

PRO/II CASEBOOK

Vinyl Chloride Monomer (VCM) Plant

ABSTRACT

A PRO/II[®] simulation model of a VCM plant has been completed. It comprises 31 unit operations, which include four columns, three reactor systems, and 6 recycle streams. An advanced extension to the SRK equation of state (SRKM) has been used to model the system thermodynamics. All required product purity specifications are achieved. The model can be used for economic evaluations, setpoint selections for achieving product quality, and as a tool for control system design/revamp.

Casebook #1. Vinyl Chloride Monomer Plant
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INTRODUCTION

A typical vinyl chloride monomer (VCM) plant comprises five sections (as described later in the Process Outline section) which may be simulated as five separate flowsheet sections. Once the flowsheet model of each section has been finalized, they may then be combined for an overall plant simulation. Although the overall plant simulation has 6 recycle loops and is CPU intensive, simulation of individual sections may be sufficient for most needs including training and localized troubleshooting during operations. It is, however, useful to have a tool to investigate interactions between different parts of the plant. For this purpose the application has been extended to simulate the entire plant with all the complexities imposed by the recycle loops. Within the context of the total plant flowsheet, this application emphasizes the purification trains for 1,2-dichloroethane (EDC) and VCM. Simple models have been used for the three reactor systems. This provides a tool for the realistic assessment of VCM plant operations.

This application demonstrates PRO/II's capability to rigorously simulate a flowsheet processing a large number of species in a wide range of concentrations. The chemical species in a VCM plant are generally non-ideal and somewhat polar. The SRKM equation of state (developed at SimSci) has been used to simulate this flowsheet. All of the desired separation efficiencies are achieved.

RELEVANCE OF MODELING VCM PLANTS

There are several possible objectives for the simulation of a VCM plant. For example:

- Tighten VCM product purity specifications for downstream polymerization to PVC;
- Improve heat integration and energy efficiency;
- Establish on-line optimization and control philosophies;
- Debottlenecking;
- Establish emission levels for comparison with environmental targets.

It is necessary to have a simulation model of the plant for assessment of advanced process control applications and improvements. On the basis of this model, it is possible to establish a base case from which achievable improvements in performance can be estimated. The resulting economic benefits can then be evaluated and compared against the cost of implementing the changes. In a similar way, plant bottlenecks and constraints may be investigated.

BACKGROUND

Commercial processes for the production of vinyl chloride from ethylene and chlorine have been operating successfully since the 1950s. These processes include direct chlorination of ethylene to produce EDC followed by pyrolysis of EDC to produce vinyl chloride. Commercial EDC cracking furnaces operate in the 480-550 C range with pressures up to 30-40 atmospheres. Single pass conversion of EDC is in the 50-60% range. This conversion level optimizes costs between coking cycles, utilities and yields. The resulting HCl is recycled to oxychlorination reactors where fresh ethylene reacts with HCl in the presence of oxygen to produce more EDC. Since HCl is totally consumed within the plant and is not a product, this process is often referred to as the "balanced oxychlorination process."

Pyrolysis of EDC is very selective towards VCM. Typical yields of VCM are greater than 95% at EDC conversion levels in the 50-60% range. The byproducts include acetylene, ethylene, methylchloride, butadiene, vinylacetylene, benzene, chloroprene and various other chlorinated hydrocarbons in trace amounts. Many of these chlorinated species are environmentally harmful.

The pyrolysis reactor establishes the yield slate and raw VCM product composition. While there is a high selectivity towards vinyl chloride, the correct prediction of impurities in the reactor feed and byproduct formation in the effluent is important. Some trace species in the feed inhibit the cracking reactions; others serve as promoters. Ninety-nine percent EDC feed purity is desirable. At the other end of the process, a purity of 99.9+% is specified for polymer grade VCM. This is achieved by two means: first, by controlling the cracking process to minimize byproduct formation; second, by proper operation of the VCM purification section to reduce the concentration of various trace contaminants to low ppm levels.

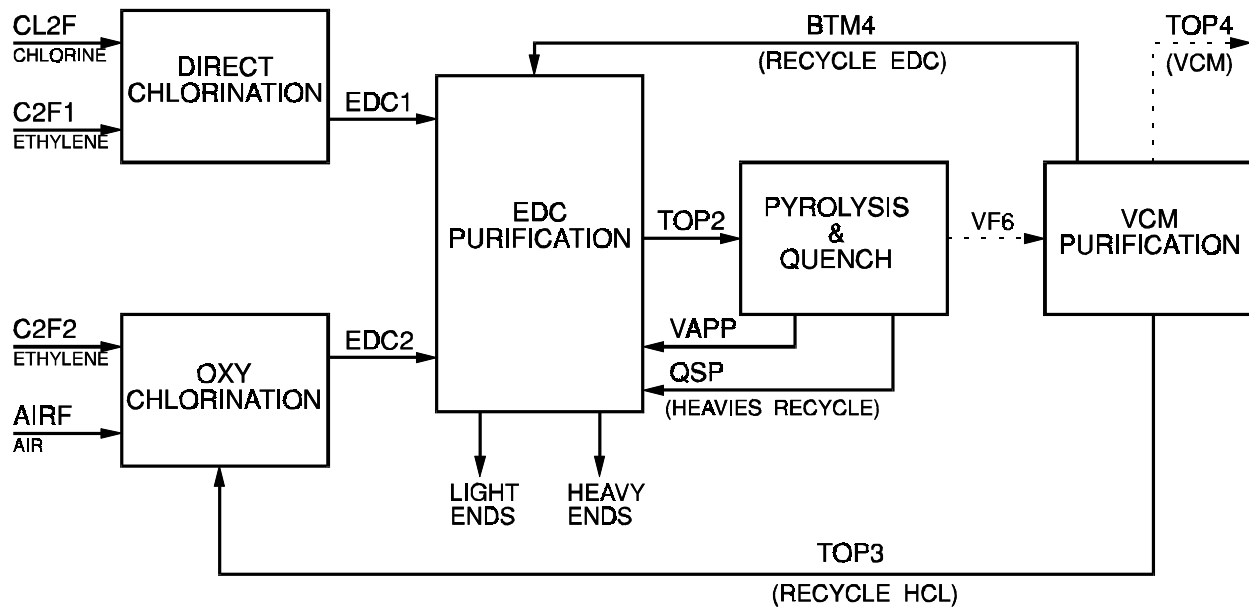
High purity VCM product is necessary for subsequent polymerization to polyvinyl chloride (PVC). For example, the presence of methylchloride and butadiene as impurities in the VCM product interferes with its polymerization to PVC. The typical upper limit to acceptable methyl chloride content in VCM is in the 60-150 ppm range.

