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Emissions Model of Waste Treatment Operations at the Idaho Chemical Processing Plant

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ABSTRACT

An integrated model of the waste treatment systems at the Idaho Chemical Processing Plant (ICPP) was developed using a commercially-available process simulation software (ASPEN Plus) to calculate atmospheric emissions of hazardous chemicals for use in an application for an environmental permit to operate (PTO). The processes covered by the model are the Process Equipment Waste evaporator, High Level Liquid Waste evaporator, New Waste Calcining Facility and Liquid Effluent Treatment and Disposal facility. The processes are described along with the model and its assumptions. The model calculates emissions of NO_x, CO, volatile acids, hazardous metals, and organic chemicals. Some calculated relative emissions are summarized and insights on building simulations are discussed.

SUMMARY

An integrated model of the waste treatment systems at the Idaho Chemical Processing Plant (ICPP) was developed to calculate atmospheric emissions of hazardous chemicals for use in an application for an environmental permit to operate (PTO). The model is a steady-state model developed using a commercially-available process simulation software (ASPEN Plus). The objectives of the simulation are 1) to calculate emissions at maximum operating capacity for each specie known or suspected to be emitted from the ICPP stack and 2) to trace each specie of concern through the waste systems.

The ICPP liquid wastes are mixed radioactive-hazardous aqueous wastes of variable composition usually composed of solutions of nitric acid, sodium nitrate and aluminum nitrate contaminated with low concentrations of chloride, fluoride, hazardous metals, organic compounds and radionuclides. The aqueous wastes can be divided into: 1) concentrated wastes from past operations which are stored in large stainless steel tanks, and 2) dilute, low-level wastes which are generated by current laboratory and clean-up operations.

The ICPP solidifies and treats liquid wastes with an integrated waste treatment system which interconnects the waste calciner (NWCF), two evaporators (PEW and HLLW), and an acid fractionator (LET&D). The core of the waste treatment system is the calciner which solidifies concentrated aqueous wastes for storage in the calcined solids storage bins. The Process Equipment Waste (PEW) evaporator separates the dilute wastes into low- and high-boiling fractions and sends the smaller high-boiling fraction to liquid waste storage before being solidified by the calciner. The condensate from the PEW evaporator goes to the LET&D system which uses an acid fractionator with a partial condenser to vaporize most of the liquid for atmospheric discharge. The concentrated nitric acid collected by the LET&D system will be transferred to the calciner for reuse as scrubber acid. The High Level Liquid Waste evaporator (HLLWE) is being installed to concentrate the more dilute of the liquid wastes in storage thereby improving calciner operation and reducing waste volumes. All gaseous effluents are treated with two or more high-efficiency, particulate aerosol filters.

The waste treatment system is modeled as an integral system because of the many interactions between the individual treatment processes. The simulation strategy was to provide an extensive, but not intensive, simulation covering every significant process and stream but using the simplest adequate simulation block. A steady state approximation, which appears conservative, is used to model the many batch processes.

The resulting simulation is a complex array with many process blocks, many streams and five internal recycle loops. The simulation program is able to converge the recycle loops (after many iterations), calculate emissions and show the disposition of all the species. The calculated emissions of nonvolatile metals are very low because all effluents are filtered by several stages of filtration. Emissions of significant fractions of the chloride and fluoride are calculated because of the volatilities of HCl, Cl_2 and HF.

The experience gained in building the simulation model confirms that large simulation models should be built a few blocks and species at a time so that problems can be located readily. Convergence is improved if insignificant reactions are deleted from the chemistry. Also, it is important to balance ion charge in each feed stream.

CONTENTS

FIGURES

TABLES

ACRONYMS

APS	Atmospheric Protection System
ICPP	Idaho Chemical Processing Plant
HLLWE	High Level Liquid Waste Evaporator
LET&D	Liquid Effluent Treatment and Disposal
PEW	Process Equipment Waste
VLE	Vapor-Liquid Equilibria
VOG	Vessel Off Gas

Emissions Model of Waste Treatment Operations at the Idaho Chemical Processing Plant

1. INTRODUCTION

The Idaho Chemical Processing Plant (ICPP) recovered uranium for about 40 years from a variety of government-owned, high-enriched, spent nuclear reactor fuels by a solvent-extraction process. The reprocessing raffinates (approximately six million gallons) have been essentially all solidified by a fluidized-bed calcination process with the resulting granular solids stored in large stainless steel bins enclosed in reinforced-concrete vaults. However, some liquid wastes from other operations remain. Fuel reprocessing has been discontinued. The current ICPP operations are 1) fuel storage, 2) treatment and solidification of the remaining radioactive liquid wastes, and 3) decontamination and decommissioning of obsolete facilities.

The ICPP has both concentrated wastes, which are stored in large stainless steel tanks, and dilute wastes which are generated by current operations. The concentrated wastes are mixed radioactive-hazardous aqueous wastes accumulated primarily from past decontamination efforts and low level liquid waste treatment. The dilute waste, which is called process equipment waste (PEW), is low level liquid waste from laboratory and other operations. The PEW is evaporated with the concentrate being added to the existing concentrated wastes in storage.

The ICPP waste treatment system interconnects the waste calciner (NWCF), two evaporators (PEW and HLLW), and an acid fractionator (LET&D) as shown in Figure 1. The core of the waste treatment system is the calciner which solidifies concentrated aqueous wastes for storage in the calcined solids storage bins. The Process Equipment Waste (PEW) evaporator separates the dilute wastes into low- and high-boiling fractions and sends the smaller high-boiling fraction to liquid waste storage before being solidified by the calciner. The condensate from the PEW evaporator goes to the LET&D system which uses an acid fractionator with a partial condenser to vaporize most of the liquid for atmospheric discharge. The concentrated nitric acid collected by the LET&D system will be transferred to the calciner for reuse as scrubber acid. The High Level Liquid Waste evaporator (HLLWE) is being installed to concentrate the more dilute of the liquid wastes in storage thereby improving calciner operation and reducing waste volumes. All gaseous effluents are treated with two or more high-efficiency, particulate aerosol filters.

The model of the waste treatment systems was developed to calculate maximum atmospheric emissions of hazardous chemicals for use in an application for an environmental permit to operate (PTO). The species included are the bulk chemicals and some species listed by the Clean Air Act. The objectives are 1) to provide an emission at maximum operating capacity for each specie known or suspected to be emitted from the ICPP stack, and 2) to trace each specie of concern through the waste systems.

The waste treatment system is modeled as an integral system because of the many interactions between the individual treatment processes. The emissions model uses a commercially-available process simulation program (ASPEN Plus). The ASPEN program is used for calculating the emissions because of its ability to 1) do material balances with large numbers of streams and species, 2) calculate recycle loops, and 3) calculate vapor-liquid equilibria. A steady state approximation, which appears conservative, is used to model the many batch processes.

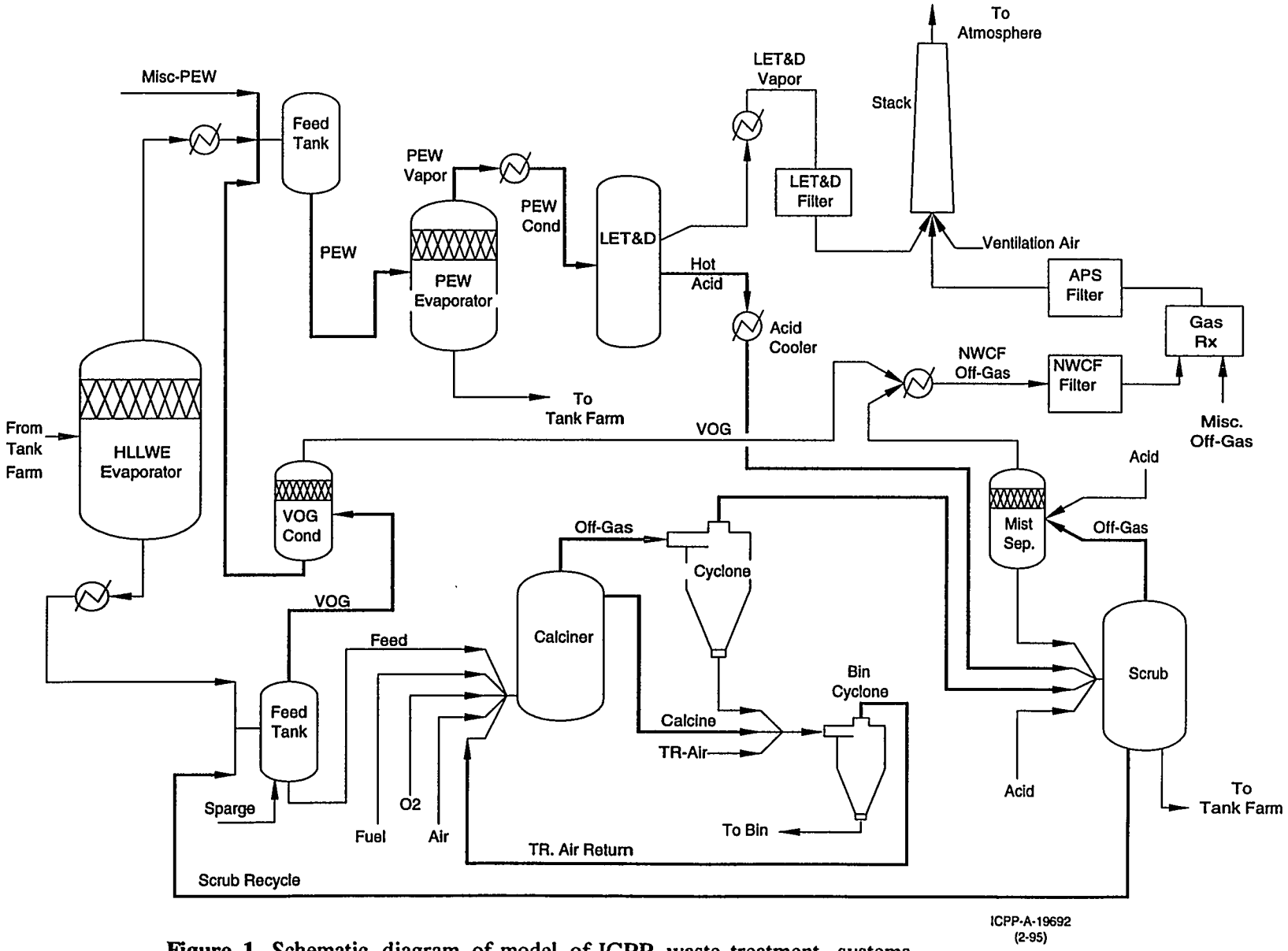


Figure 1 Schematic diagram of model of ICPP waste treatment systems.

2. WASTE TREATMENT PROCESSES

The liquid wastes, waste treatment processes and waste treatment facilities are described in this section to provide background information on the processes modeled. The liquid wastes are acidic solutions of sodium and aluminum nitrates contaminated with low and varying concentrations of chloride, fluoride, heavy metals, radionuclides and organics. The chemistry of the waste solutions is very complex because of the large number of species and the many reactions between the species. In particular, the complexing of the halides with many of the metal ions (e. g., to form AlF^{+2} and $HgCl_2$) is significant. Also, many of the solutions are very concentrated.

2.1 Liquid Waste Storage Tanks

Concentrated liquid wastes (with densities of 1.1 to 1.3 g/ml) are stored, pending calcination, in a set of 11 storage tanks each of which has a nominal capacity of 300,000 gal. and is enclosed in a concrete vault. These concentrated aqueous wastes are a mixture of 1) PEW evaporator concentrates, 2) the more-concentrated decontamination wastes, 3) evaporator de-scaling solutions and 4) solvent clean-up solutions from reprocessing. About 1.8 million gallons of concentrated wastes are currently stored in seven tanks. For modeling purposes, the wastes in the storage tanks are grouped into three representative wastes :

1) The "Na waste" represents the six tanks with high sodium concentrations. Its primary solutes are HNO_3, $NaNO_3$ and $Al(NO_3)_3$.

2) The "dilute F waste" represents one tank of dilute waste resulting mostly from calciner decontamination. It consists primarily of HNO_3, HF and $Al(NO_3)_3$.

3) The "reprocessing heel" represents the small volume of reprocessing raffinate remaining as tank heels in two tanks. It is a concentrated solution of HNO_3, HF and $Al(NO_3)_3$ which enters the waste process when blended with concentrate from the HLLWE.

For the calculation of upper-limit emissions, the concentrations of hazardous species are set at the maximum concentrations measured in any of the tanks plus a contingency. A "trace organics" specie with a concentration equal to the analytical detection limit for the tanks is included to represent a number of organic species whose presence is suspected but whose concentrations are below detectable limits. The concentrations of methanol, hexone and ethylene glycol are conservative estimates based on past usage practices.

Liquids are transferred from nine of the tanks with steam jets and from the other two tanks with air lifts. The result of transfer by steam jets is the warming and a 6 to 8 percent dilution of the solutions. The result of transfer with the air lifts is the partial volatilization of solutes and the entrainment of part of the liquid. The tanks vent to the vessel off-gas (VOG) system.

2.2 PEW Evaporator

The process equipment waste (PEW) is a variable mixture of dilute acidic solutions (The aqueous wastes are kept acidic as a part of the criticality- and corrosion-control strategies.) consisting of analytical laboratory wastes, fuel storage basin wastes, dilute decontamination solutions and rinses,

and wastes from other INEL facilities. They usually contain nitric acid (typically 0.1 to 0.5 M), dilute sodium and aluminum nitrate, chloride and trace concentrations of heavy metals and organics.

The "PEW evaporator" is a pair of redundant thermosyphon evaporators (one on standby) which separate PEW into low- and high-boiling fractions. The maximum capacity of 550 gph is sometimes reduced by heat exchanger fouling. Operation is semi-batch with a steady feed rate until the bottoms reach a temperature or density limit or it runs out of feed. The bottoms are then cooled and transferred, and the evaporator waits, often several days, for sufficient PEW for another operating cycle. The evaporator boil-down (feed-to-bottoms) ratio, which varies greatly with feed composition, is typically in the 25 to 100 range. Aluminum nitrate is added to fluoride-containing PEW to control corrosion in the evaporator by complexing the fluoride.

The PEW evaporator condensate is contaminated by HNO_3, HCl and HF volatilized from the evaporator and also by small quantities of nonvolatile solutes entrained by the vapor. The volatilization of the HNO_3, HCl and HF depends on the vapor-liquid equilibria (VLE) in the evaporator; it can be on the order of 50 percent with high boil-down ratios. A wire-mesh mist separator limits carryover[1] of entrained liquid during normal operation to less than 1E-4 based on the feed. However, a corroded mist separator can increase entrainment to 1E-3 (of the feed).

2.3 Liquid Effluent Treatment and Disposal

The Liquid Effluent Treatment and Disposal Facility[2,3] (LET&D) uses acid fractionators (one operating and one on standby) with partial condensers to vaporize nearly all of the water in the condensate from the PEW evaporator. The acid fractionators have 15 seive trays and are sized with the same capacity as the PEW evaporators. The overhead vapor, which contains about 1 percent of the nitric acid and 0.01 percent of the nonvolatile solutes from the feed, is superheated, filtered with two HEPA filters in series and discharged to the stack.

Most (99 %) of the nitric acid in the feed is collected in the bottom of the fractionator and concentrated usually to 10 to 12 M. The concentrated acid will be pumped to a storage tank near the NWCF and later fed with an air lift to the NWCF scrub system as make-up acid. Chloride is oxidized to chlorine gas by concentrated nitric acid (possibly catalyzed by chromate ion) in the bottom of the fractionator and then discharged in the overhead vapor.

2.4 New Waste Calcining Facility

The New Waste Calcining Facility (NWCF) calcines concentrated liquid wastes from the tank farm forming granular solids. The water and volatile acids are vaporized at 500°C, and the cations are converted to oxides, halides and other solid forms. The NWCF feed rate is often limited because of constraints in environmental permits on NO_x emissions. A schematic diagram of the NWCF is shown in Figure 2.

2.4.1 Calciner

The heart of the NWCF is the fluidized-bed calciner in which the liquid wastes are solidified at 500°C. A five-foot diameter bed of granular solids is fluidized by introducing air from below and heated to 500°C. When the liquid waste is atomized and sprayed into the hot fluidized bed:

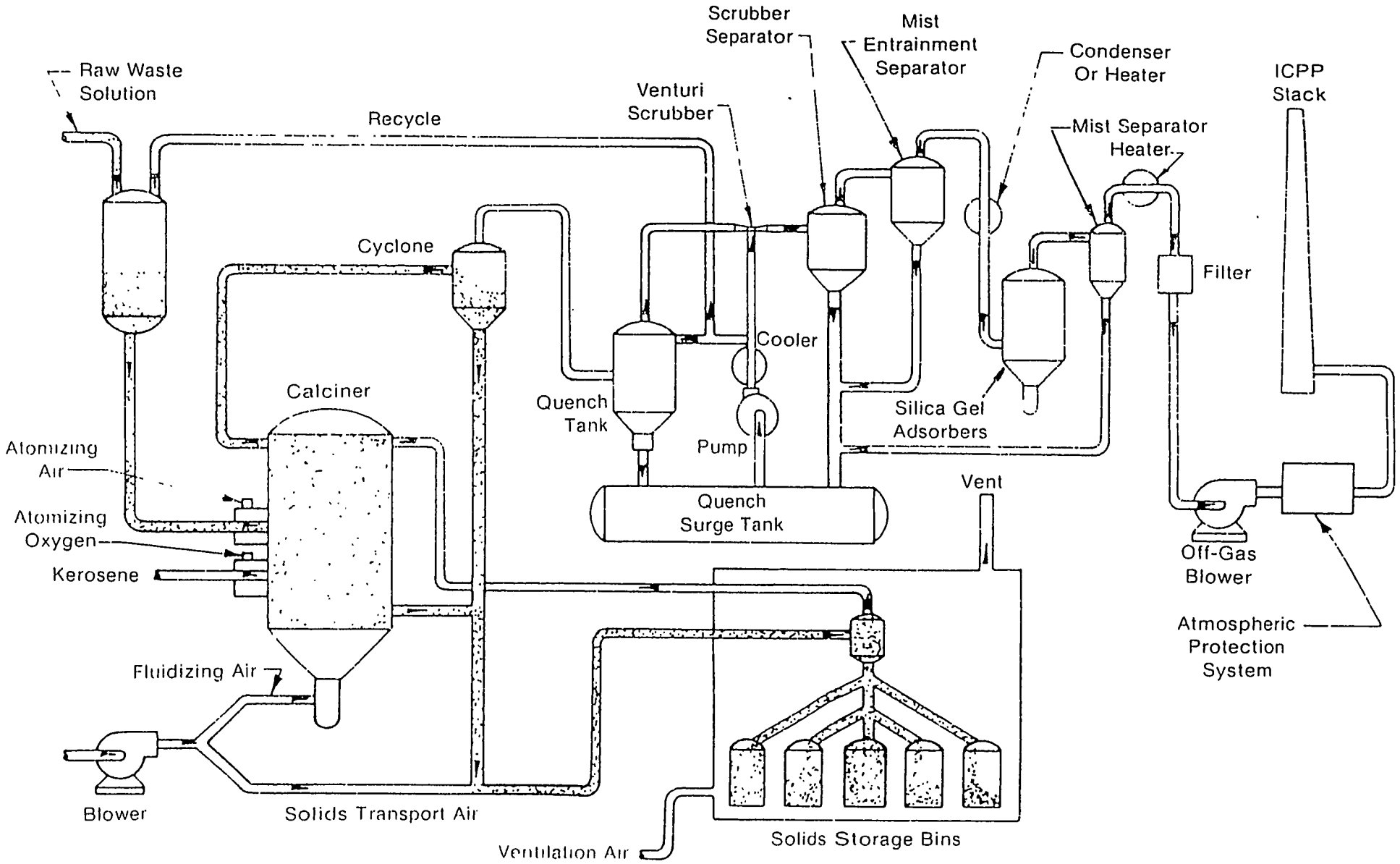


Figure 2. Schematic diagram of the New Waste Calcining Facility. ICPP-A-0008

- the water is vaporized,
- the nitric acid and most of the nitrates are decomposed to NO_x,
- the dissolved metals are converted to oxides, halides and other stable solids which mostly coat on the existing solids, and
- some of the HCl and HF vaporize.

Process heat is provided by in-bed combustion of fuel sprayed with oxygen into the fluidized bed. The combustion is incomplete. Some CO and volatile hydrocarbons are formed in the flame (in addition to CO_2 and water vapor).

2.4.2 Product Transfer

The calcined solids are removed from the fluidized bed and from a cyclone in the calciner off gas (Figure 2) and transferred pneumatically to sets of large (mostly 12- or 13.5-ft diameter) stainless steel bins, enclosed in reinforced-concrete vaults for interim storage. The transport air is returned to the calciner.

2.4.3 Feed System

The NWCF feed system is a set of interconnected vessels for the blending of wastes from different tanks with chemicals (e. g., aluminum nitrate, calcium nitrate and boric acid) added to improve calcine stability. The use of air sparges for mixing and air lifts for transfer generates vessel off gases containing acid vapors and some entrained liquids.

2.4.4 Scrub System

The NWCF scrub system cools the calciner off gas and collects entrained solids that are carried through the cyclone (Figure 2) on the calciner outlet. First, a quench tower cools the calciner off gas nearly to its dew point. Next, a Venturi scrubber removes most of the entrained solids and cools the off gas a little more. The liquids from the quench tower and scrubber drain to a surge tank from which they are recycled through a cooler back to the quench tower and scrubber.

The solids collected by the scrubber are (mostly) dissolved by the nitric acid in the scrub solution. Nitric acid (either nonradioactive acid or acid from LET&D) is added regularly to maintain the solution's nitric acid concentration. A small amount of water vapor is condensed from the off gas to dilute the accumulating dissolved solids and maintain the scrub solution at its desired density. The scrub solution density and accumulation rate are controlled by adjusting the solution temperature (which controls condensation rate). The accumulated scrub solution is periodically recycled to the calciner feed tanks for calcination. In addition, batches of scrub solution are occasionally purged to the tank farm to limit the build up of the chloride concentration in the solution.

The scrubber is followed by a mist separator which collects spray entrained from the scrubber. Nitric acid is added continuously ahead of the mist separator to dissolve any solids collected. Some of the nitric acid vaporizes into the off gas. The liquid from the mist separator drains to the scrub surge tank (forming a recycle loop).

2.4.5 Equipment Vent System

The vessel off gases from the NWCF feed vessels and air lifts, the HLLWE feed vessels and air lift, and the LET&D acid storage vessel and air lift are collected by the NWCF equipment vent system and fed to a condenser which condenses most of the moisture and acid vapors and drains them to the PEW system. The off gas from the condenser enters the NWCF off gas system downstream of the scrub system.

