SLURRY HYDROCRACKER PROJECT

Appendix B - VMG Simulation

PREPARED FOR

Frank Nolte, PEng

Worley Limited

PREPARED BY

Team 15: TR Solutions

Jaryl Schmidt, Student

Jose Te Eng Fo, Student

Naira Correia, Student

Xingming Shan, Student

Yichun Zhang, Student

DATE: April 9th, 2020

Table of Contents

B.1 SUMMARY

This Appendix contains all files and information related to the development/design and utilization of the VMG Symmetry simulation of the proposed design. Included files/documents relating to the simulation include current outputs, current and previous simulation files, and a supplementary simulation file for amine unit model estimations.

A total of 50 iterations were completed in simulation development. The thermodynamic model used was the refinery characterization of Advanced Peng Robinson. Simulation development was done through a review of current refinery processing and assistance from our academic advisor.

B.2 SIMULATION OUTPUTS

A copy of the simulation PFD is provided below. A copy of the VMG Symmetry-generated simulation report is included with the simulation supporting files.

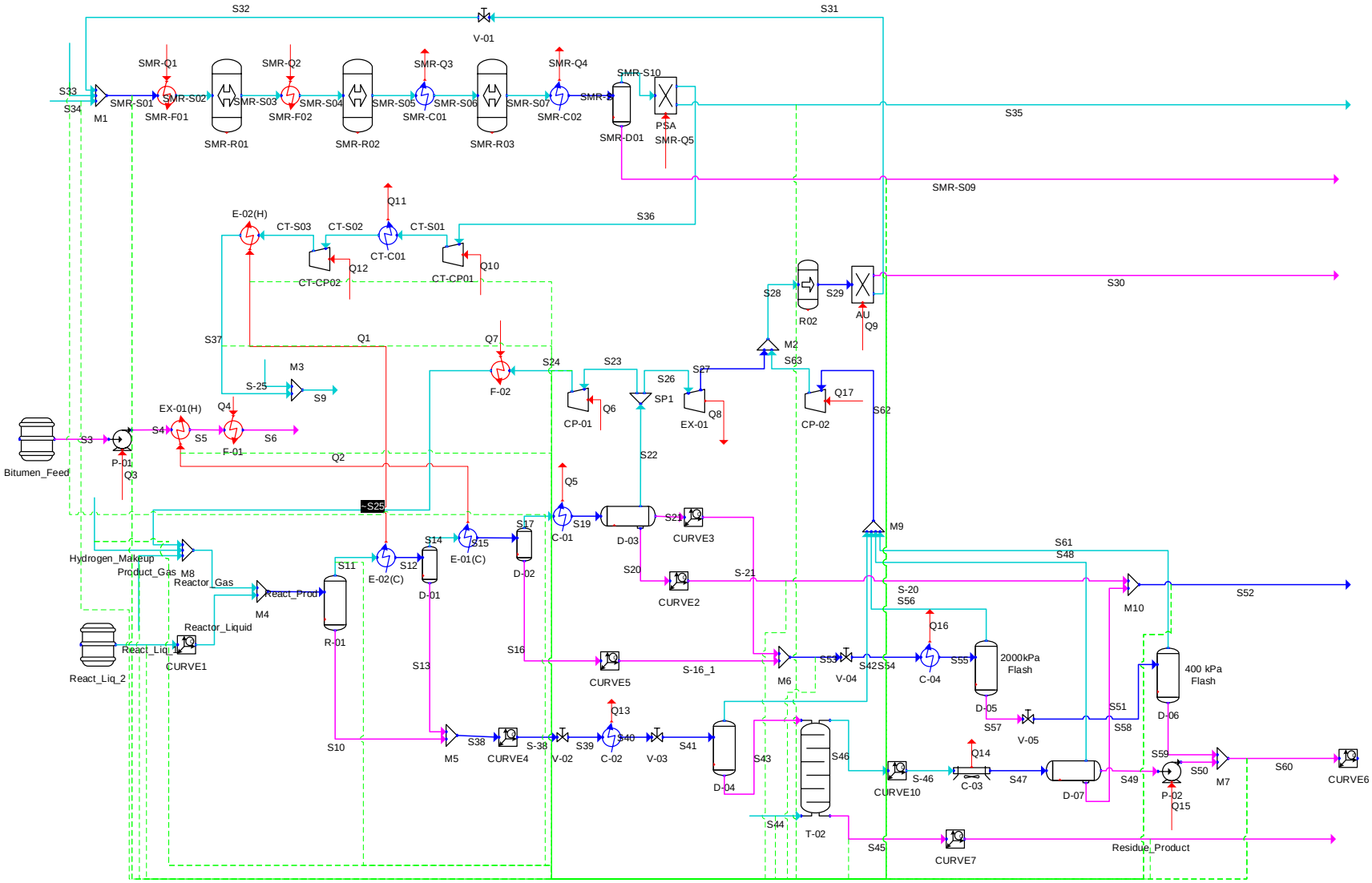

Figure B1. Simulation Process Flow Diagram

B.3 SIMULATION COMPONENTS

Certain simulation components are either not simulated or have not undergone detailed design (due to them being outside the scope of our project).

B.3.1 Bubble Column Reactor

Since the proposed hydrocracker design was based on an existing process, final product composition (using the catalyst of choice) was known, and therefore did not require reactor modelling to predict. As a result, no slurry bubble column reactor was modelled in Symmetry. Instead, the known CANMET product data was characterized in VMG with pseudo components (based on a carbon number distribution). In lieu of a modelled reactor, known liquid and gaseous product streams were mixed in a combined reactor product stream and placed into a two-phase separator to re-create the separation that would occur in the real slurry bubble column reactor.

It was found that most of the liquid product vaporized in the separator, and in conferring with our academic advisor, it was determined that this would be unlikely in the real process. The consequence of this is that our overheads are likely oversized (but this of little concern).

Additionally, VMG Symmetry does not have component support for iron (II) sulfate (the chosen process catalyst), so catalyst flows were not simulated at any time. For operation, it was assumed that catalyst flows would be added to the inlet bitumen stream and would flow out of the column with the liquid product. From there it would be completely removed from the system with the final residue product.

B.3.2 Amine Unit