PROCESS OUTLINE

An overview of the VCM plant is shown in Figure 1. Each of the five major sections of the plant are shown and discussed in more detail as described below.

- Direct chlorination of ethylene to form EDC. Figure 2.
- Oxychlorination section where ethylene is reacted with recycled HCl and O₂ to form more EDC. Figure 3.
- Purification of EDC. Figure 4.
- Thermal cracking of EDC to form VCM and HCl. The raw VCM product is quenched and cooled. Figure 5.
- Purification of VCM. The HCl formed is recycled to the oxychlorination reactor. Unreacted EDC is recycled to the EDC purification system. Figure 6.

Figure 1 Vinyl Chlorid Monomer (VCM) Plant

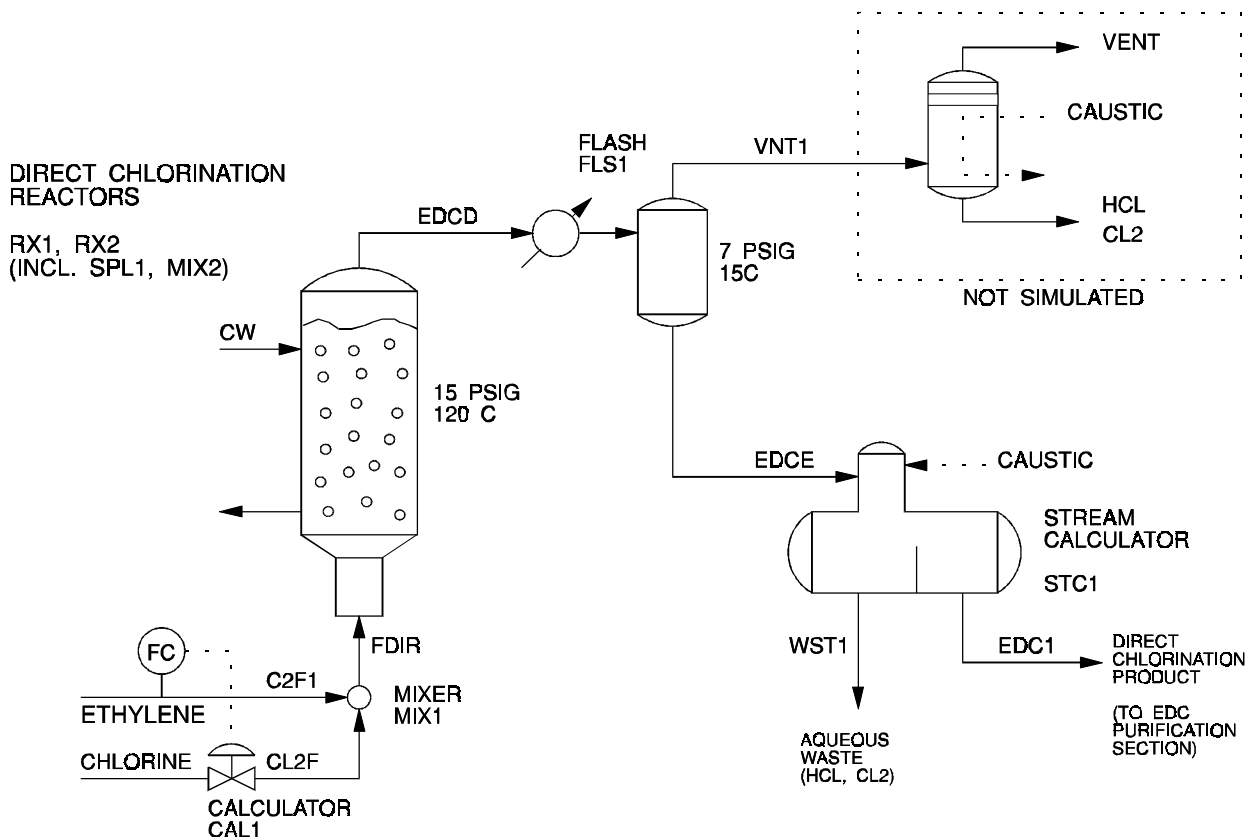


PROCESS DESCRIPTION AND SIMULATION MODEL

Direct Chlorination

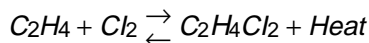
A process flow diagram for this section of the plant is shown below in Figure 2.

Figure 2 Direct Chlorination Section



Reaction

Direct chlorination of ethylene to EDC is conducted in a liquid phase reactor by intimately mixing ethylene and chlorine in liquid EDC. The operating conditions are 120-150 C and 0-30 psig pressure.