2.4.6 Remainder of NWCF Off-Gas System

The section of the NWCF off-gas system downstream of the scrub system contains silica-gel absorbers, heaters, filters and blowers. The silica-gel absorbers, which were installed to adsorb ruthenium vapors, are sometimes by-passed when ruthenium vapors are absent and are omitted from the process simulation. The off gas from the scrub system is superheated and then filtered through a filter set containing four parallel lines of filters each containing three high-efficiency particulate aerosol (HEPA) filters in series. Credit is normally taken for two HEPA filters in series each operating at the nominal efficiency of 99.97 percent. The filters are followed by blowers which boost the off-gas pressure from the process vacuum to atmospheric pressure.

2.5 Vessel Off Gas

The vessel off gas (VOG) system collects process off gas from vessels and air lifts in the fuel reprocessing building, and from the tank farm vessels and air lifts. The combined VOG flow is filtered through one HEPA filter before going to the APS system.

2.6 Atmospheric Protection System

The Atmospheric Protection System (APS) provides one additional stage of filtration through HEPA filters for the combined off gases from the NWCF, the VOG system, and some other facilities. The filtered effluent is discharged to the stack.

Nitric acid vapors decompose to NO_x in the off-gas systems. The equilibrium between nitric acid and NO_x varies with temperature and composition. The temperature and composition at the discharge from the APS probably controls the equilibrium concentrations because the discharge into the stack quenches the reactions by cooling and dilution.

2.7 Process Interactions

The ICPP waste treatment system is designed as an integrated system in which the operation of every process effects other processes. The NWCF equipment vent system channels vessel off gas from the NWCF feed vessels, the HLLWE feed vessels, and the LET&D acid recycle tank into a condenser which sends its condensate to PEW and its vapor to the NWCF off-gas system.

The LET&D system recycles acids from the PEW to the NWCF scrub system. The HLLWE concentrates the NWCF feed (thus altering its operation) and sends condensate to PEW. The PEW evaporator and HLLWE have no direct atmospheric emissions, but they strongly effect the emissions from the NWCF and LET&D via the APS. Because of these interactions and the recycle streams, the ICPP waste treatment system is best evaluated as an intregal system.

3. MISCELLANEOUS SOURCES

In order to make the simulation cover the whole ICPP, some additional sources were included which themselves combined several miscellaneous sources:

- PEW-MISC

  The source labeled PEW-MISC is a source to the PEW evaporator representing base-line PEW from chemical analyses, vessel flushes from the fuel reprocessing area, and fuel basin operation. The flow is adjusted so that the total feed to the PEW evaporator is equal to its capacity.

- VOG-601

  The VOG-601 source represents vessel off gas from fuel reprocessing vessels being decontaminated (and sparged) with nitric acid and from the tank farm. It contains nitric acid vapors and moisture from both. One tank farm air lift is included as a separate source.

- PILOT-PL

  The PILOT-PL source represents the combined VOG hazardous species input of the ICPP pilot plants that transfer off gas into the VOG system.

- FUG-EMIS

  The FUG-EMIS source represents the input into the VOG system from the breathing of nitric acid storage tanks.

- NWCF-PEW

  The NWCF-PEW source represents miscellaneous PEW sources, in addition to equipment vent condensate, from NWCF operation.

4. PROCESS SIMULATION

The ASPEN Plus process simulation program is used for calculating the emissions because of its ability to 1) do material balances with large numbers of streams and species, 2) calculate recycle loops, and 3) calculate vapor-liquid equilibria. The simulation strategy is to be extensive but not intensive. The process simulation seeks to cover every ICPP process with a significant effect on emissions, but it uses relatively simple blocks especially for processes within recycle loops. For example, the LET&D acid fractionator is represented by a SEP block, which puts stated fractions of each feed component in the vapor stream, rather than a fractionation block. The chemistry is restricted to the most significant reactions. The simulation diagram for the ASPEN simulation is shown in Figure 3. The program input file is given in Appendix A. The development of the physical properties parameters used in the VLE calculations is given in Appendix B.

The emissions are calculated to the extent feasible as conservative, upper-limit values. The NWCF flowsheet on which the simulation is based was chosen to provide the highest concentrations of hazardous species in the NWCF feed. Also, upper-limit values are selected for concentrations of hazardous species in the liquid waste tanks. A steady state approximation, which appears conservative, is used to model many batch processes. The simulation centers on the NWCF which is operated at the maximum feed rate allowed by NO_x discharge limits. The HLLWE processing rate is set to provide the NWCF feed.

4.1 Bases of Emissions Calculations

The emissions calculations are a combination of calculated emissions and specified emissions:

- NO_x

  The HLLWE and NWCF feeds are adjusted until the calculated NO_x emission is slightly below the ICPP emission limit.

- CO

  The CO emission is specified based on extrapolating the highest measured $CO:CO_2$ ratio in the NWCF to the maximum achievable NWCF fuel input. The specified CO emission is written into the in-bed combustion block.

- HNO_3

  The HNO_3 concentration in the scrub system off gas is calculated by the simulation from its vapor pressure (vapor-liquid equilibrium calculation) in the NWCF scrubber and mist eliminator (NCC-110). The HNO_3 concentration in the APS off gas is an upper-limit value obtained by calculating the gas-phase chemical equilibrium (by Gibbs free energy minimization) between HNO_3 and NO_x with the $NO:NO_x$ ratio set at a lowest observed value of 0.1.

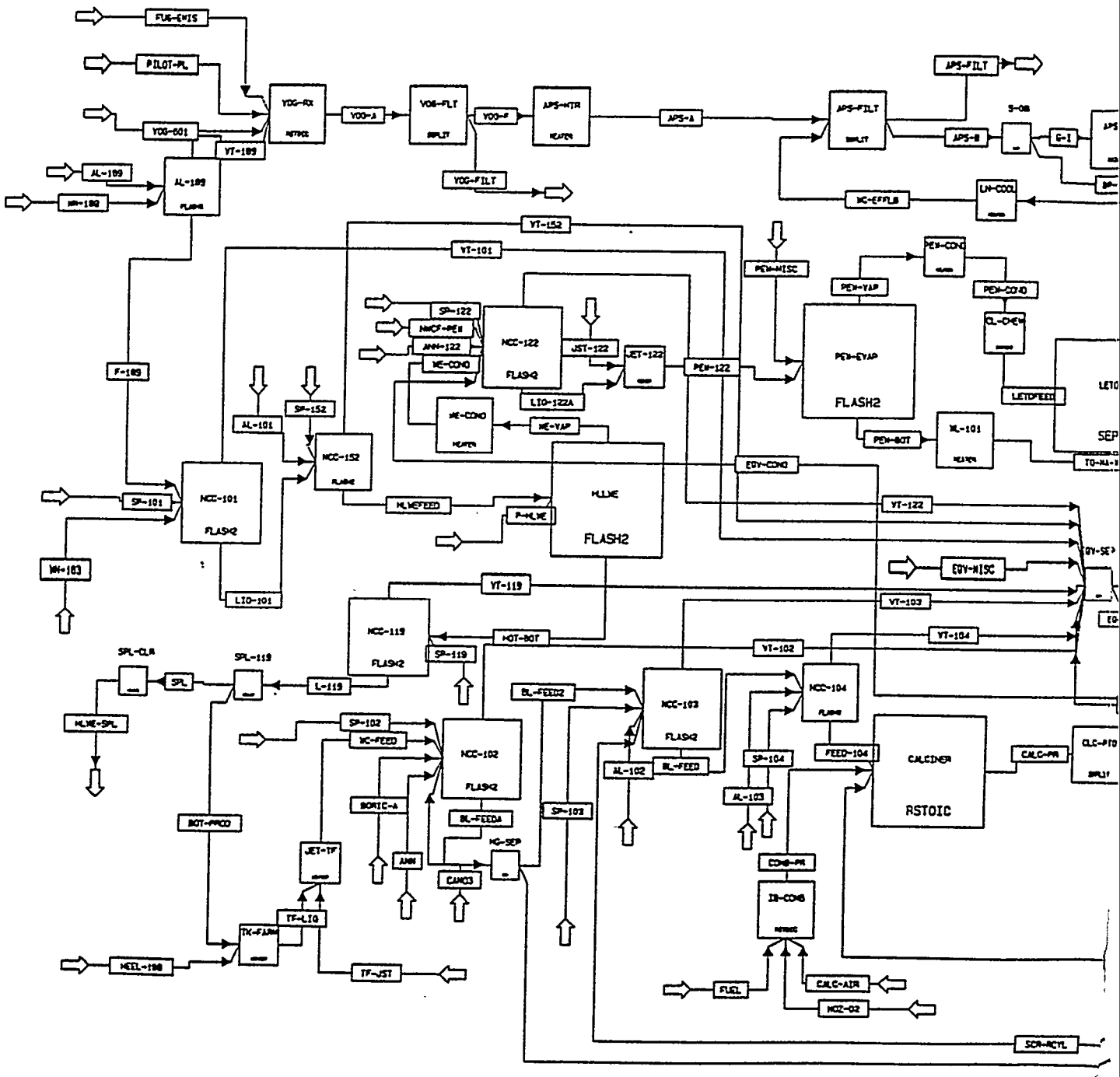
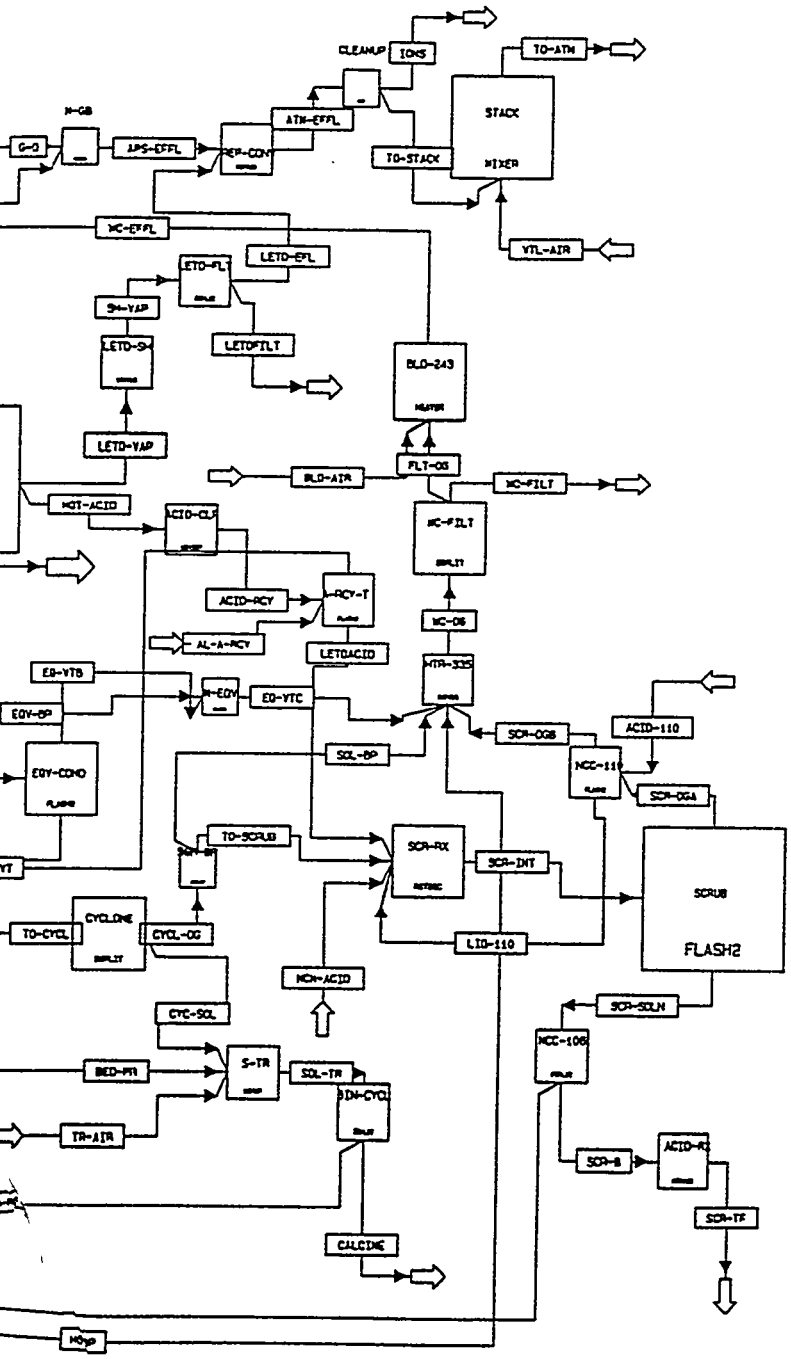


Figure 3. Simulation diagram for ASPEN simulation of ICPP waste treatment systems.


CLEANUP
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VC-EFFL
YTL-AIR
LETD-EFL
LETD-FL
LETDFILT
BLO-243
LETD-VAP
BLO-AIR
FLT-OS
MC-FILT
MST-ACID
ACID-RCY
AL-A-RCY
LETDACID
MC-OS
EQ-VTB
EQV-BP
EQ-VTC
SCR-OGS
ACID-110
SCL-BP
SCR-OGA
EQV-COND
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SCR-RX
SCR-INT
SCRUB
FLASH2
TO-CYCL
CYCLONE
CYCL-OG
LID-110
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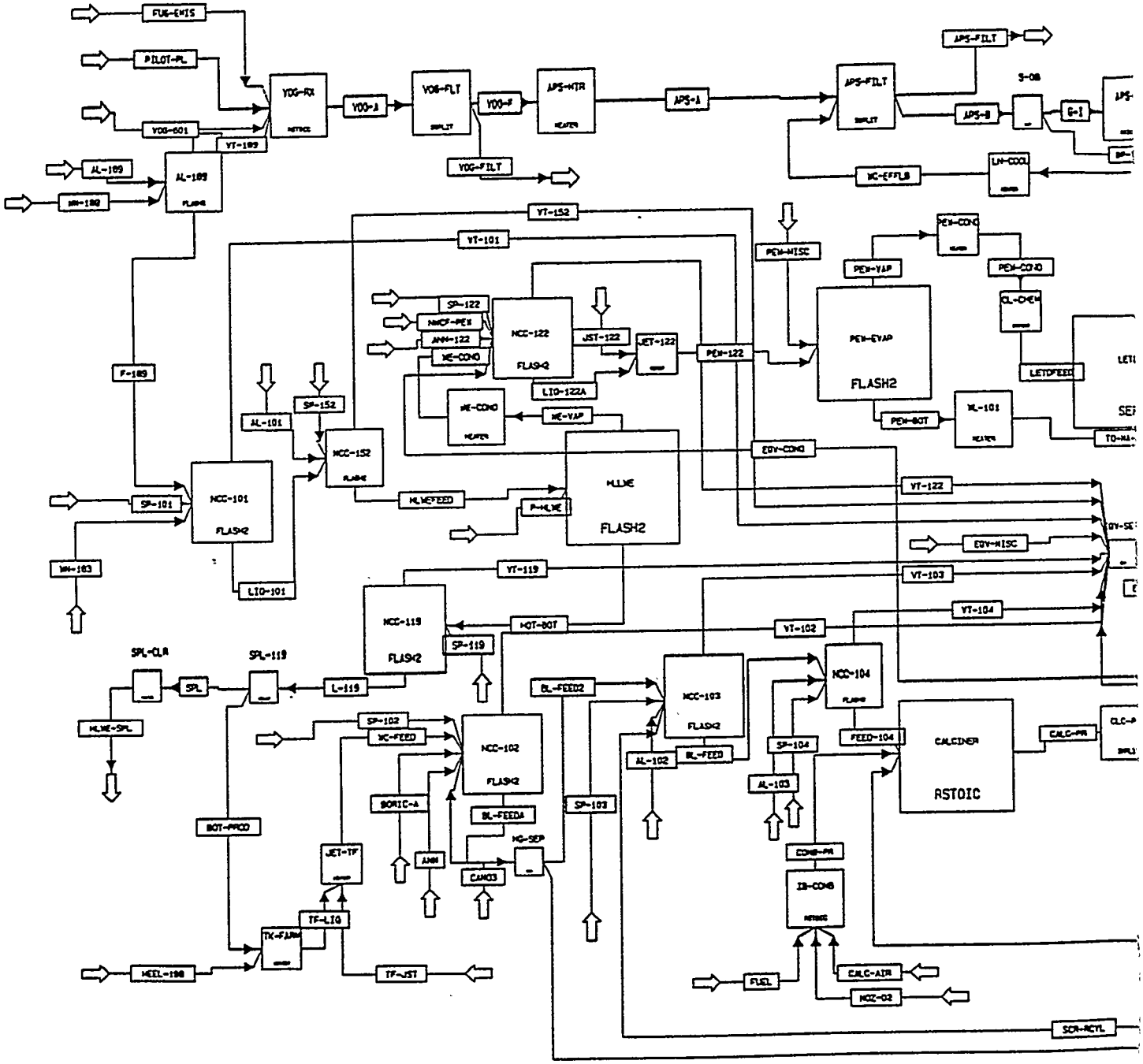

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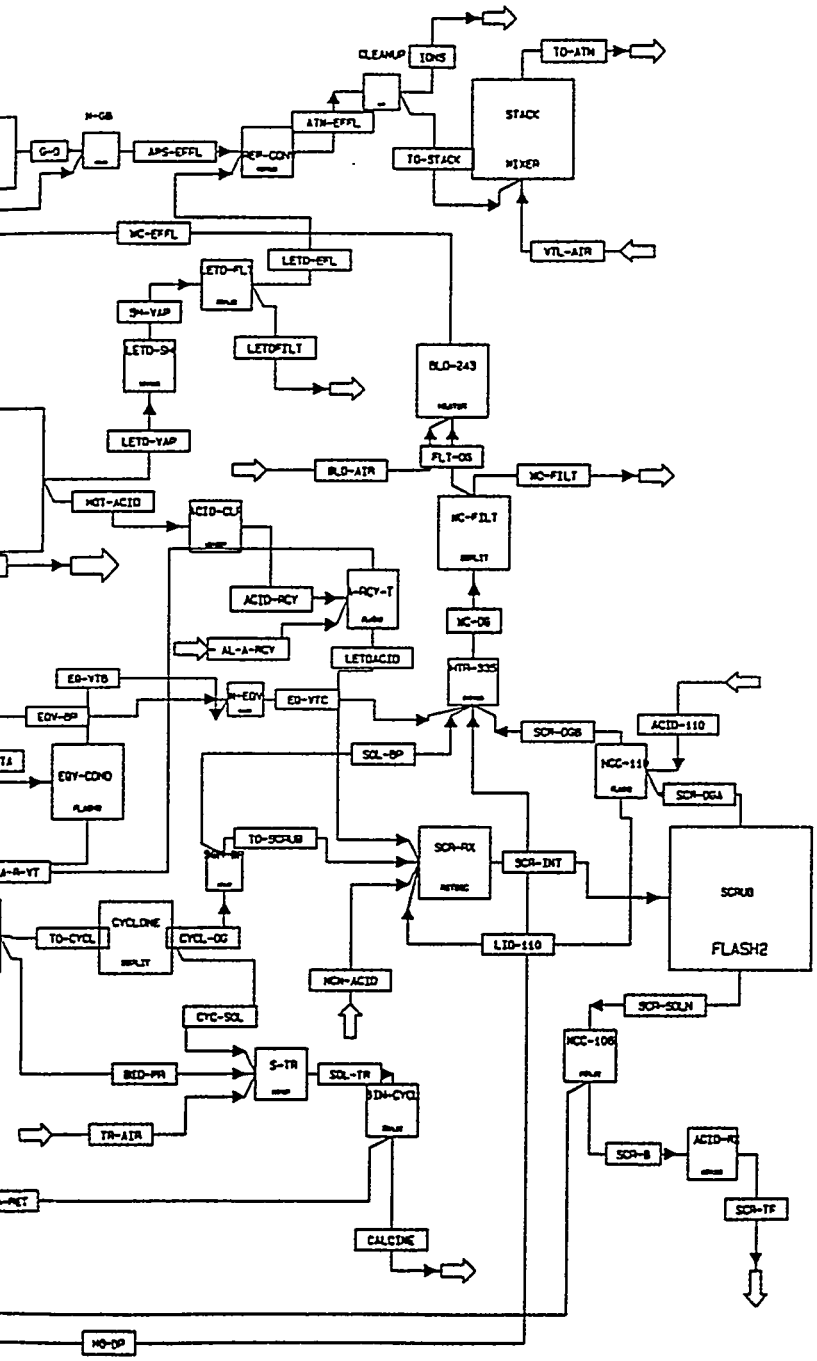
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VTL-AIR
MC-EFFL
LETD-EFFL
LETD-FLT
LETDFILT
BLO-243
LETD-VAP
BLO-AIR
FLT-OS
MC-FILT
ACID-RCY
AL-A-RCY
LETDACID
EQ-VTB
EQV-CDMO
TO-SCRUB
SCR-FIX
SCR-INT
SCRUB
FLASH2
TO-CYCL
CYCLONE
CYCL-OG
LID-110
MCN-ACID
CYC-SCL
SCR-SOLN
BED-PR
S-TR
SOL-TR
TR-AIR
SCR-B
SCR-TF
CALCINE
MO-DP

- HF

  Emission of HF is calculated based on vapor-liquid equilibrium (i. e., saturated solutions) in the NWCF scrub system and the sparged feed vessels.

- HCl

  Emission of HCl is calculated based on vapor-liquid equilibrium in the NWCF scrub system and the sparged feed vessels. The HCl in the PEW system is not included because the LET&D converts it to Cl_2.

- Cl_2

  The Cl_2 emission is based on the LET&D fractionator converting all of the chloride in its feed into Cl_2.

- SO_2

  The SO_2 emission is based on the NWCF burning lower grade kerosene (0.3 % S) at its maximum feasible rate. (It normally burns low S kerosene.)

- Hg

  The Hg emission target value is a fraction of the Hg in the NWCF feed based on the highest concentration in the stack observed during NWCF operation. The Hg emission is written into a SEP block bypassing the scrub system.

- Particulate solids

  The emission of particulate solids is based on 1) entrainment in sparged vessels and air-lifts of 0.0001 lb of entrained liquid per lb of off gas, 2) penetration of 1/2000 of the solids from the calciner through the NWCF scrub system (based on WCF scrub system performance[4]) and 3) evaporator entrainment of 0.001 of the feed. The dominant particulate emission source is the WM-189 air lift which discharges through two HEPA filters (one less than the other routes).

- Unburned hydrocarbons

  The largest source of volatile organic carbons is unburned hydrocarbons from the NWCF in-bed combustion system. The emission of unburned hydrocarbons is based on the fraction of unburned hydrocarbons in one WCF sample[5], doubled for contingency, and extrapolated to the maximum NWCF fuel capacity.

- Other volatile organics

  Emissions of the other volatile organics are based on vapor-pressure calculations for the sparged feed tanks, air lifts and the NWCF scrub system. Most of them are nearly totally discharged to the stack.

4.2 Substreams

The ASPEN simulation accounts for the components in two separate substreams: 1) a "mixed" substream containing gases, liquids and ions, and 2) a "CISolid" substream containing inert solids (i. e., do not participate in phase equilibria calculations). The separate substreams are useful for the filters which collect only solids. The reported stream tables for streams containing both substreams will list the substreams separately. Components are moved to the other substream by chemical reactions.

