 299.90 | 1.0000 | 0.24182E-02 |
| 0.30000 | 5.0000 | 299.90 | 1.0000 | 0.36640E-02 |
| 0.40000 | 5.0000 | 299.90 | 1.0000 | 0.49098E-02 |
| 0.50000 | 5.0000 | 299.90 | 1.0000 | 0.61556E-02 |
| 0.60000 | 5.0000 | 299.90 | 1.0000 | 0.74013E-02 |
| 0.70000 | 5.0000 | 299.90 | 1.0000 | 0.86471E-02 |
| 0.80000 | 5.0000 | 299.90 | 1.0000 | 0.98929E-02 |
| 0.90000 | 5.0000 | 299.90 | 1.0000 | 0.11139E-01 |
| 1.0000 | 5.0000 | 299.90 | 1.0000 | 0.12384E-01 |
| LENGTH METER | DUTY CAL/SEC | LIQUID HOLDUP | | |
| 0.0000 | 0.0000 | 0.0000 | | |
| 0.10000 | -2357.7 | 0.0000 | | |
| 0.20000 | -2357.7 | 0.0000 | | |
| 0.30000 | -2357.7 | 0.0000 | | |
| 0.40000 | -2357.7 | 0.0000 | | |
| 0.50000 | -2357.7 | 0.0000 | | |
| 0.60000 | -2357.7 | 0.0000 | | |
| 0.70000 | -2357.7 | 0.0000 | | |
| 0.80000 | -2357.7 | 0.0000 | | |
| 0.90000 | -2357.7 | 0.0000 | | |
| 1.0000 | -2357.7 | 0.0000 | | |

U-O-S BLOCK SECTION

BLOCK: PFREAC MODEL: RPLUG (CONTINUED)

*** TOTAL MOLE FRACTION PROFILE (PROCESS STREAM) ***

| LENGTH METER | METHA-01 | CARBO-01 | WATER | HYDRO-01 |
|-----------------|----------|-------------|---------|-------------|
| 0.0000 | 0.0000 | 0.20000 | 0.0000 | 0.80000 |
| 0.10000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.20000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.30000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.40000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.50000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.60000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.70000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.80000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 0.90000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |
| 1.0000 | 0.33318 | 0.91306E-04 | 0.66636 | 0.36523E-03 |

*** TOTAL MASS FRACTION PROFILE (PROCESS STREAM) ***

| LENGTH METER | METHA-01 | CARBO-01 | WATER | HYDRO-01 |
|-----------------|----------|-------------|---------|-------------|
| 0.0000 | 0.0000 | 0.84515 | 0.0000 | 0.15485 |
| 0.10000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.20000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.30000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.40000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.50000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.60000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.70000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.80000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 0.90000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |
| 1.0000 | 0.30800 | 0.23155E-03 | 0.69173 | 0.42424E-04 |

STREAM SECTION

CO2 H2 IN OUT

| STREAM ID | CO2 | H2 | IN | OUT |
|---------------------|------------|-----------|------------|------------|
| FROM : | ---- | ---- | ---- | PFREAC |
| TO : | ---- | ---- | PFREAC | ---- |
| SUBSTREAM: MIXED | | | | |
| PHASE: VAPOR | | | | |
| COMPONENTS: KMOL/HR | | | | |
| METHA-01 | 0.0 | 0.0 | 0.0 | 0.1997 |
| CARBO-01 | 0.1000 | 0.0 | 0.1997 | 5.4717-05 |
| WATER | 0.0 | 0.0 | 0.0 | 0.3993 |
| HYDRO-01 | 0.0 | 0.4000 | 0.7989 | 2.1887-04 |
| CARBO-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | |
| KMOL/HR | 0.1000 | 0.4000 | 0.9986 | 0.5993 |
| KG/HR | 4.4010 | 0.8064 | 10.4000 | 10.4000 |
| L/MIN | 21.4616 | 85.8304 | 79.5424 | 94.5668 |
| STATE VARIABLES: | | | | |
| TEMP C | 500.0000 | 500.0000 | 299.9000 | 299.8962 |
| PRES BAR | 5.0000 | 5.0000 | 10.0000 | 5.0000 |
| VFRAC | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| LFRAC | 0.0 | 0.0 | 0.0 | 0.0 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | |
| CAL/MOL | -8.8871+04 | 3323.1509 | -1.6706+04 | -4.2002+04 |
| CAL/GM | -2019.3382 | 1648.4865 | -1604.0657 | -2420.1950 |
| CAL/SEC | -2468.6298 | 369.2390 | -4633.9676 | -6991.6745 |
| ENTROPY: | | | | |
| CAL/MOL-K | 7.5482 | 3.4830 | 1.5318 | -9.6462 |
| CAL/GM-K | 0.1715 | 1.7278 | 0.1471 | -0.5558 |
| DENSITY: | | | | |
| MOL/CC | 7.7658-05 | 7.7673-05 | 2.0924-04 | 1.0562-04 |
| GM/CC | 3.4177-03 | 1.5658-04 | 2.1791-03 | 1.8329-03 |
| AVG MW | 44.0098 | 2.0159 | 10.4147 | 17.3546 |

PROBLEM STATUS SECTION

BLOCK STATUS

```
*****  
*  
* Calculations were completed normally  
*  
* All Unit Operation blocks were completed normally  
*  
* All streams were flashed normally  
*  
*****
```