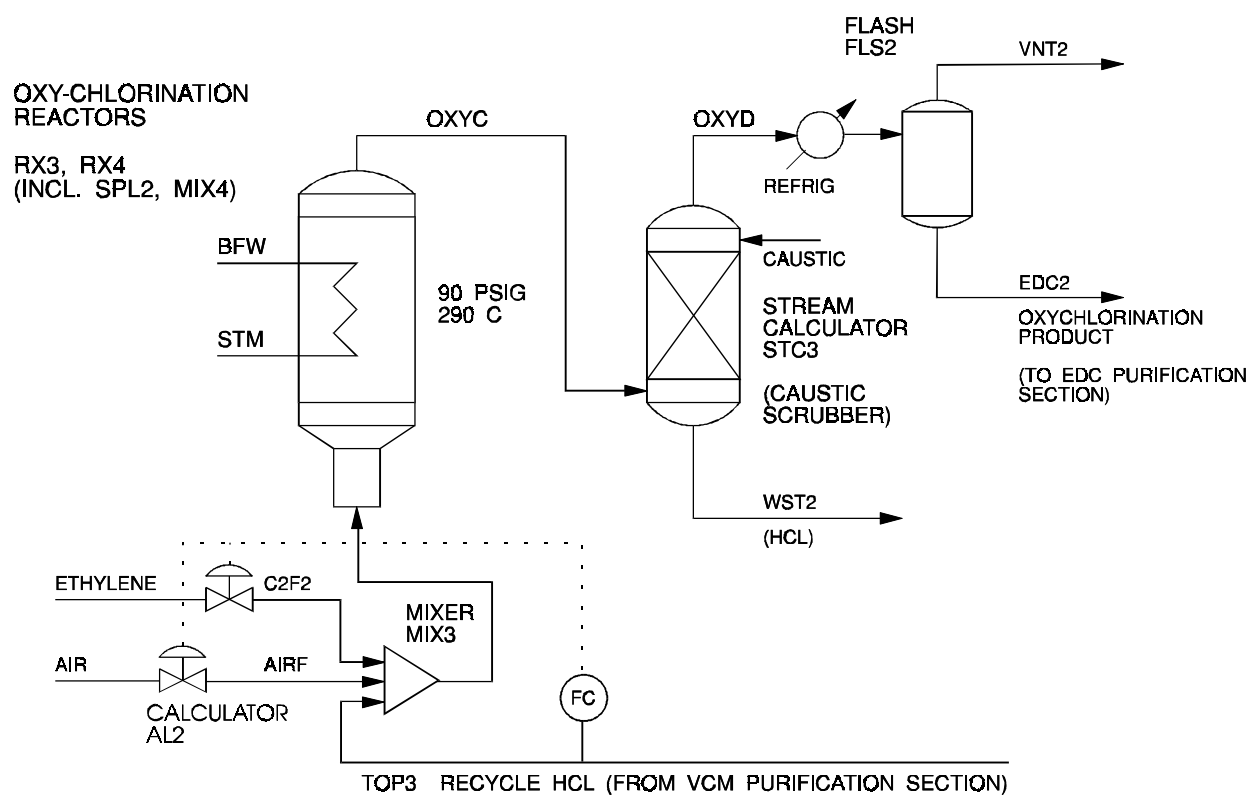


The heat of reaction is removed by circulating cooling water or by recirculating the liquid EDC through external coolers. In most commercial processes ferric chloride is used as a catalyst. The reactions are often run with a small excess of ethylene to maintain the vent gases fuel-rich for incineration. Conversion of the lean component is usually 100 % with selectivity for EDC greater than 99 %.

EDC Product Treatment

There are two major variations to recover the EDC product. In some designs, EDC is withdrawn as a liquid; in others, the heat of reaction is utilized to boil off sufficient EDC as a vapor product. In this application, product EDC is removed as a vapor phase which also contains unreacted ethylene and chlorine. Liquid EDC is recovered by two stage condensation. Any HCl and Cl₂ remaining in the vent gas are removed in a caustic scrubber. The liquid EDC goes to a caustic wash vessel where dissolved chlorine and byproduct HCl are removed. EDC overflows from the caustic wash to a decanter where it combines with the oxychlorinator product.

Figure 3 Oxychlorination Section



Simulation

The main feeds to the plant are ethylene and chlorine. The flow of ethylene (C2F1) is set by the desired VCM production rate (154 tpd). Calculator CAL1 adjusts the flow of chlorine (CL2F) such that the chlorine-to-ethylene ratio in the reactor feed is 0.99. In actual operations, the reaction takes place in a liquid EDC medium in the presence of ferric chloride as the catalyst. The conversion of the lean component (chlorine) is nearly 100% with 99% selectivity for EDC. Therefore, this reaction system has been modeled by two reactors functioning in parallel. The combined total feed (FDIR) is split (SPL1) such that a 0.985 fraction goes to the first reactor (RX1) and the remaining to the second reactor (RX2). Unit RX1 is a Gibbs reactor where most of the EDC forms. For unit RX2 a stoichiometric model has been used. A reaction stoichiometry has been balanced and fitted to expected yields of byproducts. The reaction conditions for both the reactors are 120 C and 15 psig pressure.

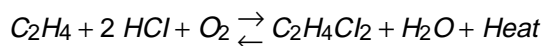
The resulting product streams from the reactors are combined (MIX2). The effluent stream (EDCD) is cooled and flashed (FLS1) to separate a vent stream (VNT1) and a raw product stream (EDCE). The raw product stream EDCE is then washed and scrubbed with caustic to remove any HCl and unconverted chlorine. This process is highly efficient in practice and is modeled with a stream calculator (STC2) to remove all of the HCl and Cl₂.

Oxychlorination

A process flow diagram for this section of the plant is shown below in Figure 3.

Reaction

The reaction between ethylene, hydrogen chloride and oxygen is conducted at temperatures of 225-325 C and in the pressure range of 15-225 psig.



In a balanced oxychlorination plant, dry hydrogen chloride gas is produced mainly from the thermal cracking of EDC. Compressed air supplies the oxygen. This reaction is conducted in either a fixed bed or a fluidized bed reactor containing a catalyst. It is highly exothermic and good temperature control is essential for the successful production of EDC. Temperatures above 325 C deactivate the catalyst, increase byproduct formation and burn ethylene to carbon monoxide and carbon dioxide. The heat of reaction is removed by circulating boiler feed water (BFW) through coils embedded in the reactor and generating steam.

Typical results from this operation are 93-97 % ethylene conversion, 94-97 % HCl conversion and 93-96 % EDC selectivities. This reaction yields more byproducts than the direct chlorination step. These byproducts must be minimized and removed in the EDC purification step. Some of the byproducts (chloral, for example) readily polymerize and tend to foul operating lines and controls. One way to reduce byproduct formation is to provide feeds of good purity. For example, the recycle HCl stream from the VCM purification section should contain less than 0.1 % of acetylene. Presence of acetylene leads to the formation of highly chlorinated byproducts and tars.

Production control is related to HCl mass flow established by the pyrolysis reactor severity and HCl column operation. Air and ethylene flowrates are then ratioed in slightly greater than stoichiometric amounts.