4.3 Major Block Types

The unit operations blocks used most in the simulation are:

- FLASH2

  The FLASH2 block calculates chemical and vapor-liquid equilibria (VLE) at the stated conditions which are pressure and either temperature or vapor fraction (fraction of the total moles in the feed put in the vapor).

- RSTOICH

  A RSTOICH block does the stated chemical reactions to the extent (fraction or moles) specified.

- SEP

  A SEP block does a component by component separation of a feed into two streams with the specified fraction or quantity of each component going to the specified stream.

- SSPLIT

  A SSPLIT block does a substream separation of a feed into two streams with the specified fraction or quantity of each substream going to the specified stream (e. g., 0.9997 of the CISolids on the filter).

4.4 Process and Vessel Simulation

The major process steps and vessels are represented by one or more blocks as described below.

- HLLWE

  The HLLWE is represented by a FLASH2 block (HLLWE) which calculates VLE and entrainment. The vapor fraction (VFRAC) is adjusted to give the desired bottoms density. The evaporator entrainment is set relatively high to represent worst-case operation.

```
   PPVAL H2O ( H3O+ F- ) 406.0699
   PPVAL ( H3O+ F- ) H2O -2173.069
   PPVAL HF ( H3O+ F- ) 3120.915
   PPVAL ( H3O+ F- ) HF -6113.476
   PPVAL H2O ( AL+3 NO3- ) 915.3977
   PPVAL ( AL+3 NO3- ) H2O -445.3932

PROP-DATA GMELCE-1
   IN-UNITS SI
   PROP-LIST GMELCE
   PPVAL H2O ( H3O+ NO3- ) 34.14618
   PPVAL ( H3O+ NO3- ) H2O -2.00109
   PPVAL H2O ( H3O+ CL- ) -45.824510
   PPVAL ( H3O+ CL- ) H2O 21.501220
   PPVAL HCL ( H3O+ CL- ) 279.97210
   PPVAL ( H3O+ CL- ) HCL 44.81820

PROP-SET RHO-SCR RHOMX UNITS='GM/CC' SUBSTREAM=MIXED PHASE=L

PROP-SET SCR-R VMX UNITS='GAL/HR' SUBSTREAM=MIXED

STREAM ACID-110
   SUBSTREAM MIXED TEMP=25 PRES=15 MASS-FLOW=56 NPHASE=1  &
      PHASE=L TOL=0.0001
   MASS-FRAC H2O 0.4 / HNO3 0.6

STREAM AL-101
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.81
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-102
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.81
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-103
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.81
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-189
   SUBSTREAM MIXED TEMP=25 PRES=62 MOLE-FLOW=1.1
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-A-RCY
   SUBSTREAM MIXED TEMP=30 PRES=20 MOLE-FLOW=0.1
   MOLE-FRAC O2 .2 / N2 .8

STREAM ANN
   SUBSTREAM MIXED TEMP=25 PRES=12.1 VOLUME-FLOW=59.1  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC NO3- 6.48 <MOL/L> / AL+3 2.16 <MOL/L>
   SUBSTREAM CISOLID TOL=0.0001

STREAM ANN-122
   SUBSTREAM MIXED TEMP=30 PRES=12.2 VOLUME-FLOW=1 SOLVENT=H2O  &
      NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC NO3- 6.6 <MOL/L> / AL+3 2.2 <MOL/L>
```

```
STREAM BLO-AIR
   SUBSTREAM MIXED TEMP=25 PRES=62 MOLE-FLOW=24.3
   MOLE-FRAC O2 .21 / N2 .79

STREAM BORIC-A
   SUBSTREAM MIXED TEMP=30 PRES=12.1 VOLUME-FLOW=19.05  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC H3BO3 0.763 <MOL/L>

STREAM CALC-AIR
   SUBSTREAM MIXED TEMP=25 PRES=110 MOLE-FLOW=142
   MOLE-FRAC O2 .21 / N2 .79

STREAM CANO3
   SUBSTREAM MIXED TEMP=25 PRES=12.1 VOLUME-FLOW=3.4  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC NO3- 8.6 <MOL/L> / CA+2 4.3 <MOL/L>

STREAM CYCL-OG
   SUBSTREAM MIXED TEMP=500 PRES=10.8
   MOLE-FLOW H2O 99 / HCL .027 / HF .005 / O2 46 / N2  &
      125 / NO 1 / NO2 9.2 / SO2 .0265 / CO 8 / CO2  &
      11 / HGCL2 .23 / E-GLYCOL .0008 / HEXONE .001 /  &
      METHANOL .0022 / UNB-FUEL .3 / H2 .05
   SUBSTREAM CISOLID TEMP=500 PRES=10.8
   MOLE-FLOW AL2O3 .148 / CAO .0092 / CDO .0026 / NANO3S  &
      .1 / B2O3 .011 / NACLS .003 / CASO4 .0015 / PBO  &
      .00023 / NIO .001 / CR2O3 .00084 / MN2O3 .0032

STREAM EQV-COND
   SUBSTREAM MIXED TEMP=28 PRES=12
   MOLE-FLOW H2O 4.78 / HNO3 .029 / HCL .00032 / HF  &
      .0002 / NO2 .00014 / HEXONE .0001 / METHANOL .001

STREAM EQV-MISC
   SUBSTREAM MIXED TEMP=30 PRES=12.1 MOLE-FLOW=6.5
   MOLE-FRAC H2O .04 / O2 .2 / N2 .76

STREAM FUEL
   SUBSTREAM MIXED TEMP=25 PRES=100 VOLUME-FLOW=45.6  &
      TOL=0.0001
   MASS-FRAC S .003 / FUEL .997

STREAM FUG-EMIS
   SUBSTREAM MIXED TEMP=30 PRES=12.2
   MASS-FLOW HNO3 .01

STREAM HEEL-188
   SUBSTREAM MIXED TEMP=30 PRES=12.2 VOLUME-FLOW=6.1  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC
;      Concentrations are listed here.

STREAM JST-122
   SUBSTREAM MIXED PRES=115 VFRAC=1 MASS-FLOW=50
   MOLE-FRAC H2O 1
```

4.5 Recycle Loops

The process simulation of Figure 3 contains five recycle loops:

- Transport air return TA-RET from the calcine bins to the calciner;
- NWCF scrub recycle from the scrub system to a NWCF feed vessel (NCC-103);
- Liquid drain (LIQ-110) from the NWCF mist separator to the scrubber;
- Acid vapors venting from the NWCF feed vessels (NCC-103 and -104) to the equipment vent condenser which drains condensate to the PEW evaporator and LET&D which collects the nitric acid in its bottoms and recycles it to the NWCF scrub system; and
- Acid vapors venting from the acid recycle vessel (A-RCY-T) to the equipment vent condenser also are returned to the PEW evaporator and LET&D.

5. RESULTS

The simulation program (ASPEN Plus, Rel 9), which operates in a sequential-modular mode, converged the recycle loops in 15 iterations. The calculated distributions of hazardous species are summarized in Table 1 which shows relative fractions (of the total of all input streams) in each product stream. The listed species are 1) F/HF, and 2) Cl/HCl and Cl_2, whose emissions depend on vapor-liquid equilibria, and 3) Cd which is typical of non-volatile ionic species. (Species whose emissions are specified to the program are not listed.) The calculated fractions to atmosphere are intended to be upper-level limits. Actual emissions will be lower than listed in Table 1. The calculated Cd emission to atmosphere is very low because of the multiple HEPA filters on each discharge stream. The overall material balances are successful.

Table 1. Calculated fractions in product streams of typical hazardous species.

Product Stream	Calcine	to Atm.	PEW Bot. to Tank Farm	NWCF Scr. to Tank Fm
F/HF.	0.948	0.026	0.021	0.0052
Cl/HCl[a]	0.461	0.13	0.036	0.013
Cl/Cl_2[a]		0.215		
Cd	0.995	2.4E-13	0.0007	0.004

a. Both HCl and Cl_2 are fractions of total Cl in feeds.

Some principles learned in developing the ICPP process simulation are of general application for development of large process simulations:

- Large simulations are best built in small sections and tested before adding more blocks. This approach facilitates locating the problems. It is especially desirable to add and test recycle loops one at a time. It is often helpful to test a recycle loop open (i. e., with a product stream) before closing the loop.

- The use of approximate initial values for recycle streams expedites the conversion of the recycle loop.

- It is desirable to add components and chemical reactions a few at a time so that problems of missing parameters or chemistry non-convergence can be located readily.

- Chemical reactions converge best when written in steps adding one molecule or ion at a time. For example, the reaction of mercuric ion with two chlorides does not converge unless written in two steps adding one chloride ion at a time. It is sometimes necessary to guess and enter a plausible intermediate with estimated properties to allow calculation of complex reactions.

- The convergence of chemical equilibria calculations and recycle loops are expedited if insignificant reactions are pruned out of the chemistry paragraph.

- It is important to have a charge balance for ionic species for every input stream. The results of chemical analyses, which seldom balance charges, should be adjusted to balance the charges of the ionic species.

6. REFERENCES

1. H. W. Godbee, "Use of Evaporation for the Treatment of Liquids in the Nuclear Industry", ORNL-4790, 1973.

2. R. E. Schindler, "Low Level Liquid Waste Treatment at the Idaho Chemical Processing Plant", WINCO-11721, 1991.

3. R. L. Hastings, "Idaho Chemical Processing Plant Liquid Effluent Treatment and Disposal Facility Hot Test Report", WINCO-1146, September 1993.

4. R. E. Schindler, "Removal of Particulate Solids from the Off-Gas of the WCF and NWCF", ICP-1157, June, 1978, p. 17.

5. J. A. Weilang, et. al., "The Fourth Processing Campaign in the Waste Calcining Facility, FY-1971", ICP-1004, 1972.

Appendix A

Aspen Input File

Appendix A

Aspen Input File

An annotated copy of the ASPEN input file is provided in this appendix for reference. The connectivity of the streams and blocks is shown in Figure 3.

A1 HELPS FOR READING FILE

Explanations of samples of some major blocks are given below to help in reading the input file.

A1.1 Flash Block

The FLASH block paragraph

```
BLOCK NCC-119 FLASH2
   PARAM TEMP=75 PRES=12 ENTRN=1.35E-5
```

asks block NCC-119 to calculate chemical and vapor-liquid equilibria for all species at 75 °C and 12 psia. The entrainment is 1.3E-5 (fraction) of the liquid into the vapor.

A1.2 RSTOIC Block

The RSTOIC block paragraph

```
BLOCK IB-COMB RSTOIC
   PARAM TEMP=500 PRES=10.8 NPHASE=2 SERIES=YES
   STOIC 1 MIXED FUEL -1 / UNB-FUEL 6 / H2 1
   STOIC 2 MIXED FUEL -2 / O2 -25 / CO 24 / H2O 26
   STOIC 4 MIXED FUEL -2 / O2 -37 / CO2 24 / H2O 26
   STOIC 3 MIXED S -1 / O2 -1 / SO2 1
   EXTENT 2 0.33469
   CONV 1 MIXED FUEL .03
   CONV 4 MIXED FUEL 1
   CONV 3 MIXED S 1
```

tells block IB-COMB to react the components (at 500 °C and 10.8 psia) in series:

1. react 0.03 (fraction) of the FUEL to UNB-FUEL and H_2,
2. react 0.33469 moles of FUEL to CO and H_2O,

3. react all the remaining FUEL to CO_2 and H_2O, and

4. react all the S to SO_2.

A1.3 SSPLIT Block

The SSPLIT block paragraph

```
BLOCK VOG-FLT SSPLIT
   FRAC MIXED VOG-FILT 0
   FRAC CISOLID VOG-FILT .9997
```

tells block VOG-FLT to put 0.9997 (fraction) of the incoming CISOLIDs into stream VOG-FILT and leave everything else in the other output stream.

A1.4 SEP Block

The SEP block paragraph

```
BLOCK HG-SEP SEP
   FRAC STREAM=HG-BP SUBSTREAM=MIXED COMPS=H2O HNO3 H3O+  &
      NO3- HCL CL- NANO3 NA+ HF F- AL+3 ALF+2 ALF2+ K+  &
      H3BO3 CD+2 CA+2 FE+3 SO4-2 O2 N2 NO NO2 SO2 CO CO2  &
      FUEL HGCL2 HGCL3- HGCL4-2 PB+2 NI+2 CR+3 MN+3 SE AS  &
      BENZENE E-GLYCOL CCL4 CHCL3 TR-ORGAN 111-TCA 112-TCA  &
      PERCHLOR HEXONE TOLUENE XYLENE METHANOL UNB-FUEL H2  &
      FRACS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  &
      0 0 0 0 0 0 0 0 0 .005 0 0 0 0 0 0 0 0 0 0  &
      0 0 0 0 0 0 0 0 0 0 0 0 0
   FRAC STREAM=HG-BP SUBSTREAM=CISOLID COMPS=AL2O3 FE2O3  &
      K2SO4 KNO3S CAF2 CACL2 CAO CDO NANO3S B2O3 NACLS  &
      CASO4 PBO NIO CR2O3 MN2O3 "SE(S)" "AS(S)" FRACS=0 0  &
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

tells block HG-SEP to separate 0.005 (fraction) of the HG from the mixed substreams of the feed into stream HG-BP, and leave everything else in the other output stream.

2.0 TEXT OF INPUT FILE

The input file is listed below with annotation in lines beginning with a semi-colon.

```
;
;Input Summary created by ASPEN PLUS Rel. 9.1-3  on  12:22:49 Tue Dec 20, 1994
;Directory D:\ASPENRUN\NWCF  Filename D:\ASPENRUN\NWCF\wc-per-c.inp
```

```
;

TITLE 'WASTE SYSTEMS SIMULATION FOR PTO PERMIT    '

;
;Input file created by ModelManager Rel. 3.3-6 on Mon Dec 20 10:25:10 1993
;Directory C:\ASPENRUN\PR-TEST  Runid EV-PROP3
;

; The following units are default units used unles specified
; otherwise.
IN-UNITS ENG VOLUME-FLOW='GAL/HR' TEMPERATURE=C VOLUME=GAL  &
      DELTA-T=C HEAD=INCH MOLE-DENSITY='MOL/L'  &
      MASS-DENSITY='GM/CC' MOLE-VOLUME='CUM/KMOL'

DEF-STREAMS MIXCISLD ALL

SIM-OPTIONS
   IN-UNITS ENG
   SIM-OPTIONS TLOWER=0 <C> TUPPER=1000 <C> PUPPER=200  &
      MW-CALC=NO

RUN-CONTROL MAX-TIME=9000

DESCRIPTION "
      CONTAINS PARAMETERS FROM ALNO3-PR, MHNO3R3, MHCLR1, MHF
      Simplified Case with WM-189 "

DATABANKS AQUEOUS  / ASPENPCD  / SOLIDS  / PURE856  /  &
      COMBUST  / INORGANIC

PROP-SOURCES AQUEOUS  / ASPENPCD  / SOLIDS  / PURE856  /  &
      COMBUST  / INORGANIC

COMPONENTS
   H2O H2O H2O /
   HNO3 HNO3 HNO3 /
   H3O+ H3O+ H3O+ /
   NO3- NO3- NO3- /
   HCL HCL HCL /
   CL- CL- CL- /
   NANO3 NANO3 NANO3 /
   NA+ NA+ NA+ /
   HF HF HF /
   F- F- F- /
   "AL(NO3)3" "AL(OH)3" "AL(NO3)3" /
   AL+3 AL+3 AL+3 /
   ALF+2 ALF+2 ALF+2 /
   ALF2+ ALF2+ ALF2+ /
   KNO3 KNO3 KNO3 /
   K+ K+ K+ /
   H3BO3 H3BO3 H3BO3 /
   CD+2 CD+2 CD+2 /
   CA+2 CA+2 CA+2 /
```

FE+3 FE+3 FE+3 /
SO4-2 SO4-2 SO4-2 /
O2 O2 O2 /
N2 N2 N2 /
NO NO NO /
NO2 NO2 NO2 /
S S S /
SO2 O2S SO2 /
CO CO CO /
CO2 CO2 CO2 /
CL2 CL2 CL2 /
FUEL C12H26 FUEL /
AL2O3 AL2O3-2 AL2O3 /
FE2O3 FE2O3 FE2O3 /
K2SO4 K2SO4 K2SO4 /
KNO3S KNO3 KNO3S /
CAF2 CAF2 CAF2 /
CACL2 CACL2 CACL2 /
CAO CAO CAO /
CDO CAO CDO /
NANO3S NANO3 NANO3S /
B2O3 B2O3 B2O3 /
NACLS NACL NACLS /
HGCL2 PBCL2 HGCL2 /
HGCL3- HGCL3- HGCL3- /
HGCL4-2 SO4-2 HGCL4-2 /
CASO4 CASO4 CASO4 /
HG HG HG /
CD CD CD /
PB PB PB /
PB+2 PB+2 PB+2 /
PBO PBSO4 PBO /
NI NI NI /
NI+2 NI+2 NI+2 /
NIO NIO NIO /
CR CR CR /
CR+3 CR+3 CR+3 /
CR2O3 CR2O3 CR2O3 /
MN MN MN /
MN+3 MN+3 MN+3 /
MN2O3 MN2O3 MN2O3 /
SE PB SE /
"SE(S)" PB "SE(S)" /
AS AS AS /
"AS(S)" AS "AS(S)" /
BENZENE C6H6 BENZENE /
E-GLYCOL C2H6O2 E-GLYCOL /
CCL4 CCL4 CCL4 /
CHCL3 CHCL3 CHCL3 /
TR-ORGAN CH3CL TR-ORGAN /
111-TCA C2H3CL3-D0 111-TCA /
112-TCA C2H3CL3 112-TCA /
PERCHLOR C2H2CL4-D2 PERCHLOR /
HEXONE C6H12O-2 HEXONE /
TOLUENE C7H8 TOLUENE /
XYLENE C8H10-1 XYLENE /

```
   METHANOL CH4O METHANOL /
   UNB-FUEL C2H4 UNB-FUEL /
   H2 H2 H2

; HENRY-COMPS are super-critical components whose VLE is
; calculated by Henry's Law using the coefficients in paragraph
; HENRY-1.
HENRY-COMPS NWCF O2 N2 NO SO2 CL2 CO CO2 UNB-FUEL TR-ORGAN  &
      H2

; Equilibria for the chemical reactions listed below is
; calculated for every stream and block in the global section.
CHEMISTRY CPP
   IN-UNITS MET
   DISS "AL(NO3)3" AL+3 1.0 / NO3- 3.0
   DISS NANO3 NA+ 1.0 / NO3- 1.0
   DISS KNO3 K+ 1 / NO3- 1
   STOIC 1 HCL -1.0 / H2O -1.0 / H3O+ 1.0 / CL- 1.0
   STOIC 2 HNO3 -1.0 / H2O -1.0 / H3O+ 1.0 / NO3- 1.0
   STOIC 3 HF -1.0 / H2O -1.0 / H3O+ 1.0 / F- 1.0
   STOIC 4 AL+3 -1 / F- -1 / ALF+2 1
   STOIC 5 ALF+2 -1 / F- -1 / ALF2+ 1
   K-STOIC 1 A=52.229750 C=-5.0 D=-.05057952
   K-STOIC 2 A=119.89190 B=-8608.460 C=-12.069460 D=-.06584351

FLOWSHEET
   BLOCK HLLWE IN=P-HLWE LIQ-104 OUT=WE-VAP HOT-BOT
   BLOCK WE-COND IN=WE-VAP OUT=WE-COND
   BLOCK JET-122 IN=LIQ-122A JST-122 OUT=PEW-122
   BLOCK PEW-EVAP IN=PEW-122 PEW-MISC OUT=PEW-VAP PEW-BOT
   BLOCK WL-101 IN=PEW-BOT OUT=TO-NA-WA
   BLOCK SCRUB IN=SCR-INT OUT=SCR-OGA SCR-SOLN
   BLOCK NCC-108 IN=SCR-SOLN OUT=SCR-RCYL SCR-B
   BLOCK SCR-RX IN=TO-SCRUB LETDACID NCM-ACID LIQ-110 OUT= &
      SCR-INT
   BLOCK NCC-119 IN=HOT-BOT SP-119 OUT=VT-119 L-119
   BLOCK NCC-104 IN=BL-FEED AL-103 SP-104 OUT=VT-104  &
      FEED-104
   BLOCK NCC-103 IN=SCR-RCYL AL-102 SP-103 BL-FEED2 OUT= &
      VT-103 BL-FEED
   BLOCK EQV-COND IN=EQ-VTA OUT=EQ-VTB EQV-COND
   BLOCK NCC-102 IN=CANO3 ANN BORIC-A WC-FEED SP-102 OUT= &
      VT-102 BL-FEEDA
   BLOCK NCC-122 IN=WE-COND ANN-122 NWCF-PEW SP-122 EQV-COND  &
      OUT=VT-122 LIQ-122A
   BLOCK NCC-152 IN=LIQ-101 AL-101 SP-152 OUT=VT-152 LIQ-104
   BLOCK NCC-101 IN=SP-101 F-189 WM-183 OUT=VT-101 LIQ-101
   BLOCK AL-189 IN=AL-189 WM-189 OUT=VT-189 F-189
   BLOCK NCC-110 IN=SCR-OGA ACID-110 OUT=SCR-OGB LIQ-110
   BLOCK TK-FARM IN=BOT-PROD HEEL-188 OUT=TF-LIQ
   BLOCK SPL-CLR IN=SPL OUT=HLWE-SPL
   BLOCK A-RCY-T IN=ACID-RCY AL-A-RCY OUT=A-R-VT LETDACID

FLOWSHEET PROD
   BLOCK LETD-SH IN=LETD-VAP OUT=SH-VAP
   BLOCK LETD IN=LETDFEED OUT=HOT-ACID LETD-VAP
```

```
   BLOCK PEW-COND IN=PEW-VAP OUT=PEW-COND
   BLOCK ACID-RX IN=SCR-B OUT=SCR-TF
   BLOCK JET-TF IN=TF-LIQ TF-JST OUT=WC-FEED
   BLOCK ACID-CLR IN=HOT-ACID OUT=ACID-RCY