The amine unit, represented as the component splitter AU, was designed to function like a real amine unit running with MDEA. In this, it separates 100% of the inlet H2S and NH3, and pulls out a small fraction of various other components while respecting appropriate inlet and outlet temperatures. The specific separation percentages were determined by running the inlet through an external amine unit simulation (provided in ChE 464) and converting the results into separation percentages. A copy of the amine unit simulation is provided in the supplemental materials.

B.3.3 Claus Plant

Simulations were not developed for Claus plant operation due to the highly available, well-documented nature of operating data for industrial Claus plants. Values for operation were estimated from literature data.

B.3.4 Steam Methane Reformer & Pressure Swing Adsorber

Since the simulation results regarding H_2 production were significant, it was required to simulate an SMR and a PSA (despite being outside the scope of detailed engineering). Values for SMR and PSA operation were taken from literature in order to ensure inlet and outlet conditions were correct, but specific optimization was never performed for these components.

The specific SMR reactors (SMR-R01, SMR-R02, and SMR-R03) are modelled as equilibrium reactors with the respective hydrocarbon-steam-reforming and water gas shift reactions specified.

B.3.5 Internal Gas Recycle Loop

The loop is required for maintaining high partial pressure of H2. Only basic optimization was performed during development. The target was to have exit vapour composition be 65 mol% (or greater) H2. It was found that increasing the size of the recycle loop positively increased H2 partial pressure but came at the cost of ridiculously high flow rates. The higher flowrates ultimately caused H2 partial pressure to decrease in the overheads, so a balance was struck by keeping the internal recycle fixed at 70 mass% of the total vapour overheads (from the three phase separator).

B.3.6 Conversion Reactor (Hydrotreater)

Due to the presence of sulfur and nitrogen-containing compounds from the stripping system overheads, a hydrotreater was required to prevent these compounds reaching the SMR (as they would poison the catalysts). Reactor R-05 is modelled as a conversion reactor which converts large sulfur and nitrogen containing hydrocarbons (C6 and larger) into hydrogen sulfide, ammonia, carbon dioxide and water. The unit is located just before the amine unit in order to separate out the ammonia and hydrogen sulfide.

B3.7 Product Characterization

Both bitumen feed and reactor liquid product were characterized from boiling curve data and pseudo-component selection (based on carbon number) from VMG Symmetry. Distillation curves of various hydrocarbon products are provided below.