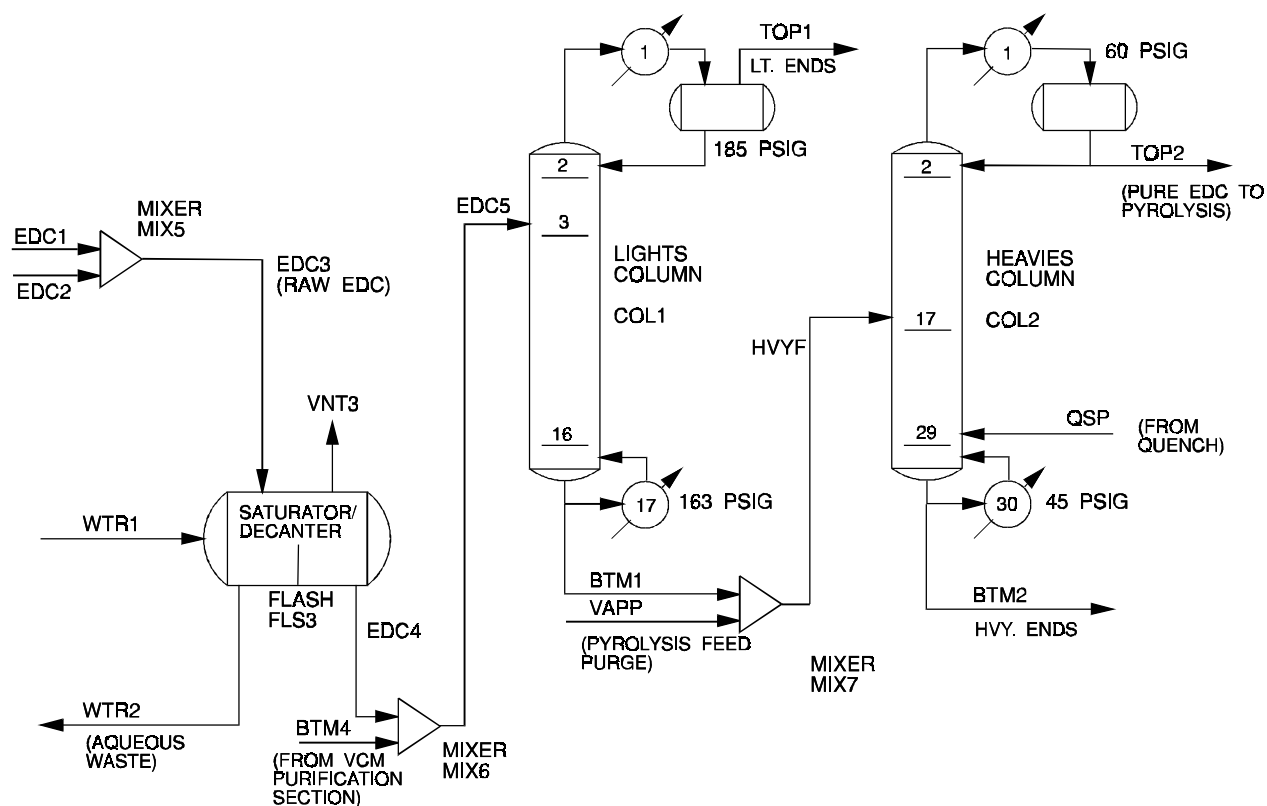
EDC Recovery

EDC, nitrogen and other gases from the oxychlorination reactor first pass through a caustic scrubbing tower where unreacted HCl is removed. The vapor then passes to a refrigerated condensation system to recover EDC and water. The crude EDC mixed with water flows to the decanter where it combines with the direct chlorination product. Uncondensed nitrogen passes to atmosphere through a venting system.

Simulation

For the oxychlorination section, the controlling flow is that of the recycle HCl stream from the top of the HCl column (VCM Purification Section). Therefore, when simulating the complete flowsheet, this section is solved

Figure 4 EDC Purification Section



as part of a recycle loop. An initial guess of the recycle HCl stream temperature, pressure, composition and flowrate is required.

Calculator CAL2 fixes the ethylene feed flowrate (C2F2) at 3% in excess of stoichiometric requirement. In a similar fashion, the flowrate of air (for oxygen) is fixed. In the absence of a specific two phase catalytic model for oxychlorination, we have used available qualitative information on the oxychlorination product composition. Accordingly, the reaction system is modeled as two Gibbs reactors in parallel. The first reactor (RX3) converts a majority of the feed to produce the desired products. The second one (RX4) processes a small fraction of the feed to yield the byproducts. The reaction system model begins with the feed streams being combined (MIX3) and then split (SPL2) into stream FOXA (96 %) and FOXB (4 %). Since it is known that selectivity for EDC is about 96 %, stream FOXA reacts in a Gibbs reactor (RX3) where the reaction is limited to the main reacting and product species: ethylene, EDC, HCl, O₂ and water. Typical operating conditions of units RX3 and RX4 are 290 C, 90 psig, and an approach of 25 C.

The product streams from the two reactors (OXYA and OXYB) are combined (MIX4). The caustic wash unit for removing unreacted HCl is modeled by a stream calculator (STC3) for ideal removal of HCl. The remaining product stream (OXYD) is cooled and flashed to remove all non-condensables (mainly nitrogen and unreacted oxygen) as a vent stream (VNT2).

EDC Purification

Figure 4 shows a process flow diagram for the EDC purification section of the plant.

Process

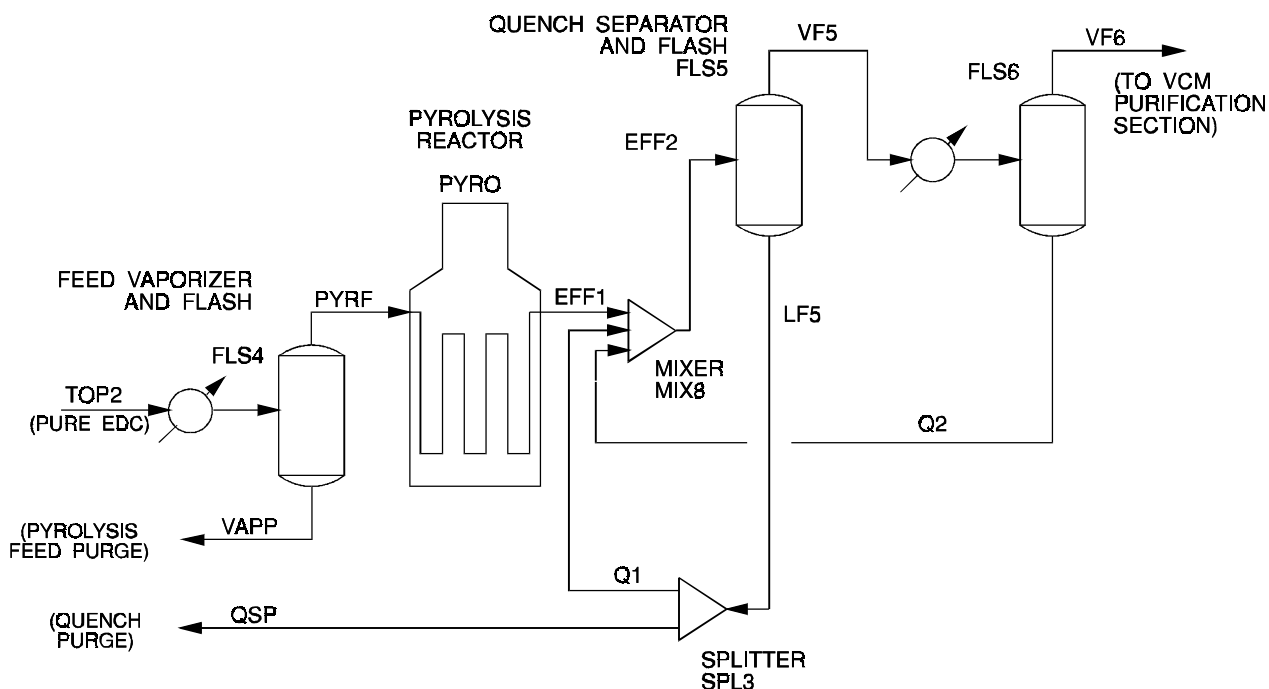
Trace amounts of impurities in the pyrolysis feed can inhibit the cracking reactions and cause fouling. In addition, EDC must also be dry to prevent excessive corrosion downstream of the reactor. Therefore, the

combined EDC from three different sources must be purified to 99 %: EDC from direct chlorination, EDC from oxychlorination and EDC recovered and recycled from the cracking step.