FLOWSHEET REACT
   BLOCK CALCINER IN=COMB-PR TA-RET FEED-104 OUT=CALC-PR
   BLOCK IB-COMB IN=FUEL NOZ-O2 CALC-AIR OUT=COMB-PR
   BLOCK CLC-PTO IN=CALC-PR OUT=TO-CYCL BED-PR
   BLOCK CYCLONE IN=TO-CYCL OUT=CYCL-OG CYC-SOL
   BLOCK S-TR IN=BED-PR TR-AIR CYC-SOL OUT=SOL-TR
   BLOCK BIN-CYCL IN=SOL-TR OUT=CALCINE TA-RET
   BLOCK SCR-BP IN=CYCL-OG OUT=SOL-BP TO-SCRUB
   BLOCK WC-FILT IN=WC-OG OUT=WC-FILT FLT-OG
   BLOCK APS-FILT IN=APS-A WC-EFFLB OUT=APS-FILT APS-B
   BLOCK REP-CONV IN=LETD-EFL APS-EFFL OUT=ATM-EFFL
   BLOCK LETD-FLT IN=SH-VAP OUT=LETDFILT LETD-EFL
   BLOCK M-EQV IN=EQ-VTB EQV-BP OUT=EQ-VTC
   BLOCK APS-HTR IN=VOG-F OUT=APS-A
   BLOCK VOG-FLT IN=VOG-A OUT=VOG-FILT VOG-F
   BLOCK VOG-RX IN=VT-189 VOG-601 PILOT-PL FUG-EMIS OUT= &
      VOG-A
   BLOCK HTR-335 IN=SOL-BP EQ-VTC SCR-OGB HG-BP OUT=WC-OG
   BLOCK SPL-119 IN=L-119 OUT=BOT-PROD SPL
   BLOCK BLO-243 IN=FLT-OG BLO-AIR OUT=WC-EFFL
   BLOCK APS-RX IN=G-I OUT=G-O
   BLOCK S-GB IN=APS-B OUT=BP-G G-I
   BLOCK M-GB IN=G-O BP-G OUT=APS-EFFL
   BLOCK EQV-SEP IN=VT-122 VT-152 EQV-MISC VT-119 VT-102 &
      VT-101 A-R-VT VT-103 VT-104 OUT=EQV-BP EQ-VTA
   BLOCK CL-CHEM IN=PEW-COND OUT=LETDFEED
   BLOCK LN-COOL IN=WC-EFFL OUT=WC-EFFLB
   BLOCK CLEANUP IN=ATM-EFFL OUT=IONS TO-STACK
   BLOCK HG-SEP IN=BL-FEEDA OUT=HG-BP BL-FEED2
   BLOCK STACK IN=VTL-AIR TO-STACK OUT=TO-ATM

PROPERTIES SYSOP15M HENRY-COMPS=NWCF CHEMISTRY=CPP &
      TRUE-COMPS=YES
   PROPERTIES SYSOP15M PROD / IDEAL REACT

PROP-REPLACE SYSOP15M ELECNRTL
   PROP PHIVMX PHIVMX03
   PROP PHILMX PHILMX39
   PROP HVMX HVMX00
   PROP HLMX HLMX15M
   PROP GVMX GVMX00
   PROP GLMX GLMX15M
   PROP SVMX SVMX00
   PROP SLMX SLMX15M
   PROP VVMX VVMX00
   PROP VLMX VLMX18A
   PROP PHIV PHIV00
   PROP HV HV00
   PROP HL HL00
   PROP GV GV00
   PROP GL GL00
```

```
   PROP SV SV00
   PROP SL SL00
   PROP VV VV00
   PROP KV KV00

PROP-DATA DATA1
   IN-UNITS SI
   PROP-LIST DHFORM / DGFORM
   PVAL HF -2.72550E+08 / -2.74640E+08
   PROP-LIST DHFORM / DGFORM / MW / TB / TC / PC / VC  &
      / ZC / OMEGA
   PVAL HNO3 -1.35060E+08 / -74720000.0 / 63.01290 /  &
      356.150 / 520.0 / 6890100.0 / .1450 / .2310 /  &
      .71440
   PROP-LIST DHFORM / TC / PC / VC / ZC / OMEGA /  &
      DGSFRM / DHSFRM / DGAQFM / DHAQFM / S025C
   PVAL H3BO3 -994.1E+6 / 2000 / 3E7 / .37 / .26 / .3 /  &
      -968.92E+6 / -1.09433E+9 / -968.75E+6 / -1.07232E+9 /  &
      162300
   PROP-LIST DHFORM / DGFORM / MW / TC / PC / VC / ZC  &
      / OMEGA / DGSFRM / DHSFRM / DGAQFM / DHAQFM /  &
      S025C
   PVAL HGCL2 -146.294E6 / -145.035E6 / 271.496 / 2000 /  &
      5E6 / 0.1 / 0.2 / 1 / -178.6E+6 / -224.3E+6 /  &
      -173.2E+6 / -216.3E-6 / 155000
   PROP-LIST DHFORM / DGSFRM / DHSFRM
   PVAL CAF2 -1.2196E+9 / -1.1673E+9 / -1.2196E+9
   PROP-LIST MW
   PVAL CDO 128.41
   PVAL PBO 223.21
   PVAL "SE(S)" 78.96
   PROP-LIST MW / DGAQFM / DHAQFM / S025C
   PVAL HGCL4-2 342.402 / -446.8E+6 / -554E+6 / 293000
   PROP-LIST MW / TB / TC / PC / VC / ZC
   PVAL SE 78.96 / 1000 / 2000 / 3E7 / .37 / .25

PROP-DATA PARAMAL
   IN-UNITS SI
   PROP-LIST CHARGE / DHSFRM / DGSFRM / MW
   PVAL "AL(NO3)3" .0 / -1042E+6 / -727.4E+6 / 213.0

PROP-DATA CORR1
   IN-UNITS SI
   PROP-LIST CPIG
   PVAL "AL(NO3)3" 100000.0 0.0 0.0 0.0 0.0 0.0 0.0  &
      1000.000 1.0000E+28 1.0000E+28 1.0000E+28
   PVAL H3BO3 82080 -10.526 .04094 -2.497E-5 6.446E-9  &
      -6.25E-13 200 1000 82080 -10.526 1
   PVAL HGCL2 53141 16.72 0.0 0.0 0.0 0.0 273 400 53141  &
      16.72 1

PROP-DATA CPD-HF
   IN-UNITS SI
   PROP-LIST CPDIEC
   PVAL HF 83.60 .0 273.150
```

```
PROP-DATA CPS-AL
   IN-UNITS SI
   PROP-LIST CPSPO1
   PVAL "AL(NO3)3" 232000.0 0.0 0.0 0.0 0.0 0.0 0.0  &
      1000.000
   PVAL H3BO3 1.45E5 183.7 0.0 -1.3E5 2.23E9 -2.27E9 250  &
      1000

PROP-DATA DATA2
   IN-UNITS SI
   PROP-LIST VLBROC
   PVAL HNO3 .04640 0.0

PROP-DATA DATA5
   IN-UNITS SI
   PROP-LIST DHVLWT
   PVAL HNO3 39040000.0 298.150 .3800000 0.0 0.0
   PVAL H3BO3 7.545E7 360 .3800000 0.0 0.0
   PVAL HGCL2 82.155E+6 400 .3256 0.0 273

PROP-DATA PLX-AL
   IN-UNITS SI
   PROP-LIST PLXANT
   PVAL "AL(NO3)3" -1.0E+28 0.0 0.0 0.0 0.0 0.0 0.0 250  &
      1000
   PVAL H3BO3 -1.0E+28 0.0 0.0 0.0 0.0 0.0 0.0 250 1000
   PVAL HGCL2 42.63 -10550 0.0 0.0 -2 0.0 0.0 273 550
   PVAL PB -1E+28 0.0 0.0 0.0 0.0 0.0 0.0 250 1000
   PVAL NI -1E+28 0.0 0.0 0.0 0.0 0.0 0.0 250 1000
   PVAL MN -1E+28 0.0 0.0 0.0 0.0 0.0 0.0 250 1000

PROP-DATA PLX-HCL
   IN-UNITS SI
   PROP-LIST PLXANT
   PVAL HCL 105.160 -3748.40 .0 .0 -15.2140 .0317370 1.0  &
      158.970 324.650

PROP-DATA PLX-HF
   IN-UNITS SI
   PROP-LIST PLXANT
   PVAL HF 59.5440 -4143.80 .0 .0 -6.17640 .0000141610 2.0  &
      189.790 461.150

PROP-DATA PLX-HNA
   IN-UNITS SI
   PROP-LIST PLXANT
   PVAL HNO3 -281.8727 0.0 0.0 -.1358019 58.15114 0.0 0.0  &
      231.55 376.1

PROP-DATA VSP-AL
   IN-UNITS SI
   PROP-LIST VSPOLY
   PVAL "AL(NO3)3" .060 0.0 0.0 0.0 0.0 0.0 1000.000
   PVAL H3BO3 .043 0.0 0.0 0.0 0.0 0.0 1000.000

PROP-DATA GMELCA-1
```

```
   IN-UNITS SI
   PROP-LIST GMELCA
   BPVAL HNO3 H2O -3.735254
   BPVAL H2O HNO3 16.31065
   BPVAL H2O HCL 5.8993890
   BPVAL H2O HF 3.227835
   BPVAL H2O HGCL2 -8
   BPVAL HCL H2O -.010413780
   BPVAL HF H2O -.8770385
   BPVAL HGCL2 H2O 5

PROP-DATA GMELCB-1
   IN-UNITS SI
   PROP-LIST GMELCB
   BPVAL HNO3 H2O 285.6733
   BPVAL H2O HNO3 -5550.353
   BPVAL H2O HCL -405.31640
   BPVAL H2O HF -2043.17
   BPVAL H2O HGCL2 3870
   BPVAL HCL H2O -83.92130
   BPVAL HF H2O -217.7091

PROP-DATA GMELCM-1
   IN-UNITS SI
   PROP-LIST GMELCM
   BPVAL H2O HF .30
   BPVAL HF H2O .30

PROP-DATA HENRY-1
   IN-UNITS ENG VOLUME-FLOW='GAL/HR' TEMPERATURE=C VOLUME=GAL  &
      DELTA-T=C HEAD=INCH MOLE-DENSITY='MOL/L'  &
      MASS-DENSITY='GM/CC' MOLE-VOLUME='CUM/KMOL'
   PROP-LIST HENRY
   BPVAL O2 H2O 147.0825 -7775.060 -18.39740 -9.4435E-3  &
      .8500061 74.85000
   BPVAL N2 H2O 167.6685 -8432.770 -21.55800 -8.4362E-3  &
      -.1499939 72.85000
   BPVAL NO H2O 170.5195 -8232.090 -22.80860 .0261350  &
      -.1499939 79.85000
   BPVAL SO2 H2O 17.72618 -2872.960 -.3028800 0.0 9.850000  &
      112.8500
   BPVAL CO H2O 174.4495 -8296.750 -23.33720 0.0 -.1499939  &
      79.85000
   BPVAL CO2 H2O 162.5395 -8741.550 -21.66900 1.10259E-3  &
      -.1499939 79.85000
   BPVAL CL2 H2O -105.7012 2428.620 19.18540 -8.9206E-3  &
      9.850000 39.85000
   BPVAL TR-ORGAN H2O 175.1895 -9768.620 -23.42400 0.0  &
      3.850000 79.85000
   BPVAL UNB-FUEL H2O 155.6105 -7959.740 -20.51080 0.0  &
      13.85000 72.85000
   BPVAL H2 H2O 182.7405 -6993.510 -26.31190 .0150431  &
      .8500061 65.85000

PROP-DATA NRTL-1
   IN-UNITS ENG VOLUME-FLOW='GAL/HR' TEMPERATURE=C VOLUME=GAL  &
```

```
   DELTA-T=C HEAD=INCH MOLE-DENSITY='MOL/L' &
   MASS-DENSITY='GM/CC' MOLE-VOLUME='CUM/KMOL'
PROP-LIST NRTL
BPVAL H2O E-GLYCOL .3184000 33.27720 .3000000 0.0 0.0 0.0 &
   30.40000 196.7000
BPVAL E-GLYCOL H2O .0531000 -174.4635 .3000000 0.0 0.0 &
   0.0 30.40000 196.7000
BPVAL H2O CO2 10.06400 -3268.135 .2000000 0.0 0.0 0.0 &
   6.10352E-6 200.0000
BPVAL CO2 H2O 10.06400 -3268.135 .2000000 0.0 0.0 0.0 &
   6.10352E-6 200.0000
BPVAL H2O BENZENE 140.0874 -5954.307 .2000000 0.0 &
   -20.02540 0.0 .8000061 77.00000
BPVAL BENZENE H2O 45.19050 591.3676 .2000000 0.0 -7.562900 &
   0.0 .8000061 77.00000
BPVAL H2O FUEL -8.414700 4175.207 .2000000 0.0 0.0 0.0 &
   25.00000 40.00000
BPVAL FUEL H2O -8.414700 4175.207 .2000000 0.0 0.0 0.0 &
   25.00000 40.00000
BPVAL H2O CCL4 491.7993 -21148.08 .2000000 0.0 -72.56400 &
   0.0 6.10352E-6 50.00000
BPVAL CCL4 H2O 196.5118 -6260.020 .2000000 0.0 -29.86000 &
   0.0 6.10352E-6 50.00000
BPVAL H2O 111-TCA 91.94810 -4284.994 .2000000 0.0 &
   -12.41430 0.0 6.10352E-6 50.00000
BPVAL 111-TCA H2O 383.3660 -14261.07 .2000000 0.0 &
   -58.13810 0.0 6.10352E-6 50.00000
BPVAL H2O 112-TCA -108.7561 4489.956 .2000000 0.0 17.46070 &
   0.0 6.10352E-6 55.00000
BPVAL 112-TCA H2O 670.9628 -26907.78 .2000000 0.0 &
   -101.3913 0.0 6.10352E-6 55.00000
BPVAL H2O CHCL3 8.843600 -1140.115 .2000000 0.0 0.0 0.0 &
   -.9999939 54.00000
BPVAL CHCL3 H2O -7.351900 3240.688 .2000000 0.0 0.0 0.0 &
   -.9999939 54.00000
BPVAL H2O PERCHLOR .4753000 676.9839 .3000000 0.0 0.0 0.0 &
   94.50000 131.5000
BPVAL PERCHLOR H2O -19.48130 8143.495 .3000000 0.0 0.0 &
   0.0 94.50000 131.5000
BPVAL H2O HEXONE 9.124600 -1482.945 .3000000 0.0 0.0 0.0 &
   87.85000 116.0000
BPVAL HEXONE H2O -6.773000 2839.433 .3000000 0.0 0.0 0.0 &
   87.85000 116.0000
BPVAL H2O TOLUENE 627.0528 -27269.36 .2000000 0.0 &
   -92.71820 0.0 -9.000000 93.00000
BPVAL TOLUENE H2O -247.8792 14759.76 .2000000 0.0 35.58200 &
   0.0 -9.000000 93.00000
BPVAL H2O XYLENE 4.238800 1246.888 .2000000 0.0 0.0 0.0 &
   6.10352E-6 25.00000
BPVAL XYLENE H2O -5.627500 2996.679 .2000000 0.0 0.0 0.0 &
   6.10352E-6 25.00000
BPVAL H2O METHANOL 4.824100 -1329.544 .3000000 0.0 0.0 &
   0.0 24.99000 188.3000
BPVAL METHANOL H2O -2.626000 828.3871 .3000000 0.0 0.0 &
   0.0 24.99000 188.3000
BPVAL H2O HF 97.28083 0.0 .3000000 0.0 0.0 0.0 25.00000 &
```

```
    110.0000
  BPVAL HF H2O -2.297253 0.0 .3000000 0.0 0.0 0.0 25.00000  &
    110.0000

PROP-DATA VLCLK-1
  IN-UNITS SI
  PROP-LIST VLCLK
  BPVAL AL+3 NO3- .0422850 .09233650
  BPVAL H3O+ NO3- .02852803 .06734272
  BPVAL NA+ NO3- .02604560 .02904670
  BPVAL ALF+2 NO3- .0423 .09233
  BPVAL K+ NO3- .037901 .024333
  BPVAL FE+3 NO3- .052586 .158299
  BPVAL CR+3 NO3- .052586 .158299
  BPVAL MN+3 NO3- .052586 .158299
  BPVAL NI+2 NO3- .052586 .158299

PROP-DATA GMELCC-1
  IN-UNITS SI
  PROP-LIST GMELCC
  PPVAL H2O ( H3O+ CL- ) 1.5501250
  PPVAL ( H3O+ CL- ) H2O -3.1792790
  PPVAL H2O ( H3O+ NO3- ) -9.3353140
  PPVAL ( H3O+ NO3- ) H2O .3928543
  PPVAL HNO3 ( H3O+ NO3- ) -8.261029
  PPVAL ( H3O+ NO3- ) HNO3 24.49516
  PPVAL HCL ( H3O+ CL- ) 4.2507620
  PPVAL ( H3O+ CL- ) HCL -2.6264610
  PPVAL ( H3O+ NO3- ) ( H3O+ CL- ) 15.0
  PPVAL ( H3O+ CL- ) ( H3O+ NO3- ) 3.253562
  PPVAL H2O ( H3O+ F- ) 14.75332
  PPVAL ( H3O+ F- ) H2O -1.153951
  PPVAL HF ( H3O+ F- ) -1.50336
  PPVAL ( H3O+ F- ) HF 6.352884
  PPVAL H2O ( AL+3 NO3- ) 7.188743
  PPVAL ( AL+3 NO3- ) H2O -3.694923
  PPVAL HNO3 ( AL+3 NO3- ) 5.327914
  PPVAL ( AL+3 NO3- ) HNO3 -2.970832
  PPVAL ( H3O+ NO3- ) ( AL+3 NO3- ) 10.0
  PPVAL ( AL+3 NO3- ) ( H3O+ NO3- ) -1.74129
  PPVAL H2O ( NA+ NO3- ) 7.1670
  PPVAL ( NA+ NO3- ) H2O -3.6450
  PPVAL HNO3 ( NA+ NO3- ) 30.0
  PPVAL ( NA+ NO3- ) HNO3 -3.370273

PROP-DATA GMELCD-1
  IN-UNITS SI
  PROP-LIST GMELCD
  PPVAL H2O ( H3O+ NO3- ) 5741.4060
  PPVAL ( H3O+ NO3- ) H2O -1504.3830
  PPVAL HNO3 ( H3O+ NO3- ) 9000.0
  PPVAL ( H3O+ NO3- ) HNO3 -8323.403
  PPVAL H2O ( H3O+ CL- ) 2933.7170
  PPVAL ( H3O+ CL- ) H2O -654.65570
  PPVAL HCL ( H3O+ CL- ) -1060.760
  PPVAL ( H3O+ CL- ) HCL 169.3420
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   PPVAL H2O ( H3O+ F- ) 406.0699
   PPVAL ( H3O+ F- ) H2O -2173.069
   PPVAL HF ( H3O+ F- ) 3120.915
   PPVAL ( H3O+ F- ) HF -6113.476
   PPVAL H2O ( AL+3 NO3- ) 915.3977
   PPVAL ( AL+3 NO3- ) H2O -445.3932

PROP-DATA GMELCE-1
   IN-UNITS SI
   PROP-LIST GMELCE
   PPVAL H2O ( H3O+ NO3- ) 34.14618
   PPVAL ( H3O+ NO3- ) H2O -2.00109
   PPVAL H2O ( H3O+ CL- ) -45.824510
   PPVAL ( H3O+ CL- ) H2O 21.501220
   PPVAL HCL ( H3O+ CL- ) 279.97210
   PPVAL ( H3O+ CL- ) HCL 44.81820

PROP-SET RHO-SCR RHOMX UNITS='GM/CC' SUBSTREAM=MIXED PHASE=L

PROP-SET SCR-R VMX UNITS='GAL/HR' SUBSTREAM=MIXED

STREAM ACID-110
   SUBSTREAM MIXED TEMP=25 PRES=15 MASS-FLOW=56 NPHASE=1  &
      PHASE=L TOL=0.0001
   MASS-FRAC H2O 0.4 / HNO3 0.6

STREAM AL-101
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.81
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-102
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.81
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-103
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.81
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-189
   SUBSTREAM MIXED TEMP=25 PRES=62 MOLE-FLOW=1.1
   MOLE-FRAC O2 .21 / N2 .79

STREAM AL-A-RCY
   SUBSTREAM MIXED TEMP=30 PRES=20 MOLE-FLOW=0.1
   MOLE-FRAC O2 .2 / N2 .8

STREAM ANN
   SUBSTREAM MIXED TEMP=25 PRES=12.1 VOLUME-FLOW=59.1  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC NO3- 6.48 <MOL/L> / AL+3 2.16 <MOL/L>
   SUBSTREAM CISOLID TOL=0.0001

STREAM ANN-122
   SUBSTREAM MIXED TEMP=30 PRES=12.2 VOLUME-FLOW=1 SOLVENT=H2O  &
      NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC NO3- 6.6 <MOL/L> / AL+3 2.2 <MOL/L>
```

```
STREAM BLO-AIR
   SUBSTREAM MIXED TEMP=25 PRES=62 MOLE-FLOW=24.3
   MOLE-FRAC O2 .21 / N2 .79

STREAM BORIC-A
   SUBSTREAM MIXED TEMP=30 PRES=12.1 VOLUME-FLOW=19.05  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC H3BO3 0.763 <MOL/L>

STREAM CALC-AIR
   SUBSTREAM MIXED TEMP=25 PRES=110 MOLE-FLOW=142
   MOLE-FRAC O2 .21 / N2 .79

STREAM CANO3
   SUBSTREAM MIXED TEMP=25 PRES=12.1 VOLUME-FLOW=3.4  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC NO3- 8.6 <MOL/L> / CA+2 4.3 <MOL/L>

STREAM CYCL-OG
   SUBSTREAM MIXED TEMP=500 PRES=10.8
   MOLE-FLOW H2O 99 / HCL .027 / HF .005 / O2 46 / N2  &
      125 / NO 1 / NO2 9.2 / SO2 .0265 / CO 8 / CO2  &
      11 / HGCL2 .23 / E-GLYCOL .0008 / HEXONE .001 /  &
      METHANOL .0022 / UNB-FUEL .3 / H2 .05
   SUBSTREAM CISOLID TEMP=500 PRES=10.8
   MOLE-FLOW AL2O3 .148 / CAO .0092 / CDO .0026 / NANO3S  &
      .1 / B2O3 .011 / NACLS .003 / CASO4 .0015 / PBO  &
      .00023 / NIO .001 / CR2O3 .00084 / MN2O3 .0032

STREAM EQV-COND
   SUBSTREAM MIXED TEMP=28 PRES=12
   MOLE-FLOW H2O 4.78 / HNO3 .029 / HCL .00032 / HF  &
      .0002 / NO2 .00014 / HEXONE .0001 / METHANOL .001

STREAM EQV-MISC
   SUBSTREAM MIXED TEMP=30 PRES=12.1 MOLE-FLOW=6.5
   MOLE-FRAC H2O .04 / O2 .2 / N2 .76

STREAM FUEL
   SUBSTREAM MIXED TEMP=25 PRES=100 VOLUME-FLOW=45.6  &
      TOL=0.0001
   MASS-FRAC S .003 / FUEL .997

STREAM FUG-EMIS
   SUBSTREAM MIXED TEMP=30 PRES=12.2
   MASS-FLOW HNO3 .01

STREAM HEEL-188
   SUBSTREAM MIXED TEMP=30 PRES=12.2 VOLUME-FLOW=6.1  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC
;     Concentrations are listed here.