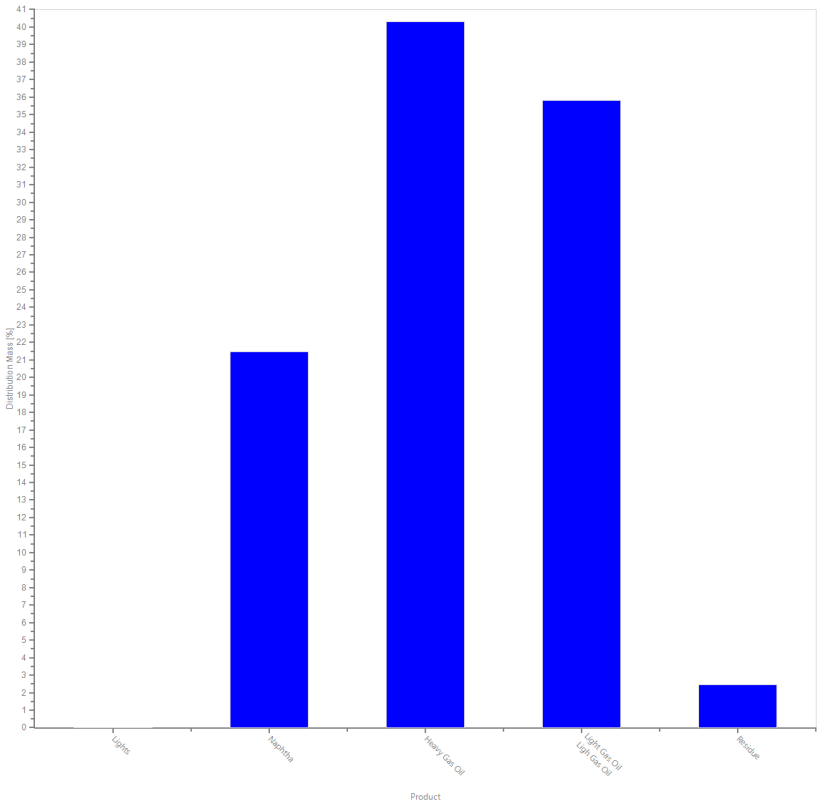

Figure B2. Product distribution of characterized reactor liquid (initial liquid product).