The combined EDC from both direct chlorination and oxychlorination sections is washed with water and scrubbed with caustic to remove chlorine, HCl and other water extractable impurities such as chloral. Free water is decanted.

The crude EDC and unconverted recycle EDC from the VCM column are combined and dried and purified in two distillation columns. In the first column (the lights column), water and lower boiling point impurities ("light ends") are separated as the overhead product. The bottoms product is mixed with a purge stream from the feed vaporizer and fed to the heavies column. Another purge stream from the quench system,

Figure 5 EDC Cracking and Quench Section



downstream of the cracker, is also directed to the bottom of the heavies column. Pure EDC of around 99 % purity is taken as the overhead product while the heavy impurities leave the column as the bottoms product ("heavy ends").

The bottoms product from the heavies column may further be processed, normally via batch distillation, to provide distilled "heavies" byproduct, mainly recovered EDC, and a residual heavy tar.

Simulation

This section begins with a simulation of a saturator/decanter unit. Streams EDC1 and EDC2 are brought together in a mixer (MIX5). The resultant EDC3 stream is combined with a large excess of water (WTR1) and flashed in a three phase flash unit (FLS3). The SRK equation of state with DECANT=ON is used for thermodynamics. While the water phase is decanted as pure water, the amount of water dissolved in the hydrocarbon phase is predicted based on solubility data. The free-water decant model reduces the computational time required to solve this unit and does not impact the overall flowsheet model.

Three streams exit unit FLS3: a small vent stream (VNT3), the aqueous phase (WTR2), and a crude, wet EDC stream (EDC4). This EDC stream is mixed with a recycle EDC stream (BTM4) from the bottoms of the VCM column (see VCM Purification Section). The combined feed (EDC5) is fed to the lights column (COL1). This column has 17 theoretical trays. The bottom product is specified to contain only 0.1 % of the water

entering the column (99.9 % dehydration). The other specification limits loss of EDC with the overheads to 0.1 %. A partial condenser is used for this column. The top vapor product (TOP1) removes most of the water and other light species with some loss of EDC. The remaining EDC and heavies (BTM1) pass on to the heavies column (COL2). Usually a surge tank is placed between the two columns to allow monitoring of the moisture content. Before being fed to the heavies column, the partially dehydrated EDC is mixed with a recycle liquid purge stream (VAPP) from the pyrolysis reactor feed vaporizer. The combined feed (HVYF) goes to COL2 which has 30 theoretical trays. The stripping section of the column also receives another recycle purge stream (QSP) from the quench separator. This purge prevents collections of heavy cracking byproducts in the quench system. The specifications for COL2 are a fixed reflux ratio of 0.6 and a maximum EDC loss of 3 % in the bottoms product (BTM2). The top product (TOP2) is about 99.9 % pure dry EDC.

The IO distillation algorithm is used to simulate the two columns in this section.

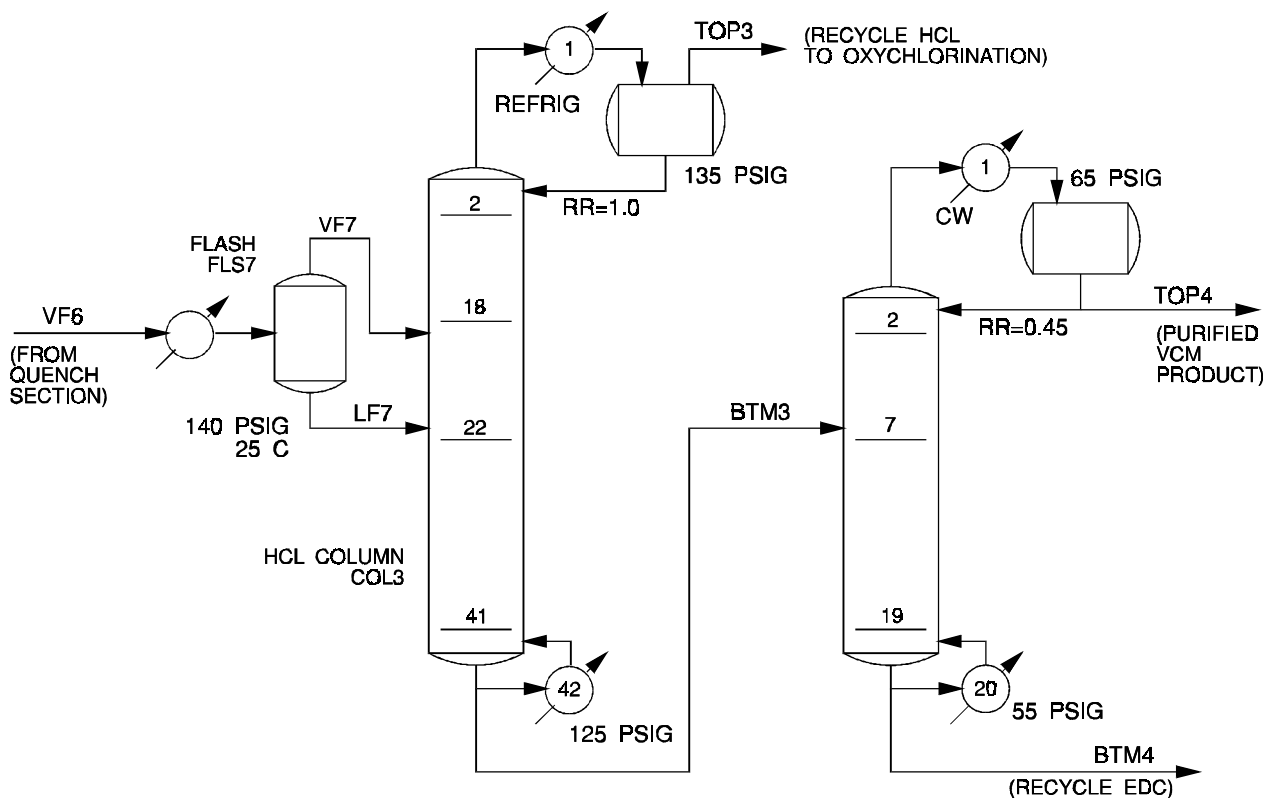
EDC Cracking and Quench

A typical flowsheet for the EDC cracking and quench section is shown below in Figure 5.