STREAM JST-122
   SUBSTREAM MIXED PRES=115 VFRAC=1 MASS-FLOW=50
   MOLE-FRAC H2O 1
```

```
STREAM NCM-ACID
   SUBSTREAM MIXED TEMP=30 PRES=15 MASS-FLOW=20 NPHASE=1  &
      PHASE=L TOL=0.0001
   MASS-FRAC H2O .4 / HNO3 .6

STREAM NOZ-O2
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=35.25
   MOLE-FRAC O2 1

STREAM NWCF-PEW
   SUBSTREAM MIXED TEMP=30 PRES=12.1 VOLUME-FLOW=2.5  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MASS-CONC HNO3 31000 <MG/L> / HCL 10 <MG/L> / NANO3  &
      1500 <MG/L> / "AL(NO3)3" 5000 <MG/L> / KNO3 50 <MG/L>

STREAM P-HLWE
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.044
   MOLE-FRAC O2 .21 / N2 .79

STREAM PEW-MISC
   SUBSTREAM MIXED TEMP=30 PRES=12.2 VOLUME-FLOW=439  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MASS-CONC HNO3 21.5 <GM/L> / HCL .05 <GM/L> / NANO3  &
      .82 <GM/L> / HF .05 <GM/L> / "AL(NO3)3" 1 <GM/L> /  &
      KNO3 .17 <GM/L> / METHANOL .01 <GM/L>

STREAM PILOT-PL
   SUBSTREAM MIXED TEMP=100 PRES=12.2
   MASS-FLOW HNO3 .2 / HCL .06 / HF .13 / SO2 .02 / CO  &
      17.6 / HGCL2 1.5E-6 / UNB-FUEL .037
   SUBSTREAM CISOLID TEMP=100 PRES=12.2
   MASS-FLOW CDO 2.5E-9 / PBO 2.5E-9 / CR2O3 2.5E-9 /  &
      MN2O3 1E-8

STREAM SCR-OGA
   SUBSTREAM MIXED TEMP=63.3 PRES=8.2
   MOLE-FLOW H2O 96 / HNO3 .24 / HCL .0063 / HF .0017 /  &
      O2 47 / N2 125 / NO 1 / NO2 9.1 / SO2 .026 /  &
      CO 8 / CO2 11.2 / HGCL2 .0001 / E-GLYCOL 3.4E-5 /  &
      HEXONE .0016 / METHANOL .0022 / UNB-FUEL .3 / H2  &
      .05

STREAM SP-101
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=2.17
   MOLE-FRAC O2 .21 / N2 .79

STREAM SP-102
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=2.17
   MOLE-FRAC O2 .21 / N2 .79

STREAM SP-103
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=2.17
   MOLE-FRAC O2 .21 / N2 .79

STREAM SP-104
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.535
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   MOLE-FRAC O2 .21 / N2 .79

STREAM SP-119
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=3.94
   MOLE-FRAC O2 .21 / N2 .79

STREAM SP-122
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=3.94
   MOLE-FRAC O2 .21 / N2 .79

STREAM SP-152
   SUBSTREAM MIXED TEMP=25 PRES=32 MOLE-FLOW=.55
   MOLE-FRAC O2 .21 / N2 .79

STREAM TA-RET
   SUBSTREAM MIXED TEMP=230 PRES=10.8
   MOLE-FLOW O2 3.4 / N2 12.8
   SUBSTREAM CISOLID TEMP=230 PRES=10.8
   MOLE-FLOW AL2O3 .04 / K2SO4 .0024 / CAF2 .007 / CAO  &
      .0026 / CDO .0008 / NANO3S .032 / B2O3 .0035 /  &
      NACLS .0013 / CASO4 .0007 / PBO .0001 / NIO .00045  &
      / CR2O3 .0004 / MN2O3 .0013 / "SE(S)" 7E-7 /  &
      "AS(S)" 7E-6

STREAM TF-JST
   SUBSTREAM MIXED PRES=112 VFRAC=1
   MASS-FLOW H2O 52

STREAM TO-ATM

STREAM TR-AIR
   SUBSTREAM MIXED TEMP=100 PRES=110 MOLE-FLOW=16.2
   MOLE-FRAC O2 .21 / N2 .79

STREAM VOG-601
   SUBSTREAM MIXED TEMP=90 <F> PRES=12
   MOLE-FLOW H2O 10 / HNO3 .002 / O2 35 / N2 133

STREAM VTL-AIR
   SUBSTREAM MIXED TEMP=25 PRES=12.2 MOLE-FLOW=12300
   MOLE-FRAC H2O .02 / O2 .206 / N2 .774

STREAM WM-183
   SUBSTREAM MIXED TEMP=30 PRES=12.2 VOLUME-FLOW=112.3  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC
;     Concentrations are listed here.

STREAM WM-189
   SUBSTREAM MIXED TEMP=30 PRES=12.2 VOLUME-FLOW=71.7  &
      SOLVENT=H2O NPHASE=1 PHASE=L TOL=0.0001
   MOLE-CONC
;     Concentrations are listed here.

BLOCK JET-122 MIXER
   PARAM PRES=20
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```
BLOCK M-EQV MIXER
  PARAM PRES=0

BLOCK M-GB MIXER

BLOCK S-TR MIXER

BLOCK STACK MIXER
  PROPERTIES IDEAL TRUE-COMPS=NO

BLOCK NCC-108 FSPLIT
  VOL-FLOW SCR-B 1

BLOCK SPL-119 FSPLIT
  FRAC SPL 1E-9

BLOCK CLEANUP SEP
  FRAC STREAM=IONS SUBSTREAM=MIXED COMPS=H3O+ NO3- CL- NA+  &
    F- AL+3 ALF+2 ALF2+ K+ CD+2 CA+2 FE+3 SO4-2 HGCL3-  &
    HGCL4-2 PB+2 NI+2 CR+3 MN+3 FRACS=1 1 1 1 1 1 1  &
    1 1 1 1 1 1 1 1 1 1 1 1 1
  FRAC STREAM=IONS SUBSTREAM=CISOLID COMPS=AL2O3 FRACS=0
  FLASH-SPECS IONS TEMP=121 PRES=12.2 NPHASE=1 PHASE=S

BLOCK EQV-SEP SEP
  FRAC STREAM=EQ-VTA SUBSTREAM=MIXED COMPS=H2O HNO3 H3O+  &
    NO3- HCL CL- NA+ HF F- AL+3 ALF+2 ALF2+ K+ H3BO3  &
    CD+2 CA+2 FE+3 SO4-2 O2 N2 NO NO2 SO2 CO CO2 FUEL  &
    HGCL2 PB+2 NI+2 CR+3 MN+3 SE AS BENZENE E-GLYCOL  &
    CCL4 CHCL3 TR-ORGAN 111-TCA 112-TCA PERCHLOR HEXONE  &
    TOLUENE XYLENE METHANOL UNB-FUEL H2 FRACS=1 .9 0 0  &
    .9 0 0 .9 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1  &
    1 0 .9 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1  &
    1 1 1
  FRAC STREAM=EQ-VTA SUBSTREAM=CISOLID COMPS=AL2O3 FE2O3  &
    K2SO4 KNO3S CAF2 CACL2 CAO CDO NANO3S B2O3 NACLS  &
    CASO4 PBO NIO CR2O3 MN2O3 "SE(S)" "AS(S)" FRACS=0 0  &
    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

BLOCK HG-SEP SEP
  FRAC STREAM=HG-BP SUBSTREAM=MIXED COMPS=H2O HNO3 H3O+  &
    NO3- HCL CL- NANO3 NA+ HF F- AL+3 ALF+2 ALF2+ K+  &
    H3BO3 CD+2 CA+2 FE+3 SO4-2 O2 N2 NO NO2 SO2 CO CO2  &
    FUEL HGCL2 HGCL3- HGCL4-2 PB+2 NI+2 CR+3 MN+3 SE AS  &
    BENZENE E-GLYCOL CCL4 CHCL3 TR-ORGAN 111-TCA 112-TCA  &
    PERCHLOR HEXONE TOLUENE XYLENE METHANOL UNB-FUEL H2  &
    FRACS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  &
    0 0 0 0 0 0 0 0 0 .005 0 0 0 0 0 0 0 0 0 0  &
    0 0 0 0 0 0 0 0 0 0 0 0 0
  FRAC STREAM=HG-BP SUBSTREAM=CISOLID COMPS=AL2O3 FE2O3  &
    K2SO4 KNO3S CAF2 CACL2 CAO CDO NANO3S B2O3 NACLS  &
    CASO4 PBO NIO CR2O3 MN2O3 "SE(S)" "AS(S)" FRACS=0 0  &
    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

BLOCK LETD SEP
  MASS-FLOW STREAM=HOT-ACID SUBSTREAM=MIXED COMPS=H2O FLOWS= &
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    60
  FRAC STREAM=HOT-ACID SUBSTREAM=MIXED COMPS=HNO3 H3O+ NO3- &
    NA+ HF F- AL+3 ALF+2 ALF2+ K+ H3BO3 CD+2 CA+2 FE+3 &
    SO4-2 O2 N2 NO NO2 S SO2 CO CO2 CL2 FUEL HGCL2 &
    HGCL3- HGCL4-2 PB+2 NI+2 CR+3 MN+3 SE AS BENZENE &
    E-GLYCOL CCL4 CHCL3 TR-ORGAN 111-TCA 112-TCA PERCHLOR &
    HEXONE TOLUENE XYLENE METHANOL UNB-FUEL H2 FRACS=.99 &
    .999 .999 .999 .95 .999 .999 .999 .999 .999 .999 &
    .999 .999 .999 .999 0 0 0 0 1 0 0 0 0 0 .9 1 &
    1 .999 .999 .999 .999 .999 .999 0 .999 0 0 0 0 0 &
    0 0 0 0 0 0 0
  FRAC STREAM=HOT-ACID SUBSTREAM=CISOLID COMPS=AL2O3 FE2O3 &
    CACL2 CAO CDO NANO3S B2O3 NACLS CASO4 PBO NIO CR2O3 &
    MN2O3 FRACS=.999 .999 .999 .999 .999 .999 .999 .999 &
    .999 .999 .999 .999 .999
  PROPERTIES SYSOP15M TRUE-COMPS=YES

BLOCK S-GB SEP
  FRAC STREAM=G-I SUBSTREAM=MIXED COMPS=H2O HNO3 H3O+ NO3- &
    HCL CL- NA+ HF F- AL+3 ALF+2 ALF2+ K+ H3BO3 CD+2 &
    CA+2 FE+3 SO4-2 O2 N2 NO NO2 S SO2 CO CO2 CL2 &
    FUEL HGCL2 PB+2 NI+2 CR+3 MN+3 SE "SE(S)" AS "AS(S)" &
    BENZENE E-GLYCOL CCL4 CHCL3 TR-ORGAN 111-TCA 112-TCA &
    PERCHLOR HEXONE TOLUENE XYLENE METHANOL UNB-FUEL H2 &
    FRACS=1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 &
    1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 &
    0 0 0 0 0 0 0 0 0 0 0 0 0
  FRAC STREAM=G-I SUBSTREAM=CISOLID COMPS=AL2O3 FE2O3 K2SO4 &
    KNO3S CAF2 CACL2 CAO CDO NANO3S B2O3 NACLS CASO4 PBO &
    NIO CR2O3 MN2O3 "SE(S)" "AS(S)" FRACS=0 0 0 0 0 0 &
    0 0 0 0 0 0 0 0 0 0 0 0 0

BLOCK ACID-CLR HEATER
  PARAM TEMP=35 PRES=12.2
  PROPERTIES SYSOP15M CHEMISTRY=CPP

BLOCK APS-HTR HEATER
  PARAM TEMP=88 PRES=12

BLOCK BLO-243 HEATER
  PARAM TEMP=200 PRES=12.6

BLOCK JET-TF HEATER
  PARAM PRES=17 DUTY=0
  PROPERTIES SYSOP15M CHEMISTRY=CPP

BLOCK LN-COOL HEATER
  PARAM TEMP=90 PRES=12.5

BLOCK PEW-COND HEATER
  PARAM TEMP=35 PRES=12.1
  PROPERTIES SYSOP15M HENRY-COMPS=NWCF CHEMISTRY=CPP

BLOCK SPL-CLR HEATER
  PARAM TEMP=25 PRES=12.2
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```
BLOCK TK-FARM HEATER
   PARAM TEMP=25 PRES=12

BLOCK WE-COND HEATER
   IN-UNITS ENG
   PARAM TEMP=25 <C> PRES=12.1

BLOCK WL-101 HEATER
   PARAM TEMP=50 PRES=12.1

BLOCK A-RCY-T FLASH2
   PARAM PRES=11.8 DUTY=0 ENTRN=2E-9

BLOCK AL-189 FLASH2
   PARAM PRES=12 DUTY=0 ENTRN=7.3E-6

BLOCK EQV-COND FLASH2
   PARAM TEMP=28 PRES=12

BLOCK HLLWE FLASH2
   PARAM PRES=12.1 VFRAC=.51 ENTRN=.001

BLOCK NCC-101 FLASH2
   PARAM TEMP=65 PRES=12 ENTRN=4E-6

BLOCK NCC-102 FLASH2
   PARAM TEMP=65 PRES=12 ENTRN=4.4E-6

BLOCK NCC-103 FLASH2
   PARAM TEMP=65 PRES=12 ENTRN=5.3E-6

BLOCK NCC-104 FLASH2
   PARAM TEMP=65 PRES=12 ENTRN=2.4E-6

BLOCK NCC-110 FLASH2
   PARAM PRES=8.2 DUTY=0

BLOCK NCC-119 FLASH2
   PARAM TEMP=75 PRES=12 ENTRN=1.35E-5

BLOCK NCC-122 FLASH2
   PARAM TEMP=50 PRES=12 ENTRN=1.25E-5

BLOCK NCC-152 FLASH2
   PARAM TEMP=65 PRES=12 ENTRN=2.4E-6

BLOCK PEW-EVAP FLASH2
   PARAM PRES=12.1 VFRAC=.97 ENTRN=.001

BLOCK SCRUB FLASH2
   PARAM TEMP=63.3 PRES=8.2

BLOCK ACID-RX RSTOIC
   PARAM TEMP=25 PRES=0
   STOIC 1 MIXED H3O+ -1 / NO3- -1 / HNO3 1 / H2O 1
   CONV 1 MIXED H3O+ 1
```

```
   PROPERTIES SYSOP15M CHEMISTRY=CPP TRUE-COMPS=NO

BLOCK CALCINER RSTOIC
   PARAM TEMP=500 PRES=10.8 SERIES=YES
   STOIC 1 MIXED ALF+2 -1 / F- 1 / AL+3 1
   STOIC 2 MIXED FE+3 -2 / H2O -9 / CISOLID FE2O3 1 / &
      MIXED H3O+ 6
   STOIC 3 MIXED K+ -2 / SO4-2 -1 / CISOLID K2SO4 1
   STOIC 4 MIXED ALF2+ -1 / F- 2 / AL+3 1
   STOIC 7 MIXED NA+ -1 / CL- -1 / CISOLID NACLS 1
   STOIC 5 MIXED HGCL3- -1 / HGCL2 1 / CL- 1
   STOIC 6 MIXED HGCL4-2 -1 / HGCL2 1 / CL- 2
   STOIC 8 MIXED H3O+ -1 / CL- -1 / HCL 1 / H2O 1
   STOIC 9 MIXED CD+2 -1 / H2O -3 / CISOLID CDO 1 / &
      MIXED H3O+ 2
   STOIC 10 MIXED H3BO3 -2 / CISOLID B2O3 1 / MIXED H2O &
      3
   STOIC 11 MIXED CA+2 -1 / F- -2 / CISOLID CAF2 1
   STOIC 12 MIXED CA+2 -1 / SO4-2 -1 / CISOLID CASO4 1
   STOIC 13 MIXED CA+2 -1 / H2O -3 / CISOLID CAO 1 / &
      MIXED H3O+ 2
   STOIC 14 MIXED K+ -1 / NO3- -1 / CISOLID KNO3S 1
   STOIC 15 MIXED NA+ -1 / NO3- -1 / CISOLID NANO3S 1
   STOIC 16 MIXED F- -1 / H3O+ -1 / HF 1 / H2O 1
   STOIC 17 MIXED AL+3 -2 / H2O -9 / CISOLID AL2O3 1 / &
      MIXED H3O+ 6
   STOIC 18 MIXED PB+2 -1 / H2O -3 / CISOLID PBO 1 / &
      MIXED H3O+ 2
   STOIC 19 MIXED CR+3 -2 / H2O -9 / CISOLID CR2O3 1 / &
      MIXED H3O+ 6
   STOIC 20 MIXED MN+3 -2 / H2O -9 / CISOLID MN2O3 1 / &
      MIXED H3O+ 6
   STOIC 21 MIXED NI+2 -1 / H2O -3 / CISOLID NIO 1 / &
      MIXED H3O+ 2
   STOIC 22 MIXED H3O+ -1 / NO3- -1 / HNO3 1 / H2O 1
   STOIC 23 MIXED HNO3 -4 / NO2 4 / O2 1 / H2O 2
   STOIC 24 MIXED NO2 -2 / NO 2 / O2 1
   STOIC 25 MIXED SE -1 / CISOLID "SE(S)" 1
   STOIC 26 MIXED AS -1 / CISOLID "AS(S)" 1
   CONV 1 MIXED ALF+2 1
   CONV 2 MIXED FE+3 1
   CONV 3 MIXED SO4-2 1
   CONV 4 MIXED ALF2+ 1
   CONV 7 MIXED CL- .6
   CONV 5 MIXED HGCL3- 1
   CONV 6 MIXED HGCL4-2 1
   CONV 8 MIXED CL- 1
   CONV 9 MIXED CD+2 1
   CONV 10 MIXED H3BO3 1
   CONV 11 MIXED F- .985
   CONV 12 MIXED SO4-2 1
   CONV 13 MIXED CA+2 1
   CONV 14 MIXED K+ 1
   CONV 15 MIXED NA+ 1
   CONV 16 MIXED F- 1
   CONV 17 MIXED AL+3 1
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   CONV 18 MIXED PB+2 1
   CONV 19 MIXED CR+3 1
   CONV 20 MIXED MN+3 1
   CONV 21 MIXED NI+2 1
   CONV 22 MIXED NO3- 1
   CONV 23 MIXED HNO3 1
   CONV 24 MIXED NO2 .10
   CONV 25 MIXED SE 1
   CONV 26 MIXED AS 1

BLOCK CL-CHEM RSTOIC
   PARAM TEMP=100 PRES=12.2 SERIES=YES
   STOIC 1 MIXED CL- -6 / HNO3 -2 / H3O+ -6 / CL2 3 / &
      NO 2 / H2O 10
   STOIC 2 MIXED HCL -6 / HNO3 -2 / CL2 3 / NO 2 / &
      H2O 4
   STOIC 3 MIXED H3O+ -1 / NO3- -1 / HNO3 1 / H2O 1
   CONV 1 MIXED CL- 1
   CONV 2 MIXED HCL 1
   CONV 3 MIXED H3O+ 1

BLOCK HTR-335 RSTOIC
   PARAM TEMP=85 PRES=5.9 SERIES=YES
   STOIC 1 MIXED NA+ -1 / CL- -1 / CISOLID NACLS 1
   STOIC 9 MIXED NA+ -1 / NO3- -1 / CISOLID NANO3S 1
   STOIC 2 MIXED ALF+2 -1 / AL+3 1 / F- 1
   STOIC 3 MIXED ALF2+ -1 / AL+3 1 / F- 2
   STOIC 4 MIXED AL+3 -2 / H2O -9 / CISOLID AL2O3 1 / &
      MIXED H3O+ 6
   STOIC 5 MIXED K+ -2 / SO4-2 -1 / CISOLID K2SO4 1
   STOIC 6 MIXED K+ -1 / NO3- -1 / CISOLID KNO3S 1
   STOIC 7 MIXED CD+2 -1 / H2O -3 / CISOLID CDO 1 / &
      MIXED H3O+ 2
   STOIC 8 MIXED FE+3 -2 / H2O -9 / CISOLID FE2O3 1 / &
      MIXED H3O+ 6
   STOIC 10 MIXED CA+2 -1 / F- -2 / CISOLID CAF2 1
   STOIC 11 MIXED CA+2 -1 / SO4-2 -1 / CISOLID CASO4 1
   STOIC 12 MIXED H3BO3 -2 / CISOLID B2O3 1 / MIXED H2O &
      3
   STOIC 13 MIXED CA+2 -1 / H2O -3 / CISOLID CAO 1 / &
      MIXED H3O+ 2
   STOIC 14 MIXED HGCL3- -1 / HGCL2 1 / CL- 1
   STOIC 15 MIXED HGCL4-2 -1 / HGCL2 1 / CL- 2
   STOIC 16 MIXED H3O+ -1 / CL- -1 / HCL 1 / H2O 1
   STOIC 17 MIXED PB+2 -1 / H2O -3 / CISOLID PBO 1 / &
      MIXED H3O+ 2
   STOIC 18 MIXED CR+3 -2 / H2O -9 / CISOLID CR2O3 1 / &
      MIXED H3O+ 6
   STOIC 19 MIXED MN+3 -2 / H2O -9 / CISOLID MN2O3 1 / &
      MIXED H3O+ 6
   STOIC 20 MIXED NI+2 -1 / H2O -3 / CISOLID NIO 1 / &
      MIXED H3O+ 2
   STOIC 21 MIXED H3O+ -1 / NO3- -1 / HNO3 1 / H2O 1
   STOIC 22 MIXED SE -1 / CISOLID "SE(S)" 1
   STOIC 23 MIXED AS -1 / CISOLID "AS(S)" 1
   CONV 1 MIXED CL- 1
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   CONV 9 MIXED NA+ 1
   CONV 2 MIXED ALF+2 1
   CONV 3 MIXED ALF2+ 1
   CONV 4 MIXED AL+3 1
   CONV 5 MIXED SO4-2 1
   CONV 6 MIXED K+ 1
   CONV 7 MIXED CD+2 1
   CONV 8 MIXED FE+3 1
   CONV 10 MIXED F- 1
   CONV 11 MIXED SO4-2 1
   CONV 12 MIXED H3BO3 1
   CONV 13 MIXED CA+2 1
   CONV 14 MIXED HGCL3- 1
   CONV 15 MIXED HGCL4-2 1
   CONV 16 MIXED CL- 1
   CONV 17 MIXED PB+2 1
   CONV 18 MIXED CR+3 1
   CONV 19 MIXED MN+3 1
   CONV 20 MIXED NI+2 1
   CONV 21 MIXED NO3- 1
   CONV 22 MIXED SE 1
   CONV 23 MIXED AS 1

BLOCK IB-COMB RSTOIC
   PARAM TEMP=500 PRES=10.8 NPHASE=2 SERIES=YES
   STOIC 2 MIXED FUEL -2 / O2 -25 / CO 24 / H2O 26
   STOIC 4 MIXED FUEL -2 / O2 -37 / CO2 24 / H2O 26
   STOIC 3 MIXED S -1 / O2 -1 / SO2 1
   STOIC 1 MIXED FUEL -1 / UNB-FUEL 6 / H2 1
   EXTENT 2 0.33469
   CONV 4 MIXED FUEL 1
   CONV 3 MIXED S 1
   CONV 1 MIXED FUEL .03