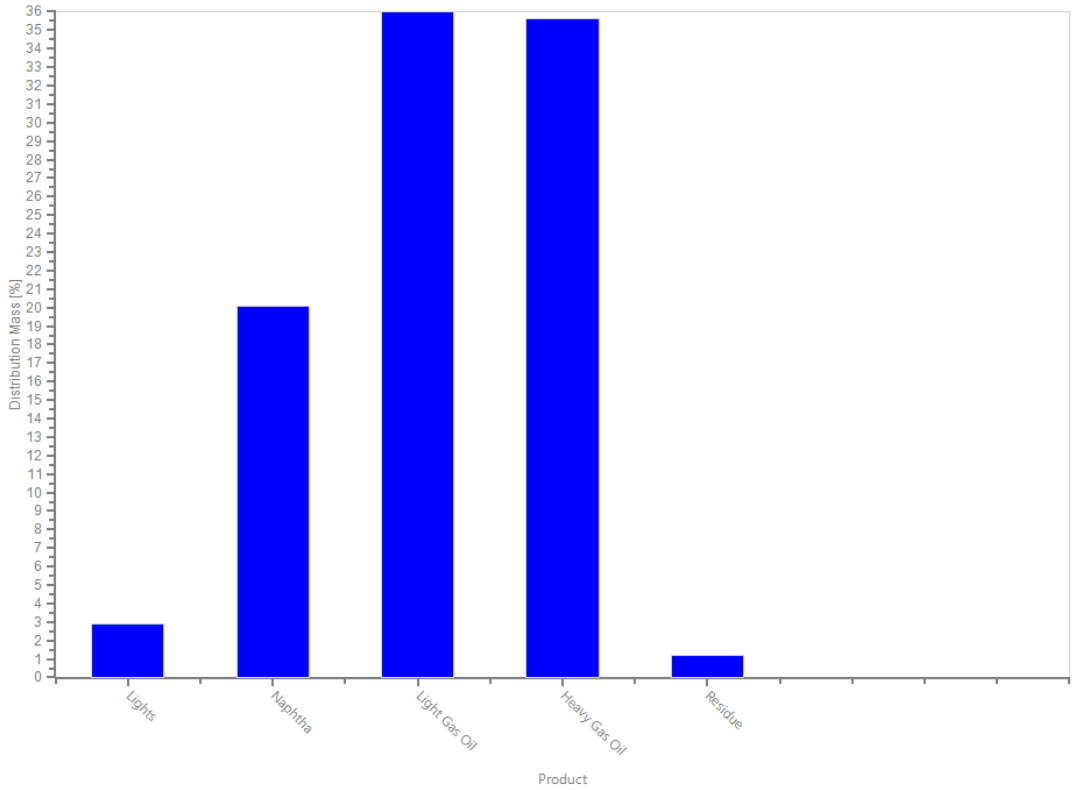

Figure B3. Product distribution of final liquid product.

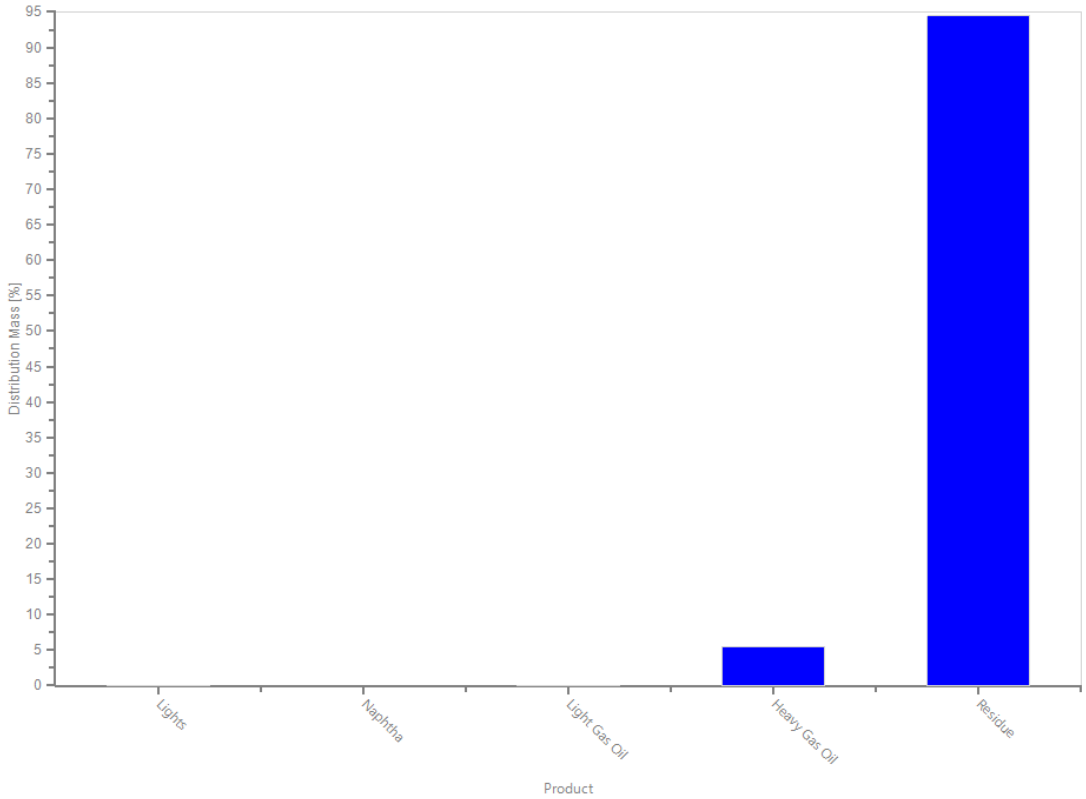

Figure B4. Product distribution of final residue product.

B.4 MODEL VALIDATION

Simulation outputs were validated by comparing a simulation product stream outlet with known material properties from literature. Results comparing simulation outputs with available data are provided in Table B1.

Table B1. Density of Athabasca bitumen vacuum reside (>524°C).

Component	Component Density (SG)
Simulation Results	1.16
Ghasemi et al., 2011	1.06
Difference:	10%

B.5 REFERENCES

Ghasemi, M. & Whitson, C. (2013). Modeling Steam-Assisted Gravity Drainage With a Black-Oil Proxy. *SPE Reservoir Evaluation & Engineering*. 16, 155-171. 10.2118/147072-PA.