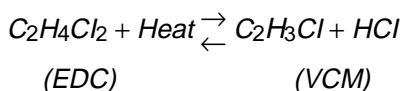
Process

Pure EDC is preheated and vaporized before being fed to the cracking furnace, where it is thermally cracked

Figure 6 VCM Purification Section



at about 500 C and 200 psig by the following reaction.



About half of the EDC entering the furnace is reacted. The product stream then contains roughly equimolar proportions of EDC, VCM and HCl. This stream is quenched by recycled liquids and cooled to about 25-50 C before being fed as both liquid and vapor to the HCl column.

There are two purges in this section of the plant. A liquid purge to prevent iron buildup and fouling of the EDC vaporizer. A quench separator purge to remove “tarry” byproducts of the cracking reaction. Both of these purges are recycled to the heavies column.

EDC furnaces are typically operated up to a maximum of 55% conversion of EDC. This optimizes conversion per pass, column tray loadings and balances the load between direct chlorination and oxychlorination reactors.

Simulation Model

The pyrolysis reactor is represented as a stoichiometric reactor. Stoichiometry of three of the major molecular reactions representing the overall reaction system is defined. For trace species in the feed and the effluent, a reaction fitted to typical plant data is specified. This simplified approach to the overall pyrolysis process is appropriate for the overall modeling of the VCM plant. If desired, a more detailed model of this reactor system could be achieved using in-line FORTRAN reaction data or incorporated as a user-added subroutine.

The top product (TOP2) from the heavies column (COL2) of the EDC purification section is sent to a pure EDC surge tank. The pyrolysis furnace receives its feed from this tank. The feed is heated and flashed (FLS4) to recover a liquid purge stream (VAPP). The balance is a vapor stream (PYRF) which is fed to the pyrolysis reactor (PYRO). The reactor effluent (EFF1) is quenched by recirculating liquid streams (Q1 and Q2) to yield a quenched product (EFF2). This stream passes to a quench separator (FLS5) where the liquid phase containing heavy byproducts is removed. A small portion is sent to the EDC purification section as purge. The remaining liquid phase constitutes the Q1 quench stream. The vapor phase (VF5) is further cooled in one or more heat exchangers and flashed (FLS6) to recover a liquid stream (Q2) which formed the other circulating quench stream.

Vinyl Chloride Purification

Process

VCM is separated from HCl and EDC in two distillation columns. The first column, called the HCl column, receives mixed phase feeds containing mainly EDC, VCM and HCl with small amounts of reaction byproducts. HCl distills off at the top; half of it is recycled to the oxychlorinator directly and the other half condensed against propane refrigerant for reflux to the column. The bottom product is fed to the VCM column for final separation of the purified VCM product as the overhead. EDC is recycled to the lights column for repurification.

Control and Specification

The HCl column is operated to achieve impurity specs of less than 100 ppm VCM in the distillate and less than 5 ppm HCl in the bottoms. Any VCM in the overhead will be converted to more highly chlorinated byproducts in the oxychlorinator, representing a decreased product conversion efficiency. A breakthrough of HCl into the bottoms results in out of spec VCM which must be rerun, reducing VCM production rates. Proper simulation can help establish better setpoints and improve the control system for a more stable operation.

Simulation

The HCl column in this application has 42 theoretical trays, including the condenser and the reboiler. The feed to this column comes from the flash unit (FLS7) upstream of the column. The vapor (VF7) is fed to tray 18 while the liquid (LF7) is fed to tray 22. One of the control specifications is for the reflux ratio to be maintained at 1.0. The other control specification is a suitable tray temperature. In this example, the temperature of tray 34 is maintained at 73 C. Examination of the resulting column temperature profile reveals that this tray provides sufficient sensitivity to changes without sacrificing stability. A top pressure of 135 psig is maintained by using a partial condenser using refrigerant propane. The top temperature is around -31 C. Simulation results show that both the top product (TOP3) and the bottom product (BTM3) purity requirements are achieved.

The top product (TOP3) is recycled to the oxychlorination section, while the bottoms pass on to the VCM column (COL4). The VCM column has 20 theoretical trays and a top pressure of 65 psig. The control specifications are the reflux ratio of 0.45 and tray 17 temperature of 140 C. The column converges with ease and provides a high purity (greater than 99.9%) VCM product as the distillate (TOP4). The bottoms product (BTM4) is unreacted EDC which is recycled to the EDC purification section.

The two columns in the VCM purification section exhibit similar behavior as the columns in the EDC purification section. Both columns successfully converge with the IO algorithm and the SRKM equation of state.

METHODS AND DATA

All of the components are available in the pure component data bank, along with pure component properties.

The SRKM equation of state is chosen for its excellent handling of light polar compounds. Binary interaction parameters for many component pairs are already present in PRO/II's thermodynamic data base. Additional pairs have been regressed for this simulation and entered in the Thermodynamic Data Category of input.

TECHNICAL RESULTS

The main feeds to a plant producing 154 MTPD of 99.9+% pure VCM product are summarized below.

Ethylene	7326	lb/hr	
Chlorine		10009	lb/hr
Air	7970	lb/hr	(Oxygen: 1856 lb/hr)

The main product is VCM. Various vent gas, decant water and purge streams containing heavies and other byproducts of reaction are also removed from the process.

PRO/II successfully determined the calculation sequence, the recycle loops and the recycle streams. The flowsheet converged in five iterations of the outermost loop. The PRO/II input file for this simulation is attached. Selected results, mainly related to the HCl column, are also presented. Examination of the results shows that all product purity specifications are achieved. Electronic copies of the input files and the complete output file are available upon request.

BENEFITS AND ECONOMICS

The VCM plant model may be used for optimization, improved product quality through setpoint selection, and as a simple control system design/revamp tool.

COMMERCIAL INFORMATION

There are roughly 125 to 150 VCM plants worldwide. About 90 % of these plants use the balanced oxychlorination process described here. The technology for these plants is available from about 15 different licensors, each specializing in one or more sections of the VCM plant. Some of the leading licensors are B. F. Goodrich, Hoechst, Stauffer, ICI, Dow, PPG and Tosoh.

APPENDIX A

Input File

This file is available on floppy disk.