BLOCK LETD-SH RSTOIC
   PARAM TEMP=150 PRES=12.2 SERIES=YES
   STOIC 1 MIXED PB+2 -1 / H2O -3 / CISOLID PBO 1 / &
      MIXED H3O+ 2
   STOIC 2 MIXED CR+3 -2 / H2O -9 / CISOLID CR2O3 1 / &
      MIXED H3O+ 6
   STOIC 3 MIXED MN+3 -2 / H2O -9 / CISOLID MN2O3 1 / &
      MIXED H3O+ 6
   STOIC 4 MIXED ALF+2 -1 / AL+3 1 / F- 1
   STOIC 5 MIXED ALF2+ -1 / AL+3 1 / F- 2
   STOIC 6 MIXED CA+2 -1 / F- -2 / CISOLID CAF2 1
   STOIC 7 MIXED K+ -2 / SO4-2 -1 / CISOLID K2SO4 1
   STOIC 8 MIXED NA+ -1 / NO3- -1 / CISOLID NANO3S 1
   STOIC 9 MIXED AL+3 -2 / H2O -9 / CISOLID AL2O3 1 / &
      MIXED H3O+ 6
   STOIC 10 MIXED K+ -1 / NO3- -1 / CISOLID KNO3S 1
   STOIC 11 MIXED CD+2 -1 / H2O -3 / CISOLID CDO 1 / &
      MIXED H3O+ 2
   STOIC 12 MIXED FE+3 -2 / H2O -9 / CISOLID FE2O3 1 / &
      MIXED H3O+ 6
   STOIC 13 MIXED CA+2 -1 / SO4-2 -1 / CISOLID CASO4 1
   STOIC 14 MIXED CA+2 -1 / H2O -3 / CISOLID CAO 1 / &
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      MIXED H3O+ 2
   STOIC 15 MIXED NI+2 -1 / H2O -3 / CISOLID NIO 1 /  &
      MIXED H3O+ 2
   STOIC 18 MIXED H3O+ -1 / NO3- -1 / HNO3 1 / H2O 1
   STOIC 17 MIXED H3BO3 -2 / CISOLID B2O3 1 / MIXED H2O  &
      3
   STOIC 16 MIXED H3O+ -1 / F- -1 / HF 1 / H2O 1
   STOIC 19 MIXED SE -1 / CISOLID "SE(S)" 1
   STOIC 20 MIXED AS -1 / CISOLID "AS(S)" 1
   CONV 1 MIXED PB+2 1
   CONV 2 MIXED CR+3 1
   CONV 3 MIXED MN+3 1
   CONV 4 MIXED ALF+2 1
   CONV 5 MIXED ALF2+ 1
   CONV 6 MIXED F- 1
   CONV 7 MIXED SO4-2 1
   CONV 8 MIXED NA+ 1
   CONV 9 MIXED AL+3 1
   CONV 10 MIXED K+ 1
   CONV 11 MIXED CD+2 1
   CONV 12 MIXED FE+3 1
   CONV 13 MIXED SO4-2 1
   CONV 14 MIXED CA+2 1
   CONV 15 MIXED NI+2 1
   CONV 18 MIXED H3O+ 1
   CONV 17 MIXED H3BO3 1
   CONV 16 MIXED F- 1
   CONV 19 MIXED SE 1
   CONV 20 MIXED AS 1
   PROPERTIES SYSOP15M CHEMISTRY=CPP TRUE-COMPS=NO

BLOCK REP-CONV RSTOIC
   PARAM PRES=12.2 DUTY=0
   STOIC 1 MIXED NO -2 / O2 -1 / NO2 2
   STOIC 2 MIXED HGCL2 -1 / HG 1 / CL2 1
   STOIC 3 CISOLID PBO -2 / MIXED PB 2 / O2 1
   STOIC 4 CISOLID NIO -2 / MIXED NI 2 / O2 1
   STOIC 5 CISOLID CR2O3 -2 / MIXED CR 4 / O2 3
   STOIC 6 CISOLID MN2O3 -2 / MIXED MN 4 / O2 3
   STOIC 7 CISOLID "SE(S)" -1 / MIXED SE 1
   STOIC 8 CISOLID "AS(S)" -1 / MIXED AS 1
   STOIC 9 CISOLID CDO -2 / MIXED CD 2 / O2 1
   CONV 1 MIXED NO 1
   CONV 2 MIXED HGCL2 1
   CONV 3 CISOLID PBO 1
   CONV 4 CISOLID NIO 1
   CONV 5 CISOLID CR2O3 1
   CONV 6 CISOLID MN2O3 1
   CONV 7 CISOLID "SE(S)" 1
   CONV 8 CISOLID "AS(S)" 1
   CONV 9 CISOLID CDO 1

BLOCK SCR-RX RSTOIC
   PARAM TEMP=70 PRES=11 SERIES=YES
   STOIC 1 MIXED HNO3 -1 / H2O -1 / H3O+ 1 / NO3- 1
   STOIC 2 CISOLID CAO -1 / MIXED H3O+ -2 / CA+2 1 /  &
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```
    H2O 3
  STOIC 3 CISOLID NANO3S -1 / MIXED NA+ 1 / NO3- 1
  STOIC 4 CISOLID KNO3S -1 / MIXED K+ 1 / NO3- 1
  STOIC 5 CISOLID CAF2 -1 / MIXED H3O+ -2 / CA+2 1 / &
    HF 2 / H2O 2
  STOIC 6 CISOLID B2O3 -1 / MIXED H2O -3 / H3BO3 2
  STOIC 7 CISOLID CDO -1 / MIXED H3O+ -2 / CD+2 1 / &
    H2O 3
  STOIC 8 CISOLID NACLS -1 / MIXED NA+ 1 / CL- 1
  STOIC 9 CISOLID K2SO4 -1 / MIXED K+ 2 / SO4-2 1
  STOIC 10 CISOLID FE2O3 -1 / MIXED H3O+ -6 / FE+3 2 / &
    H2O 9
  STOIC 11 CISOLID "AL(NO3)3" -1 / MIXED AL+3 1 / NO3- 3
  STOIC 12 CISOLID PBO -1 / MIXED H3O+ -2 / PB+2 1 / &
    H2O 3
  STOIC 13 CISOLID CR2O3 -1 / MIXED H3O+ -6 / CR+3 2 / &
    H2O 9
  STOIC 14 CISOLID AL2O3 -1 / MIXED H3O+ -6 / AL+3 2 / &
    H2O 9
  STOIC 15 CISOLID MN2O3 -1 / MIXED H3O+ -6 / MN+3 2 / &
    H2O 9
  STOIC 16 CISOLID NIO -1 / MIXED H3O+ -2 / NI+2 1 / &
    H2O 3
  STOIC 17 CISOLID H3BO3 -1 / MIXED H3BO3 1
  STOIC 18 CISOLID CASO4 -1 / MIXED CA+2 1 / SO4-2 1
  STOIC 19 CISOLID "SE(S)" -1 / MIXED SE 1
  STOIC 20 CISOLID "AS(S)" -1 / MIXED AS 1
  CONV 1 MIXED HNO3 1
  CONV 2 CISOLID CAO 1
  CONV 3 CISOLID NANO3S 1
  CONV 4 CISOLID KNO3S 1
  CONV 5 CISOLID CAF2 1
  CONV 6 CISOLID B2O3 1
  CONV 7 CISOLID CDO 1
  CONV 8 CISOLID NACLS 1
  CONV 9 CISOLID K2SO4 1
  CONV 10 CISOLID FE2O3 1
  CONV 11 CISOLID "AL(NO3)3" 1
  CONV 12 CISOLID PBO 1
  CONV 13 CISOLID CR2O3 1
  CONV 14 CISOLID AL2O3 1
  CONV 15 CISOLID MN2O3 1
  CONV 16 CISOLID NIO 1
  CONV 17 CISOLID H3BO3 1
  CONV 18 CISOLID CASO4 1
  CONV 19 CISOLID "SE(S)" 1
  CONV 20 CISOLID "AS(S)" 1

BLOCK VOG-RX RSTOIC
  PARAM PRES=12 DUTY=0 SERIES=YES
  STOIC 1 MIXED ALF+2 -1 / AL+3 1 / F- 1
  STOIC 2 MIXED ALF2+ -1 / AL+3 1 / F- 2
  STOIC 3 MIXED AL+3 -2 / H2O -9 / CISOLID AL2O3 1 / &
    MIXED H3O+ 6
  STOIC 4 MIXED K+ -2 / SO4-2 -1 / CISOLID K2SO4 1
  STOIC 5 MIXED K+ -1 / NO3- -1 / CISOLID KNO3S 1
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    STOIC 6 MIXED CA+2 -1 / SO4-2 -1 / CISOLID CASO4 1
    STOIC 7 MIXED CD+2 -1 / H2O -3 / CISOLID CDO 1 / &
      MIXED H3O+ 2
    STOIC 8 MIXED CA+2 -1 / F- -2 / CISOLID CAF2 1
    STOIC 9 MIXED FE+3 -2 / H2O -9 / CISOLID FE2O3 1 / &
      MIXED H3O+ 6
    STOIC 10 MIXED CA+2 -1 / H2O -3 / CISOLID CAO 1 / &
      MIXED H3O+ 2
    STOIC 11 MIXED PB+2 -1 / H2O -3 / CISOLID PBO 1 / &
      MIXED H3O+ 2
    STOIC 12 MIXED HGCL3- -1 / HGCL2 1 / CL- 1
    STOIC 13 MIXED HGCL4-2 -1 / HGCL2 1 / CL- 2
    STOIC 14 MIXED NA+ -1 / CL- -1 / CISOLID NACLS 1
    STOIC 15 MIXED NA+ -1 / NO3- -1 / CISOLID NANO3S 1
    STOIC 18 MIXED CR+3 -2 / H2O -9 / H3O+ 6 / CISOLID &
      CR2O3 1
    STOIC 20 MIXED H3O+ -1 / NO3- -1 / HNO3 1 / H2O 1
    STOIC 19 MIXED H3BO3 -2 / CISOLID B2O3 1 / MIXED H2O &
      3
    STOIC 16 MIXED MN+3 -2 / H2O -9 / CISOLID MN2O3 1 / &
      MIXED H3O+ 6
    STOIC 17 MIXED NI+2 -1 / H2O -3 / CISOLID NIO 1 / &
      MIXED H3O+ 2
    STOIC 21 MIXED SE -1 / CISOLID "SE(S)" 1
    STOIC 22 MIXED AS -1 / CISOLID "AS(S)" 1
    CONV 1 MIXED ALF+2 1
    CONV 2 MIXED ALF2+ 1
    CONV 3 MIXED AL+3 1
    CONV 4 MIXED SO4-2 1
    CONV 5 MIXED K+ 1
    CONV 6 MIXED CA+2 1
    CONV 7 MIXED CD+2 1
    CONV 8 MIXED F- 1
    CONV 9 MIXED FE+3 1
    CONV 10 MIXED CA+2 1
    CONV 11 MIXED PB+2 1
    CONV 12 MIXED HGCL3- 1
    CONV 13 MIXED HGCL4-2 1
    CONV 14 MIXED CL- 1
    CONV 15 MIXED NA+ 1
    CONV 18 MIXED CR+3 1
    CONV 20 MIXED NO3- 1
    CONV 19 MIXED H3BO3 1
    CONV 16 MIXED MN+3 1
    CONV 17 MIXED NI+2 1
    CONV 21 MIXED SE 1
    CONV 22 MIXED AS 1

BLOCK APS-RX RGIBBS
    PARAM TEMP=80 PRES=12 NREAC=3
    PROD N2 / O2 / H2O / NO2 / NO / HNO3
    STOIC 1 HNO3 -2 / NO -1 / NO2 3 / H2O 1
    STOIC 2 NO2 -2 / N2 1 / O2 2
    STOIC 3 NO -2 / N2 1 / O2 1
    EXTENT-SPEC 2 0 / 3 0
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```
BLOCK APS-FILT SSPLIT
   FRAC MIXED APS-FILT 0
   FRAC CISOLID APS-FILT .9997

BLOCK BIN-CYCL SSPLIT
   FRAC MIXED CALCINE 0
   FRAC CISOLID CALCINE .95

BLOCK CLC-PTO SSPLIT
   FRAC MIXED BED-PR 0
   FRAC CISOLID BED-PR .5

BLOCK CYCLONE SSPLIT
   FRAC MIXED CYC-SOL 0
   FRAC CISOLID CYC-SOL .75

BLOCK LETD-FLT SSPLIT
   FRAC MIXED LETD-EFL 1
   FRAC CISOLID LETD-EFL 9E-8

BLOCK SCR-BP SSPLIT
   FRAC MIXED SOL-BP 0
   FRAC CISOLID SOL-BP .004

BLOCK VOG-FLT SSPLIT
   FRAC MIXED VOG-FILT 0
   FRAC CISOLID VOG-FILT .9997

BLOCK WC-FILT SSPLIT
   PARAM PRES=4.6
   FRAC MIXED FLT-OG 1
   FRAC CISOLID FLT-OG 9E-8

DESIGN-SPEC LETD-A
   DEFINE WATER BLOCK-VAR BLOCK=LETD SENTENCE=MASS-FLOW  &
      VARIABLE=FLOWS ID1=MIXED ID2=HOT-ACID ELEMENT=1
   DEFINE CONC MASS-FRAC STREAM=HOT-ACID SUBSTREAM=MIXED  &
      COMPONENT=H2O
   SPEC "CONC" TO ".45"
   TOL-SPEC ".02"
   VARY BLOCK-VAR BLOCK=LETD SENTENCE=MASS-FLOW VARIABLE=FLOWS  &
      ID1=MIXED ID2=HOT-ACID ELEMENT=1
   LIMITS "5" "100"

DESIGN-SPEC SCR-RET
   DEFINE SCR STREAM-PROP STREAM=SCR-SOLN PROPERTY=SCR-R
   DEFINE RHOSCR STREAM-PROP STREAM=SCR-SOLN PROPERTY=RHO-SCR
   SPEC "SCR" TO "36"
   TOL-SPEC ".1"
   VARY BLOCK-VAR BLOCK=SCRUB VARIABLE=TEMP SENTENCE=PARAM
   LIMITS "60" "75"

TEAR
   TEAR TA-RET / CYCL-OG 0.001 / SCR-OGA .001

STREAM-REPOR NOZEROFLOW MOLEFLOW MASSFLOW MOLEFRAC  &
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      INCL-STREAMS=WM-189 WM-183 LIQ-104 WE-VAP HOT-BOT  &
      HLWE-SPL BOT-PROD WE-COND HEEL-188 TF-LIQ TF-JST  &
      WC-FEED ANN BORIC-A CANO3 BL-FEEDA SCR-RCYL BL-FEED  &
      CALCINE ATM-EFFL TO-ATM SCR-TF NCM-ACID ACID-110  &
      LETDACID TO-NA-WA FUEL NOZ-O2 CALC-AIR COMB-PR TR-AIR  &
      TA-RET CALC-PR BED-PR CYC-SOL SOL-TR CYCL-OG SCR-INT  &
      SCR-OGA SCR-OGB WC-OG SCR-SOLN SP-101 VT-101 AL-101  &
      SP-152 VT-152 P-HLWE SP-119 VT-119 SP-122 VT-122  &
      SP-102 VT-102 AL-102 SP-103 VT-103 AL-103 SP-104  &
      VT-104 EQV-MISC EQ-VTA EQV-COND EQ-VTC VOG-601 PILOT-PL  &
      FUG-EMIS AL-189 VT-189 VOG-A APS-A WC-EFFL APS-B  &
      BLO-AIR APS-EFFL NWCF-PEW ANN-122 JST-122 PEW-122  &
      PEW-MISC PEW-BOT PEW-VAP PEW-COND HOT-ACID LETD-VAP  &
      LETD-EFL VTL-AIR APS-FILT LETDFILT WC-FILT VOG-FILT G-I  &
      IONS TO-STACK