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16, 36, 0.2255, -0.0790, 0., 0., &
0.0, 0.0, 1.0, 1.0 / &
21, 33, -0.008752, 0.011038, 1.7890, -4.3071, &
0.0, 0.0, 1.10530, 0.93789 / &
22, 36, 0.1917, -0.1251, 0., 0., &
0.0, 0.0, 1.0, 1.0 / &
24, 36, 0.2429, -0.1171, 0., 0., &
0.0, 0.0, 1.0, 1.0

METHOD SET=3, SYSTEM(VLE)=SRK, DENSITY(L)=RACKETT
KVALUE(VLE) BANK=SIMSCI
WATER DECANT=ON

STREAM DATA

\$ VARIOUS FEED STREAMS:

PROP STREAM=C2F1, PHASE=V, PRES(P SIG)=15, TEMP=75, &
COMP(W)=1,100, NORMALIZE, RATE(W)=4000

PROP STREAM=CL2F, PHASE=V, PRES(PSIG)=15, TEMP=75, &
COMP(W)=2,100
PROP STREAM=C2F2, PHASE=V, PRES(PSIG)=105, TEMP=75, &
COMP(W)=1,100

PROP STREAM=AIRF, PHASE=V, PRES(PSIG)=105, TEMP=75, &
COMP(M)=34,21/35,79, NORMALIZE

PROP STREAM=WTR1, PHASE=L, PRES(PSIG)=12, TEMP=40, &
COMP=36,100, NORMALIZE, RATE(W)=1000

\$ RECYCLE STREAMS (STARTING GUESS):

PROP STREAM=Q1, PHASE=L, PRES(PSIG)=165, TEMP=160, &
COMP(W)=3,56133/4,33/5,30/6,0.2/13,121/15,0.3/ &
18,14.9/21,3800/24,49/26,0.02/27,0.7/ &
30,20/31,0.02/32,298/33,576/ &
NORMALIZE, RATE(W)=62000

PROP STREAM=Q2, PHASE=L, PRES(PSIG)=150, TEMP=90, &
COMP(W)=3,42944/4,31/5,29/6,0.25/13,92/15,0.4/ &
18,14.7/21,5207/24,49/26,0.03/27,0.97/ &
30,19/31,0.03/32,240/33,829/ &
NORMALIZE, RATE(W)=50000

PROP STREAM=VAPP, PHASE=L, TEMP=200, PRES(PSIG)=200, &
COMP(W)=1,5.4295E-04/3,9889.6846/4,20.3888/5,6.3502/ &
6,0.0281/8,0.0280/9,5.4295E-04/10,5.4295E-04/ &
11,0.3703/12,2.9903E-06/13,11.3615/14,1.3128E-03/ &
15,0.0286/16,0.1162/17,0.0272/18,3.8722/19,0.2392/ &
20,0.0270/21,21.2816/22,0.5113/23,1.9886/24,8.3884/ &
25,1.0862/26,0.0110/27,0.0261/29,5.4348E-03/30,2.5708/ &
31,5.5609E-03/32,28.6818/33,2.9158/34,5.4295E-04/ &
35,5.4295E-04/36,1.6774E-03, &
NORMALIZE, RATE(W)=10000

PROP STREAM=TOP3, PHASE=L, TEMP=-31, PRES(PSIG)=135, &
COMP(W)=33,100, NORMALIZE, RATE(W)=9865

PROP STREAM=BTM4, PHASE=LIQUID, TEMP=155, PRES(PSIG)=74, &
COMP(W)=3,19555 / 4,120 / 5,22 / 13,40 / &
18,11 / 21,9 / 24,39 / 30,15 / 32,120, &
NORMALIZE, RATE(W)=19932

\$ REFERENCE STREAMS:

PROP STREAM=C2F0, REFSTREAM=C2F1

UNIT OPERATIONS DATA

\$ _____-\$
\$ DIRECT CHLORINATION REACTOR SECTION
\$ _____-\$

CALC UID=CAL1, NAME=RATIO CALC 1
SEQU STREAM=C2F0,CL2F
PROCEDURE
R(1) = 0.99 * SMR(C2F0)
CALL SRXSTR(SMR,R(1),CL2F)
RETURN

MIXER UID=MIX1, NAME=FEED MIXER 1
FEED C2F1, CL2F
PROD V=FDIR

SPLIT UID=SPL1, NAME=FD SPLT 1
FEED FDIR
PROD V=DIRA, V=DIRB
SPEC STREAM=DIRA, RATE, RATIO, REFFEED, VALUE=0.985

GIBBS UID=RX1, NAME=DIR CL RX 1
FEED DIRA
PROD M=EDCA
OPER ISOTHERMAL, PRES(PSIG)=15, TEMP=120
ELEM REACTANTS(M)=1,2/2,0/3,722/22,1

REAC UID=RX2, NAME=DIR CL RX 2
FEED DIRB
PROD M=EDCB
OPER ISOTHERMAL, PRES(PSIG)=15, TEMP=120
RXCA MODEL=STOIC
STOI 1,-0.5/2,-0.5/ &
3,0.021/4,0.015/5,0.018/6,0.04/8,0.02/ &
11,0.012/12,0.0115/13,0.019/14,0.012/15,0.05/ &
16,0.021/17,0.023/18,0.022/19,0.016/20,0.014/ &
21,0.0348/22,0.015/23,0.0183/24,0.020/25,0.015/ &
26,0.037/27,0.030/33,0.0599
BASE COMPONENT=2
CONV 0.995

MIXER UID=MIX2, NAME=RX MIX 1
FEED EDCA,EDCB
PROD M=EDCD

FLASH UID=FLS1, NAME=D-CLO OV FLS
FEED EDCD
PROD L=EDCE, V=VNT1
ISOT TEMP=25, PRES(PSIG)=13

STCALC UID=STC2, NAME=CAUSTIC WASH
FEED EDCE
OVHD L=EDC1
BTMS L=WST1
FOVHD 1,1.0/3,32,1.0/34,36,1.0
FBTMS 2,1.0/33,1.0

\$ _____\$
\$ OXY CHLORINATION REACTOR SECTION
\$ _____\$

CALC UID=CAL2, NAME=RATIO CALC 2

SEQU STREAM=TOP3,C2F2,AIRF

PROCEDURE

$R(1) = 1.03 * 0.5 * SMR(TOP3)$

CALL SRXSTR(SMR,R(1),C2F2)

$R(2) = 0.30 * (100/21) * SMR(TOP3)$

CALL SRXSTR(SMR,R(2),AIRF)