FORTRAN FORT1
F     COMMON / RGLOB / XRMISS, RMIN, ABSMIN, SCLMIN, XMIN
  DEFINE DUMMY STREAM-VAR STREAM=VOG-601 VARIABLE=MOLE-FLOW
F     RMIN = 1.0D-25
F     XMIN = 1.0D-25
  EXECUTE FIRST
;
```

Appendix B

Regression of Activity Coefficient Parameters

APPENDIX B

Regression of Activity Coefficient Parameters

The ASPEN Plus software contains property and activity coefficient parameters for many of the binary systems of interest. However, independent regressions were done in an effort to 1) obtain improved activity coefficient parameters in the concentration ranges of interest for aqueuos solutions of HNO_3, HCl and HF, and 2) obtain interaction parameters for mixtures of water and nitric acid with HCl, HF, $NaNO_3$ and $Al(NO_3)_3$. The parameters used in the emissions model are selected to provide conservative partial pressures for HNO_3, HCl and HF.

The ASPEN aqueous electrolyte model (ELECTNRTL) being used to calculate vapor pressures of nitric and hydrochloric acid solutions calculates aqueous activity coefficients using the non-random two-liquid (NRTL) theory[1,2]. The end result of the NRTL theory is a set of coefficients whose values are obtained by regression of some property data (e. g., vapor pressure).

B-1. BINARY NITRIC ACID SOLUTIONS

The data regression for aqueous nitric acid solutions used 124 data points from eight references[3,4,5,6,7,8,9,10] covering the nitric acid mole fraction range from 0.05 to 0.3 (60 wt. %) and the temperature range from 25 to 120°C. (The vapor pressure values from handbooks were avoided because they are extrapolations and interpolations[11] rather than actual data points.) The nitric acid hydrolysis equilibrium coefficients (K-STOIC) and activity coefficient parameters (GMELCX) were regressed alternately to obtain the values listed in Tables B1 and B2 respectively. (Thus, the K-STOIC values of Table B1 are those that provide the best fit of the vapor pressure data.) The K-STOIC values of Table 1 were then used to regress density data[12] for the ASPEN density parameters (VLCLK) which are also listed in Table B1. Densities calculated with the density parameters of Table B1 agree within 1 percent with handbook[12] values over the temperature range from 25 to 100°C.

The partial pressures of nitric acid calculated with the parameters of Tables B1 and B2 agree with the measured data about as well as the different data sets agree with each other. Sample comparisons are shown in Figures B1, B2, and B3 which cover cases where data from two sources can be compared.

Table B-1. Property parameters for nitric acid solutions.

Parameter	K-STOIC	VLCLK
Element 1	119.8919	0.0445218
Element 2	-8608.46	0.0247703
Element 3	-12.06946	n. a.
Element 4	-0.06584351	n. a.

Table B-2. Activity coefficient parameters for HNO_3-H_2O.

Parameter	Species Pair	Value (SI)
GMELCA	HNO3 H2O	-3.735254
GMELCA	H2O HNO3	16.31065
GMELCB	HNO3 H2O	285.6733
GMELCB	H2O HNO3	-5550.353
GMELCC	H20 (H3O+ NO3-)	-9.335314
GMELCC	(H3O+ NO3-) H2O	0.3928543
GMELCC	HNO3 (H3O+ NO3-)	-8.261029
GMELCC	(H3O+ NO3-) HNO3	24.49516
GMELCD	H20 (H3O+ NO3-)	5741.406
GMELCD	(H3O+ NO3-) H2O	-1504.383
GMELCD	HNO3 (H3O+ NO3-)	9000
GMELCD	(H3O+ NO3-) HNO3	-8323.403
GMELCE	H20 (H3O+ NO3-)	34.14618
GMELCE	(H3O+ NO3-) H2O	-2.0011

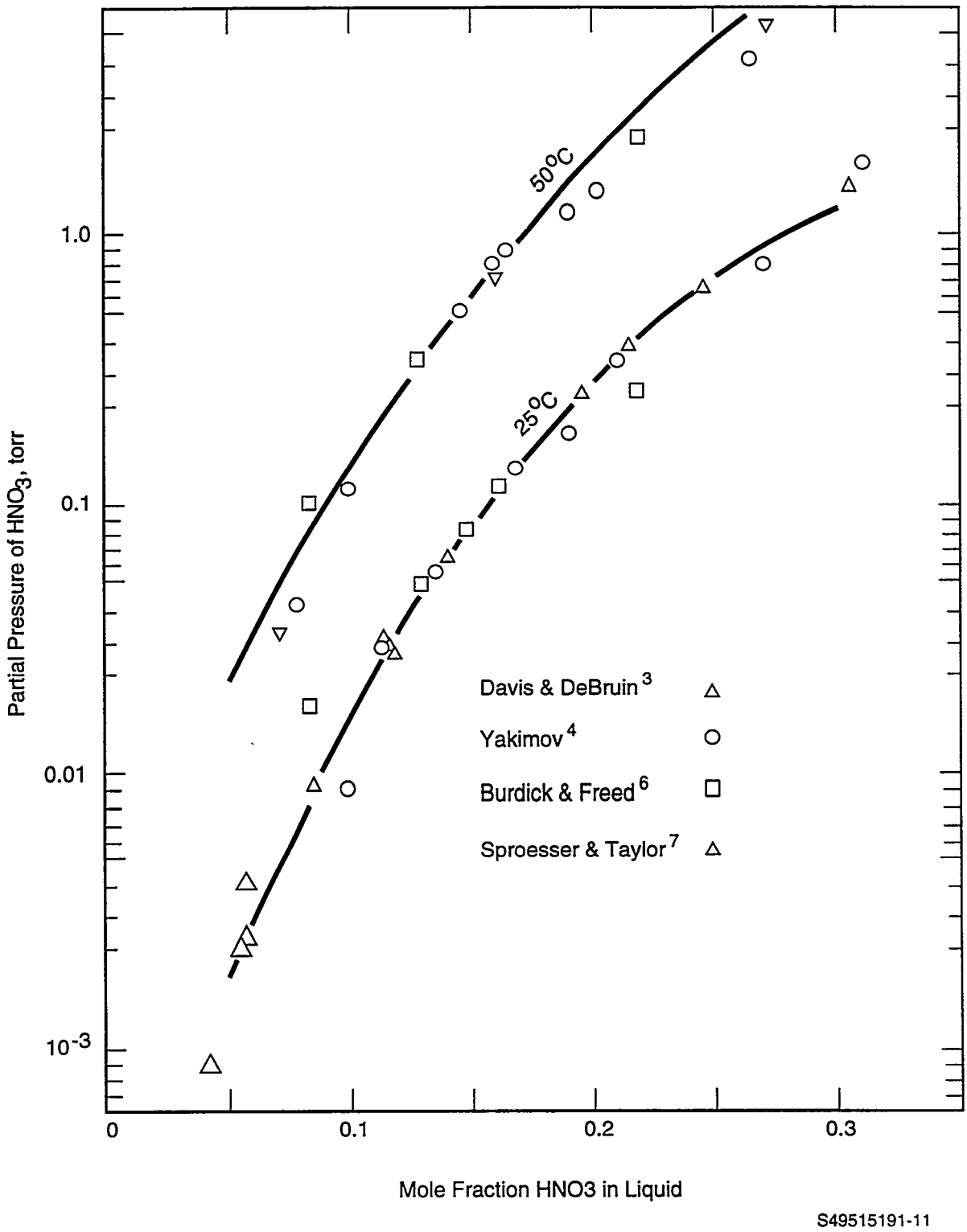

Figure B-1 Comparison of calculated and measured values for nitric acid partial pressure at 25 and 50°C.

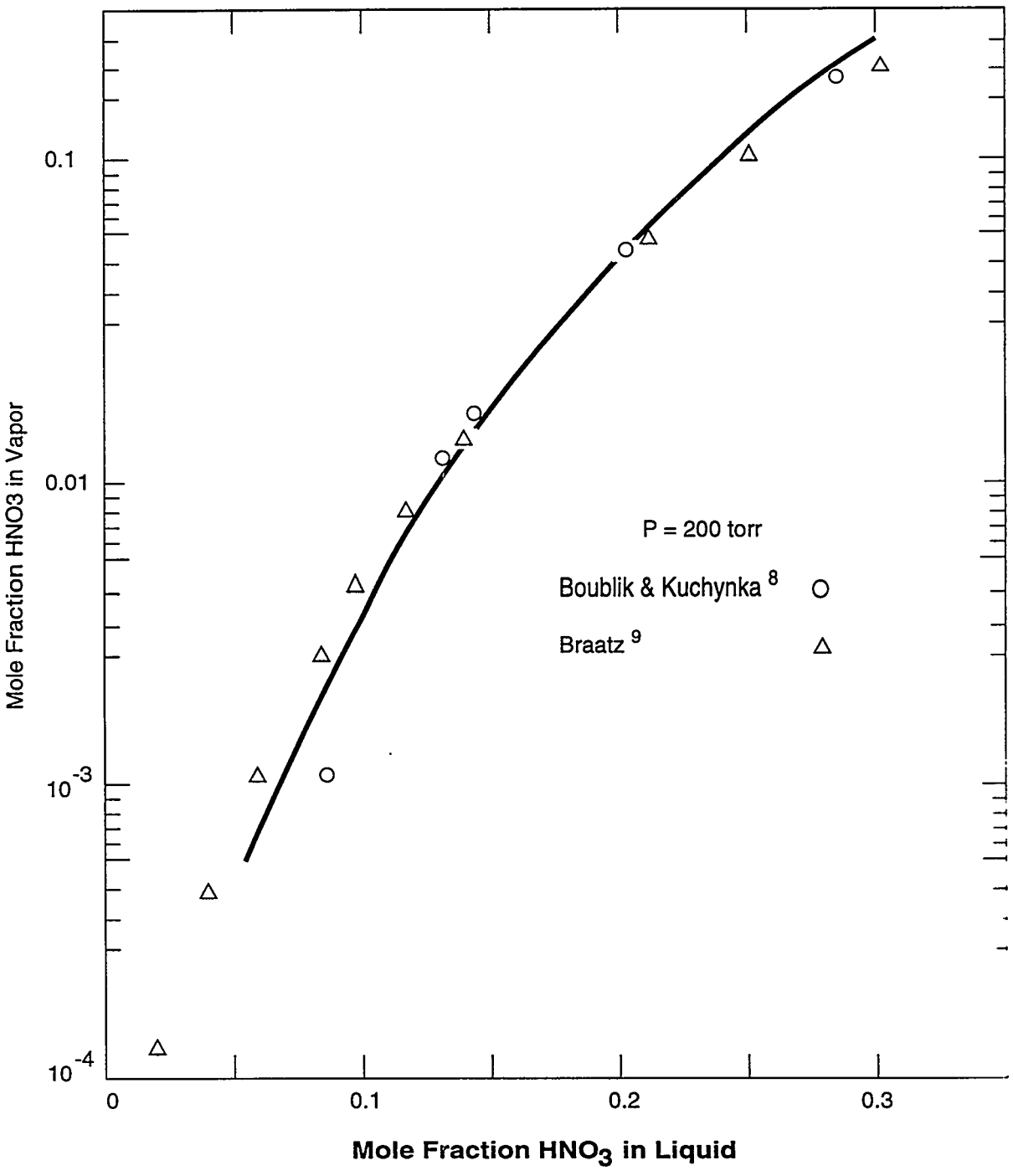

Figure B-2. Comparison of calculated and measured values for vapor-phase mole fraction of nitric acid at 200 Torr.

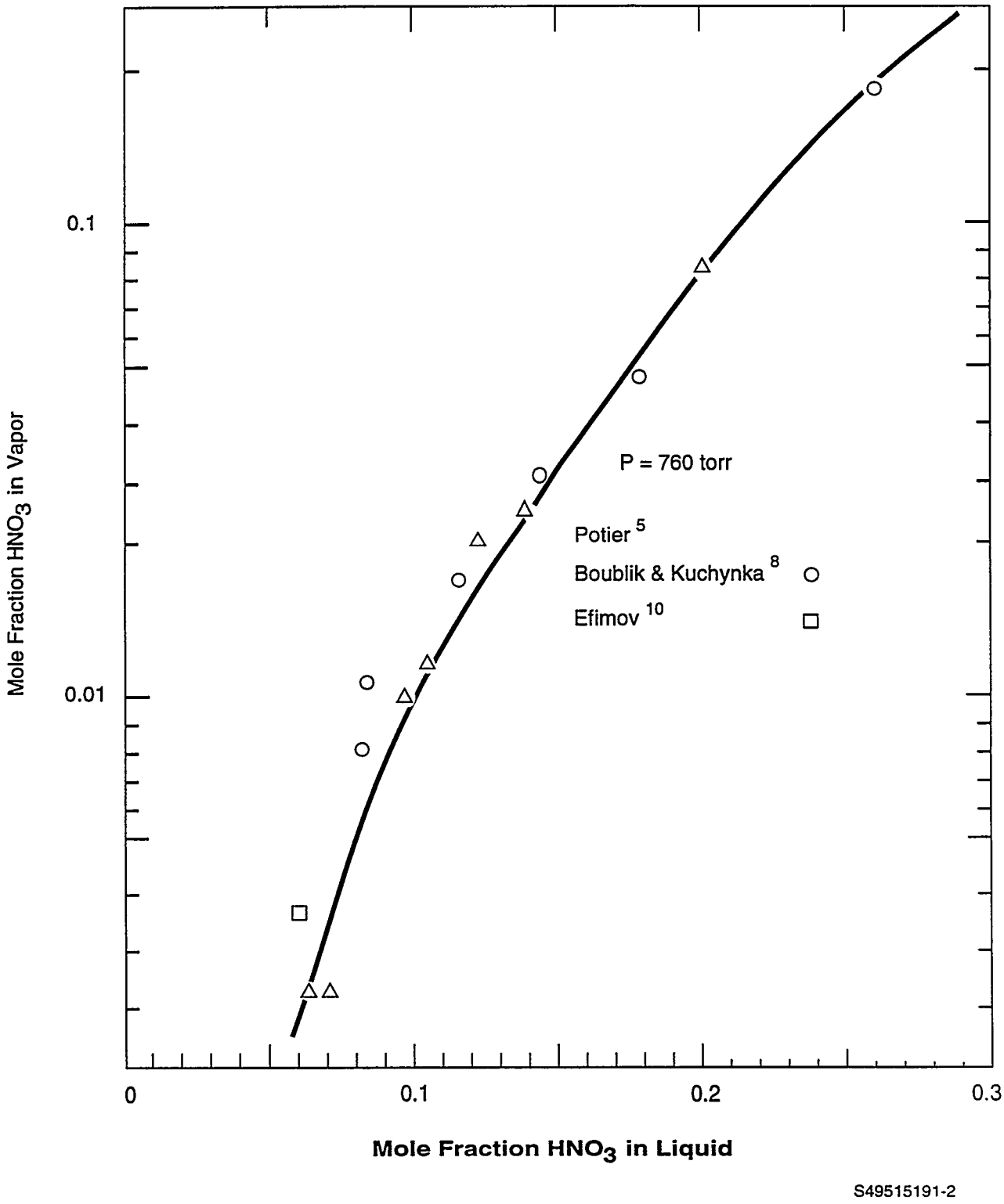

Figure B-3. Comparison of calculated and measured values for vapor-phase mole fraction of nitric acid at 760 Torr.

B-2. BINARY HYDROCHLORIC ACID SOLUTIONS

Handbook[13] partial pressure values were regressed with the ASPEN data regression system (DRS). The best results were obtained by regressing first for the HCl hydrolysis equilibrium coefficient parameters, which are listed in Table B3, and then regressing the activity coefficient parameters which are listed in Table B4. (Note that the numbers listed in Tables B3 and B4 should be taken together as a set; the equilibrium coefficients by themselves may not be valid for other applications.) Calculated and reference[13] partial pressures are compared in Figures B4 and B5.

Table B-3. Chemical equilibrium constant parameters for the hydrolysis reaction of HCl with water.

K-STOIC Parameter	Value (SI)
A (Constant)	52.22975
B (B/T)	0
C (C*lnT)	-5.0
d (D*T)	-0.05057952

Table B-4. NRTL activity coefficient coefficient parameters for HCl-H_2O.

Parameter	Pair	Value (SI)
GMELCA	HCl H2O	-0.01041378
GMELCA	H2O HCl	5.899389
GMELCB	HCl H2O	-83.9213
GMELCB	H2O HCl	-405.3164
GMELCC	H20 (H3O+ Cl-)	1.550125
GMELCC	(H3O+ Cl-) H2O	-3.179279
GMELCC	HCl (H3O+ Cl-)	4.250762
GMELCC	(H3O+ Cl-) HCl	-2.626461
GMELCD	H20 (H3O+ Cl-)	2933.717
GMELCD	(H3O+ Cl-) H2O	-654.6557
GMELCD	HCl (H3O+ Cl-)	-1060.76
GMELCD	(H3O+ Cl-) HCl	169.342
GMELCE	H20 (H3O+ Cl-)	-45.82451
GMELCE	(H3O+ Cl-) H2O	21.50122
GMELCE	HCl (H3O+ Cl-)	279.9721
GMELCE	(H3O+ Cl-) HCl	44.8182

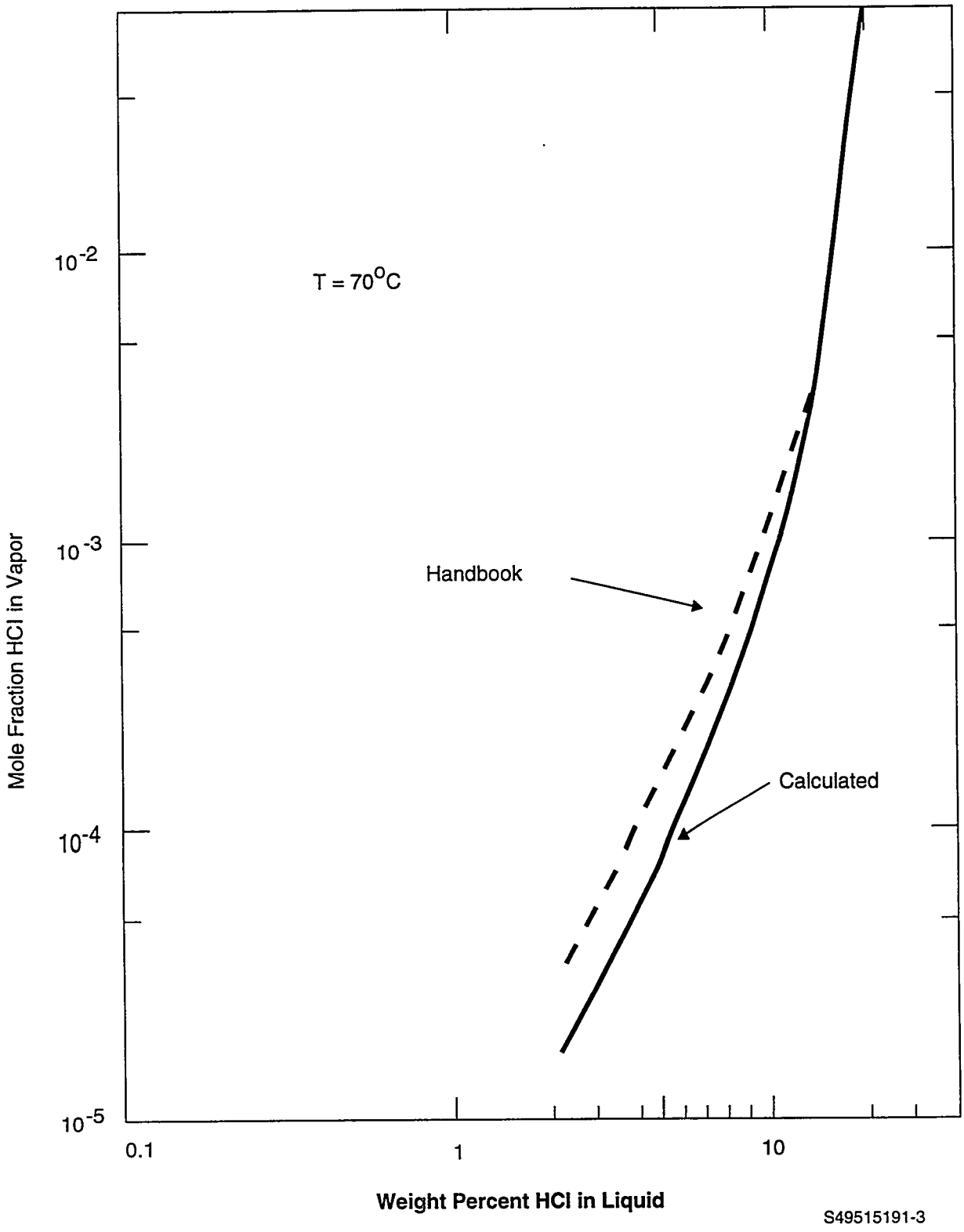