RETURN

MIXER UID=MIX3, NAME=FEED MIXER 2

FEED C2F2,AIRF, TOP3

PROD V=FDOX

SPLIT UID=SPL2, NAME=FD SPLT 3

FEED FDOX

PROD V=FOXA, V=FOXB

SPEC STREAM=FOXA, RATE, RATIO, REFFEED, VALUE=0.96

GIBBS UID=RX3, NAME=OXY CL RX1

FEED FOXA

PROD M=OXYA

OPER ISOTHERMAL, PRES(P SIG)=90, TEMP=290

ELEM REACTANTS(W)=1/3/33/34/36

CONV APPROACH=25

GIBBS UID=RX4, NAME=OXY CL RX2

FEED FOXB

PROD M=OXYB

OPER ISOTHERMAL, PRES(P SIG)=90, TEMP=290

ELEM REACTANTS(W)=1/3/4/5/6/8/9/10/13/16/ &

18/21/24/25/27/33/34/36

CONV APPROACH=25

MIXER UID=MIX4, NAME=OXY EDC MIX

FEED OXYA, OXYB

PROD M=OXYC

STCALC UID=STC3, NAME=OXY NAOH WSH

FEED OXYC

OVHD V=OXYD

BTMS L=WST2

FOVHD 1,32,1.0/34,36,1.0

FBTMS 33,1.0

FLASH UID=FLS2, NAME=OXY REFRIG

FEED OXYD

PROD L=EDC2, V=VNT2

ISOT TEMP=25, PRES(P SIG)=60

\$ _____\$
\$ EDC PURIFICATION SECTION
\$ _____\$

MIXER UID=MIX5, NAME=RAW EDC MIX
FEED EDC1, EDC2
PROD L=EDC3

FLASH UID=FLS3, NAME=SATURATOR
FEED EDC3, WTR1
PROD L=EDC4, V=VNT3, W=WTR2
ADIA DP=1.0
METHOD SET=3

MIXER UID=MIX6, NAME=EDC FD MIX
FEED EDC4, BTM4
PROD L=EDC5

COLUMN UID=COL1, NAME=EDC LT COL
PARA TRAY=17, IO=25 , DAMP=0.7
FEED EDC5,3
PROD OVHD=TOP1,5, BTMS=BTM1
ESTI MODEL=CHEM, REFLUX=10000
PSPE PTOP(PSIG)=185, DPCOL=22
COND TYPE=PART
DUTY 1,1/2,17
VARY HEAT=1,2
SPEC STREAM=TOP1, COMP=3, RATE, RATIO, &
STREAM=EDC5, COMP=3, VALUE=0.001, RTOL=0.0002
SPEC STREAM=BTM1, COMP=36, RATE, RATIO, &
STREAM=EDC5, COMP=36, VALUE=0.001, RTOL=0.0002
METH SET=2

MIXER UID=MIX7, NAME=HVY FD MIX
FEED BTM1, VAPP
PROD M=HVYF

COLUMN UID=COL2, NAME=HVY COL
PARA TRAY=30, IO
FEED HVYF,17 / QSP,29 \$ SECOND FEED NOT IGNORED
PROD OVHD=TOP2,460, BTMS=BTM2
ESTI MODEL=CONV, RRATIO=0.6
PSPE PTOP(PSIG)=60, DPCOL(Psia)=15
COND TYPE=BUBB
DUTY 1,1/2,30
VARY HEAT=1,2
SPEC RRATIO, VALUE=0.6, RTOL=0.0001
SPEC STREAM=BTM2, COMP=3, RATE, RATIO, &
STREAM=HVYF, COMP=3, VALUE=0.03, RTOL=0.0001
METH SET=2

FLASH UID=FLS4, NAME=PYRO FD FLSH
FEED TOP2
PROD V=PYRF, L=VAPP
TPSP PRES(PSIG)=200, TEST=200
SPEC STREAM=VAPP, RATE(W), VALUE=10000

\$ _____\$
\$ PYROLYSIS SECTION (EDC —> VCM + HCL)
\$ _____\$

REAC UID=PYRO, NAME=CRACKER
FEED PYRF
PROD V=EFF1
OPER TEMP=500, PRES(PSIG)=175
RXCA MODEL=STOIC, CONVERSION
STOI 3,-1 / 21,1 / 33,1
BASE COMP=3
CONV 0.55
STOI 1,-1 / 15,-1 / 31,1
BASE COMP=1
CONV 1.0
STOI 21,-0.2251 / 33,0.2251 / 15,0.2251

\$ _____\$
\$ REACTOR EFFLUENT QUENCH SECTION
\$ _____\$

MIXER UID=MIX8, NAME=QUENCH MIXER
FEED EFF1, Q1, Q2
PROD M=EFF2
OPER PRES(PSIG)=170

FLASH UID=FLS5, NAME=QUENCH FLASH
FEED EFF2
PROD V=VF5, L=LF5
TPSPEC PRES(PSIG)=165, TEST=160
SPEC STREAM=LF5, RATE(W), VALUE=64125

SPLIT UID=SPL3, NAME=QUENCH SPLIT
FEED LF5
PROD L=Q1, L=QSP
SPEC STREAM=QSP, RATE(W), VALUE=2000

FLASH UID=FLS6, NAME=POST FLASH 1
FEED VF5
PROD V=VF6, L=Q2
TPSPEC PRES(PSIG)=150, TEST=90
SPEC STREAM=Q2, RATE(W), VALUE=50000, RTOL=0.00001

\$ _____\$
\$ VINYL CHLORIDE MONOMER (VCM) PURIFICATION SECTION
\$ _____\$

FLASH UID=FLS7, NAME=POST FLASH 2

FEED VF6

PROD V=VF7, L=LF7

ISOT PRES(PSIG)=140, TEMP=25

COLUMN UID=COL3, NAME=HCL COLUMN

PARA TRAY=42, IO \$ ACTUAL NUMBER OF TRAYS = 73 + 2

FEED VF7,18/LF7,22

PROD OVHD=TOP3,270, BTMS=BTM3

ESTI MODEL=CONV, RRATIO=1.0

TEMP 1,-31/6,-31/9,-25/11,0/13,20/17,20/24,22/ &

27,40/35,78/40,80/42,90

PSPE PTOP(PSIG)=135, DPCOL=10

COND TYPE=PART

DUTY 1,1/2,42

SPEC RRATIO, VALUE=1.0, RTOL=0.0001

SPEC TRAY=34, TEMP, VALUE=73, ATOL=0.01

SPEC(CHANGE) STREAM=TOP3, COMP=21, PPM(W), VALUE=100

SPEC(CHANGE) STREAM=BTM3, COMP=33, PPM(W), VALUE=5

VARY HEAT=1,2

METH SET=2

\$ PRINT ITER=ALL

COLUMN UID=COL4, NAME=VC COLUMN

PARA TRAY=20, IO

FEED BTM3,7

PROD OVHD=TOP4,270, BTMS=BTM4

ESTI MODEL=CONV, RRATIO=0.45

PSPE PTOP(PSIG)=65, DPCOL=10

COND TYPE=BUBB

DUTY 1,1/2,20

SPEC RRATIO, VALUE=0.45, RTOL=0.0001

SPEC TRAY=17, TEMP, VALUE=140, ATOL=0.01

VARY HEAT=1,2

METH SET=2

\$ PRINT ITER=ALL

RECYCLE DATA

ACCEL TYPE=WEGS