Figure B-4. Comparison of calculated HCl partial pressures with reference[13] values at 70°C.

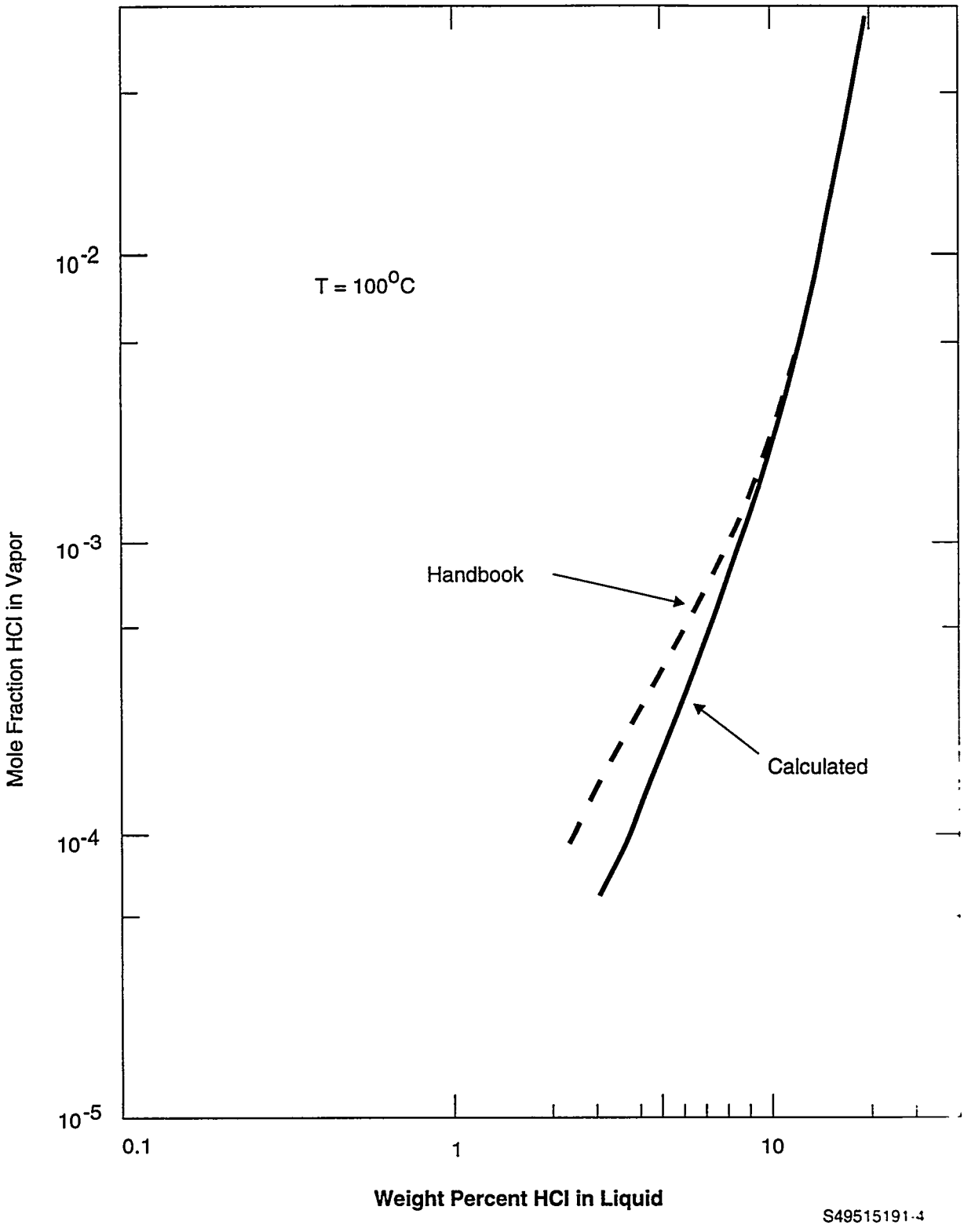

Figure B-5. Comparison of calculated HCl partial pressures with reference[13] values at 100°C.

B-3. AQUEOUS SOLUTIONS OF HNO_3 AND HCl

The need for interaction parameters was checked by calculating HCl volatility in nitric acid solutions using only the binary solution parameters of Tables B1, B2, B3, and B4. The calculated volatilities shown by the dashed lines on Figures B6 and B7 are much lower than the available data[9,14]. The data[9,14] was then regressed to obtain the ion-pair interaction parameters:

GMELCC (H3O+ NO3-) (H3O+ Cl-) = 15 and

GMELCC (H3O+ Cl-) (H3O+ NO3-) = 3.253562.

Calculations using the above ion-pair parameters provide a much improved data fit as shown by the solid lines on Figures B6 and B7. Other parameters were also tested but provided only minor improvements.

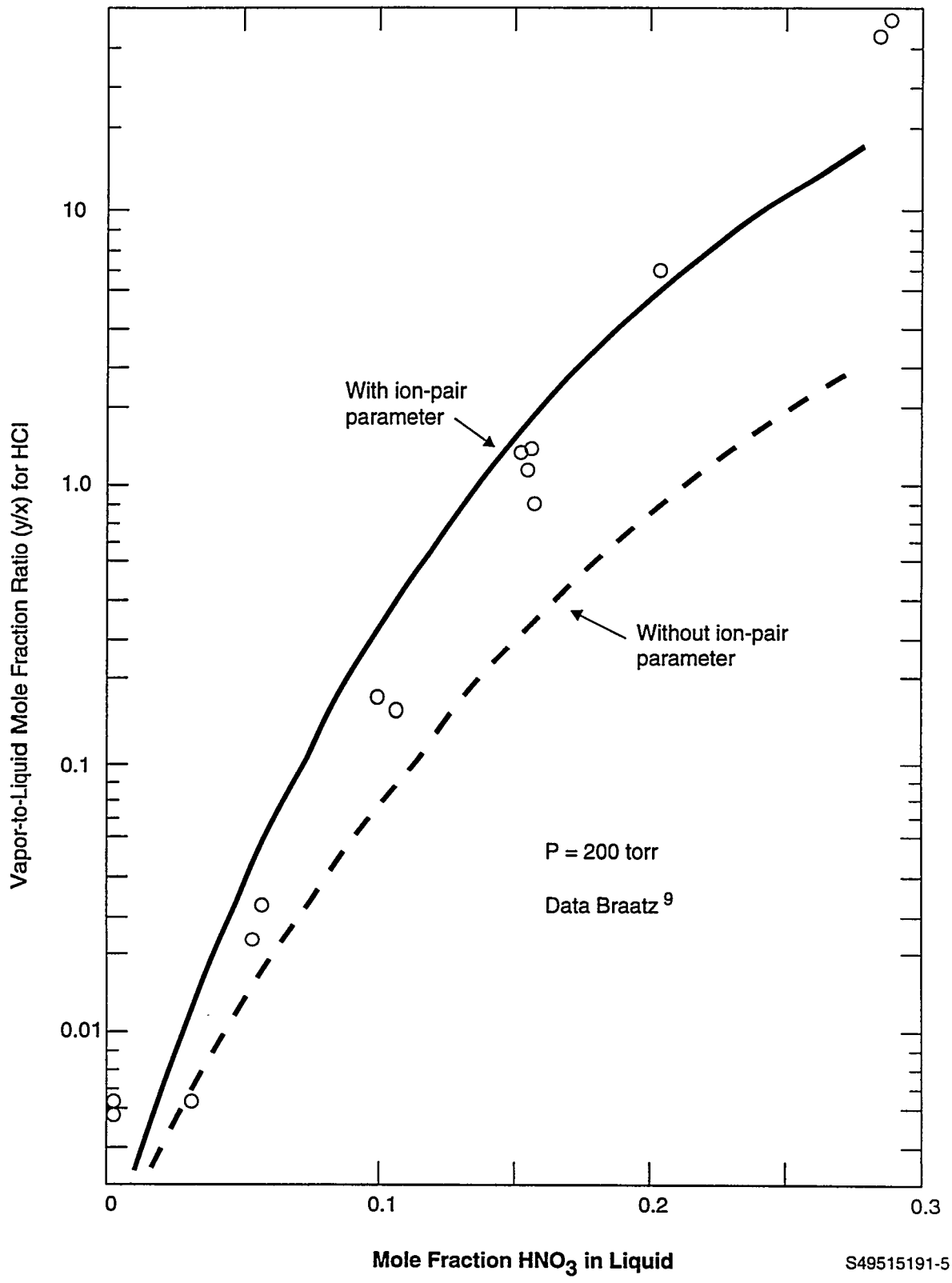

Figure B-6. Effect of nitric acid concentration on HCl volatility in boiling solutions at 200 torr.

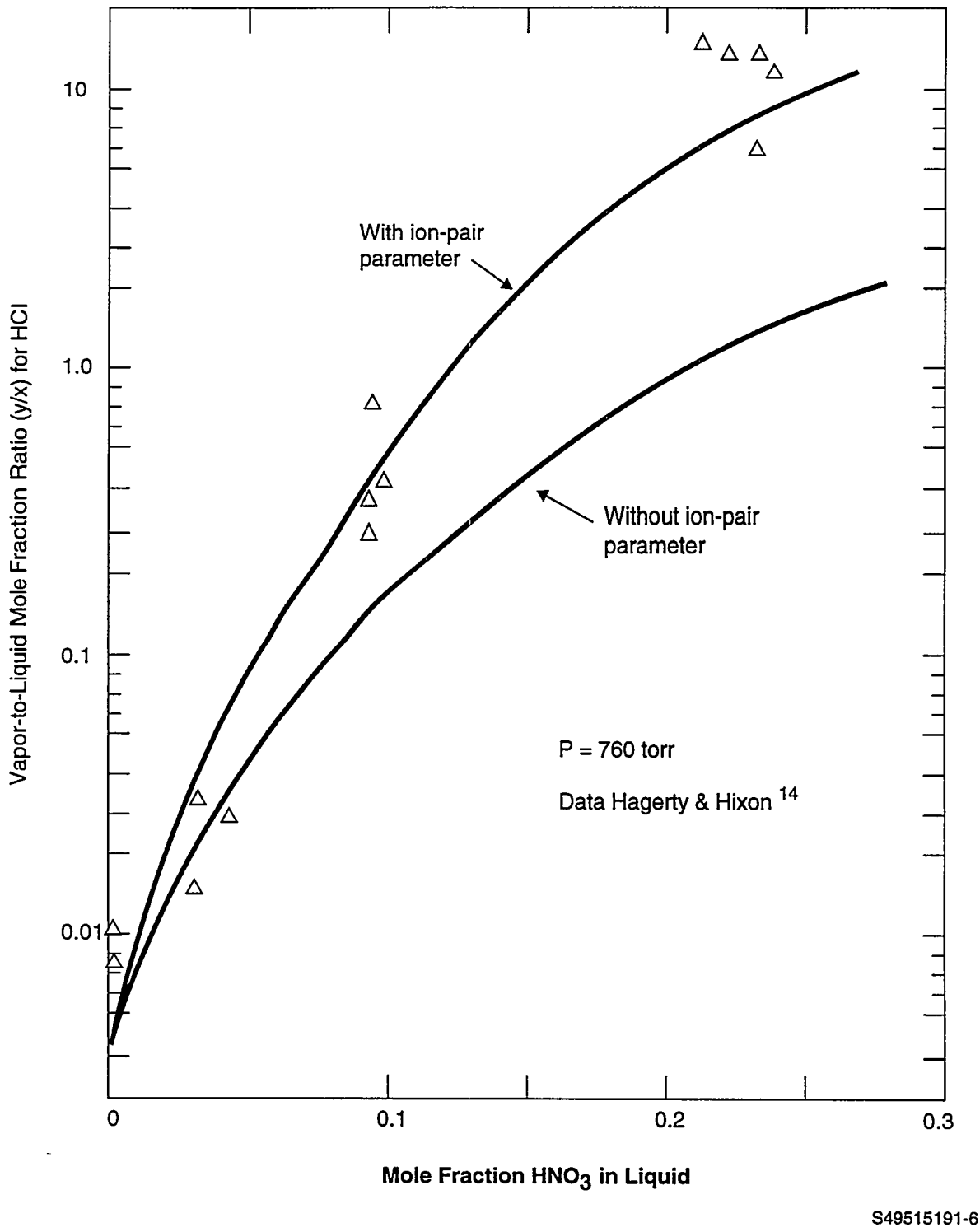

Figure B-7. Effect of nitric acid concentration on HCl volatility in boiling solutions at 760 torr.

B-4. AQUEOUS SOLUTIONS OF HNO_3 AND $NaNO_3$

The addition of sodium nitrate to nitric acid solutions increases the partial pressure of nitric acid[10] by both the common ion effect of the increased nitrate and an increase in activity coefficient. First, the vapor compositions shown as the dashed line in Figure B8, were calculated, for comparison with measured data[10], using only the nitric acid parameters from Tables B1 and B2 and the sodium nitrate-water GMELCC parameters from the ASPEN Plus internal data base. Agreement with the data is poor. Then, the data of Figure B8 was regressed to obtain the nitric acid-sodium nitrate parameters listed in Table B5. The vapor composition calculations with the additional parameters are much improved as shown by the solid line on Figure B8.

Table B-5. Activity coefficient parameters for $NaNO_3$-HNO_3-H_2O.

Parameter	Species Pair	Value (SI)
GMELCC[a]	H2O (Na+ NO3-)	7.167
GMELCC[a]	(Na+ NO3-) H2O	-3.645
GMELCC	HNO3 (Na+ NO3-)	30
GMELCC	(Na+ NO3-) HNO3	-3.37027

a. From ASPEN Plus internal data base.

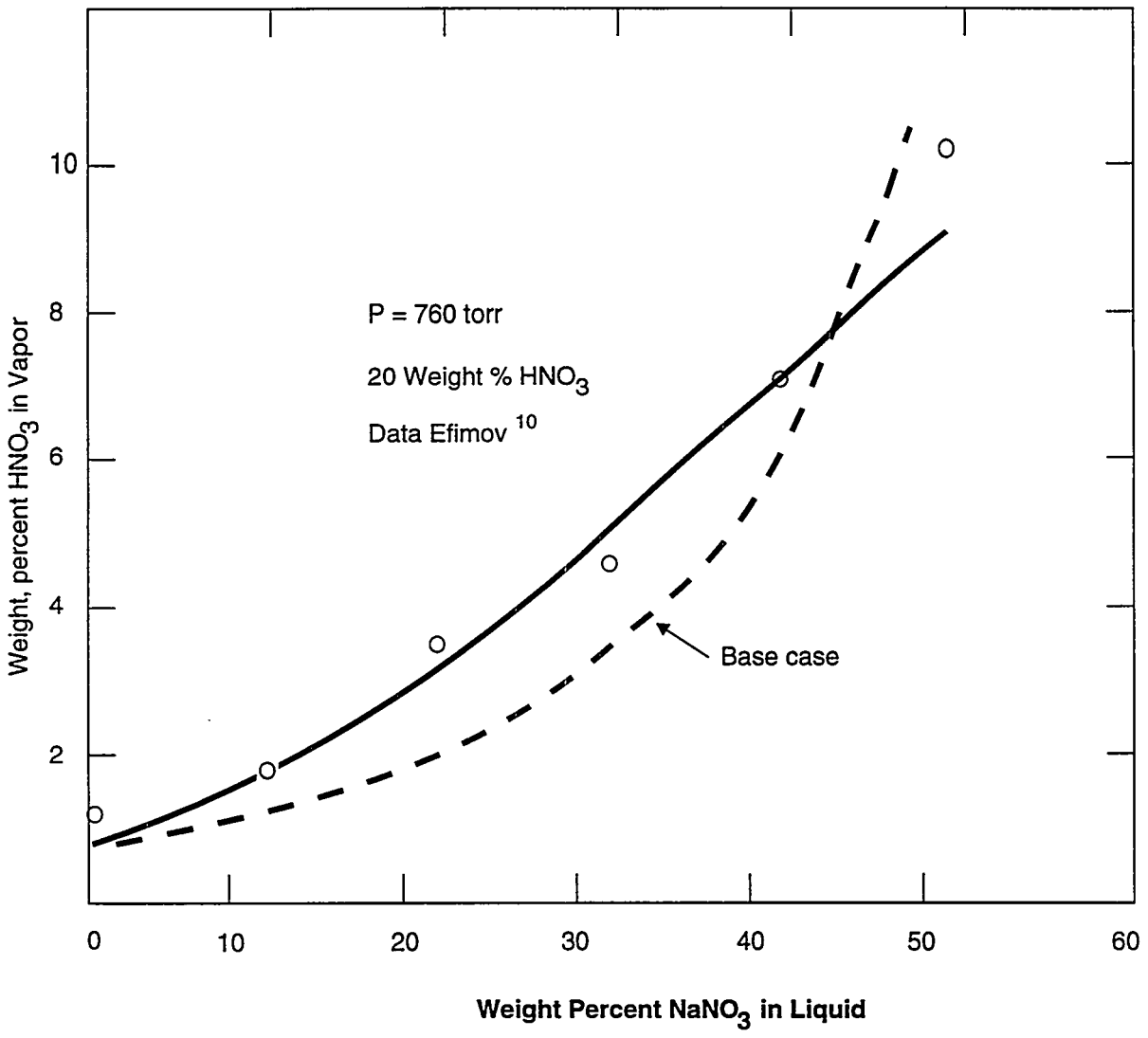

Figure B-8. Effect of $NaNO_3$ concentration on the composition of vapors from boiling 20 Percent HNO_3 solutions.

B-5. AQUEOUS SOLUTIONS OF HNO_3 AND $Al(NO_3)_3$

The addition of aluminum nitrate to nitric acid solutions increases the partial pressure of nitric acid[10] by both the common ion effect of the increased nitrate and an increase in activity coefficient. The activity coefficient parameters listed in Table B6 were obtained by simultaneous data regression of: 1) vapor compositions[10] for boiling nitric acid-aluminum nitrate solutions, 2) freezing point depression[15] of aluminum nitrate solutions, and 3) osmotic coefficients[16] of aluminum nitrate solutions. An assessment of the data fit is given by the comparisons of calculated and measured vapor compositions in Figure B9. VLCLK density parameters for $Al(NO_3)_3$ solutions of 0.04228523 and 0.09233652 were obtained by regression of density data[17].

Table B-6. Activity coefficient parameters for $Al(NO_3)_3$-HNO_3 solutions.

Parameter	Pair	Value (SI)
GMELCC	H2O (AL+3 NO3-)	7.188743
GMELCC	(AL+3 NO3-) H2O	-3.694923
GMELCD	H2O (AL+3 NO3-)	915.3977
GMELCD	(AL+3 NO3-) H2O	-445.3932
GMELCC	HNO3 (AL+3 NO3-)	5.327914
GMELCC	(AL+3 NO3-) HNO3	-2.970832
GMELCC	(H3O+ NO3-) (AL+3 NO3-)	10
GMELCC	(AL+3 NO3-) (H3O+ NO3-)	-1.741289

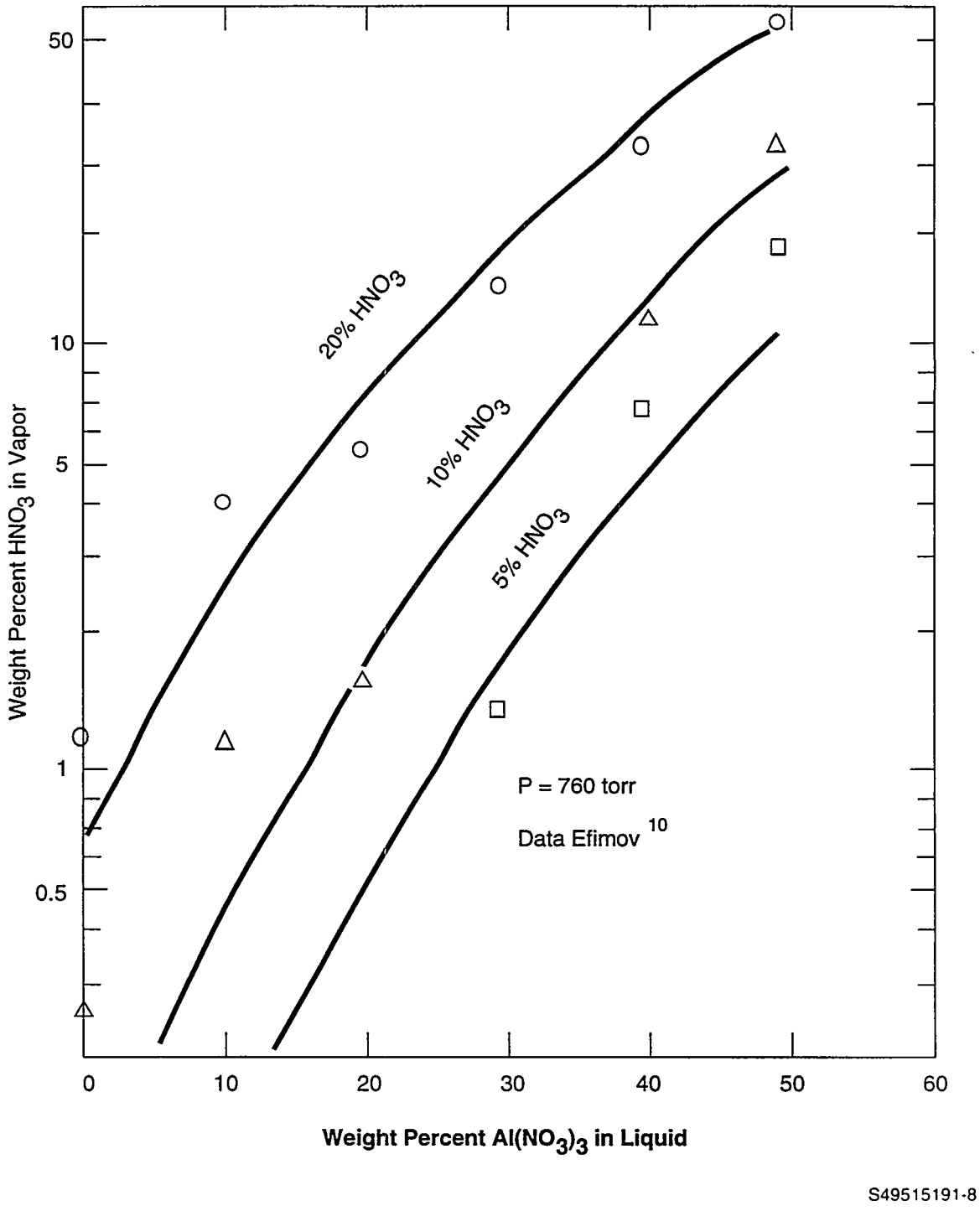

Figure B-9. Effect of $Al(NO_3)_3$ concentration on the composition of vapors from boiling HNO_3 solutions.

B-6. AQUEOUS SOLUTIONS OF HF

The activity coefficient parameters for aqueous HF solutions listed in Table B7 were obtained by regression of HF partial pressure data[18,19,20,21]. Comparisons of the measured HF partial pressures or vapor concentrations with those calculated with the parameters of Table B7 are shown in Figures B10 and B11.

The addition of nitric acid to HF solutions increases[22] the partial pressure of HF over the solution. The HF partial pressures for aqueous solutions of HF and HNO_3 calculated with the activity coefficient parameters HNO_3-H_2O and HF-H_2O were compared with measured data[22] (at 25°C) and found to be conservative by roughly a factor of two. An interaction parameter for HNO_3 solutions was not determined in order to leave a margin of conservatism in the calculations.

Table B-7. Activity coefficient parameters for HF-H_2O .

Parameter	Species Pair	Value (SI)
GMELCA	HF H2O	-0.8770385
GMELCA	H2O HF	3.227835
GMELCB	HF H2O	-217.7091
GMELCB	H2O HF	-2043.170
GMELCC	H20 (H3O+ F-)	14.75332
GMELCC	(H3O+ F-) H2O	-1.153951
GMELCC	HF (H3O+ F-)	-1.503360
GMELCC	(H3O+ F-) HF	6.352884
GMELCD	H20 (H3O+ F-)	406.0699
GMELCD	(H3O+ F-) H2O	-2173.069
GMELCD	HF (H3O+ F-)	3120.915
GMELCD	(H3O+ F-) HF	-6113.476

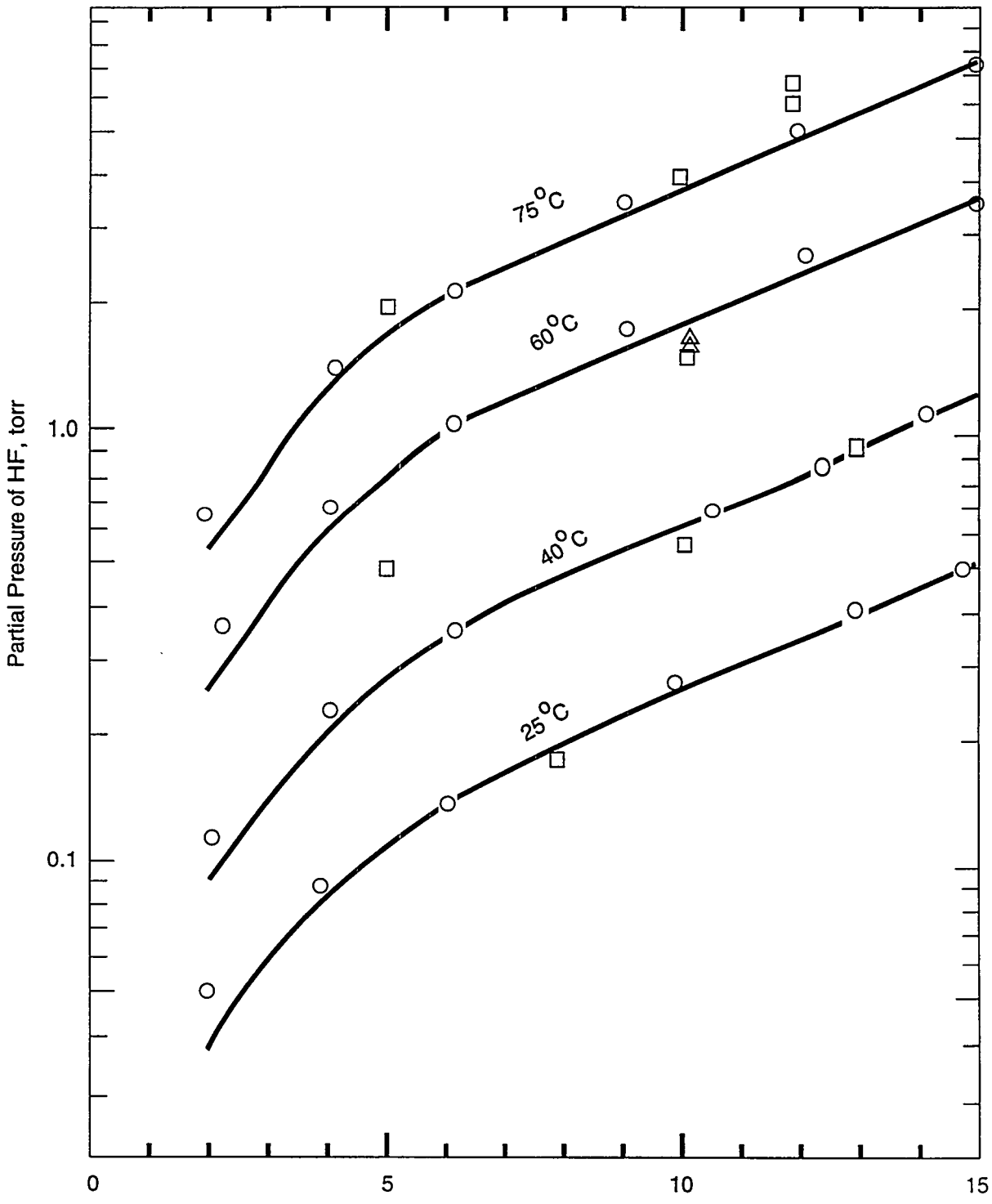

Figure B-10. Comparison of calculated and measured HF partial pressures at 25, 40, 60, and 75°C.

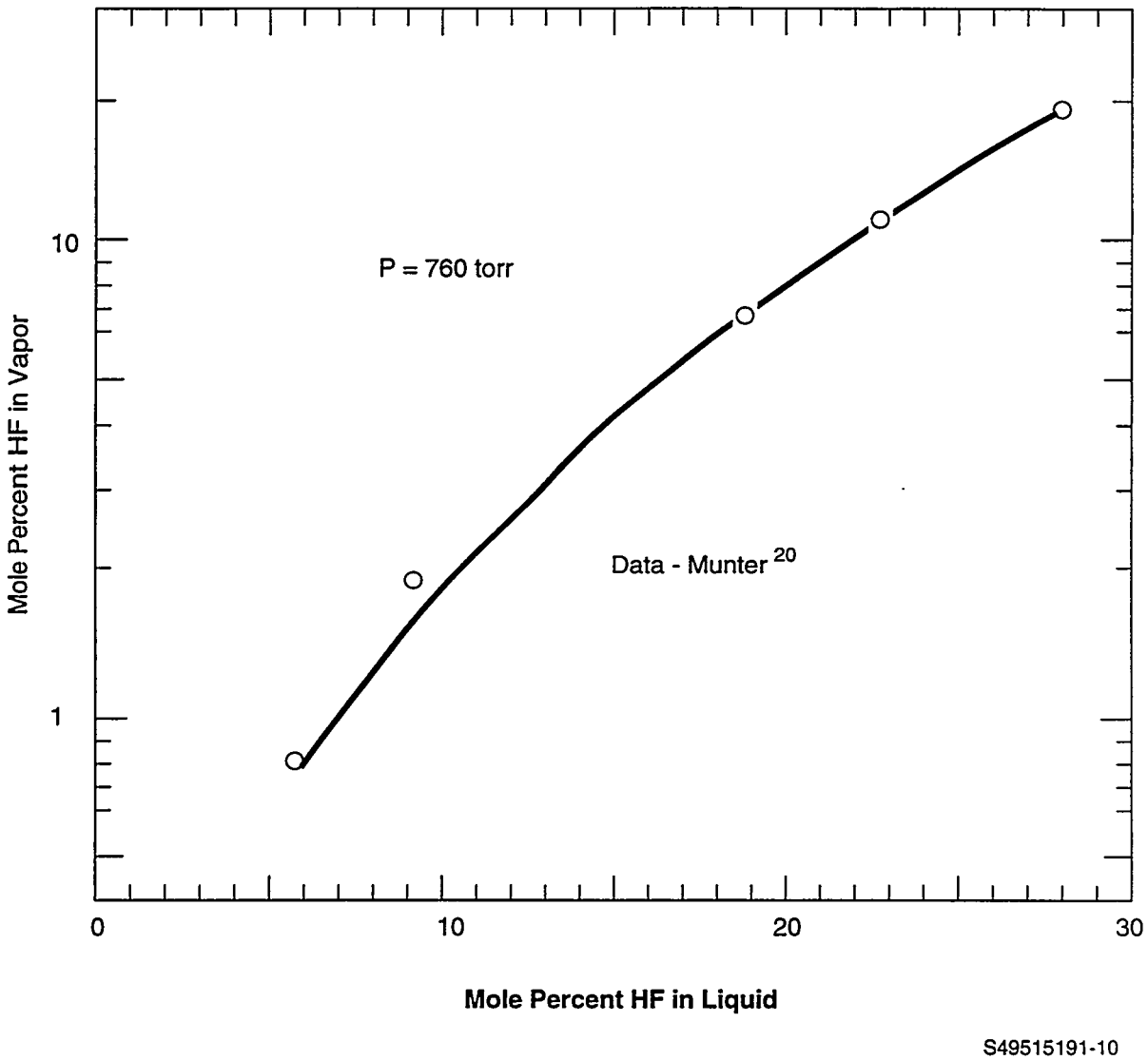

Figure B-11. Comparison of calculated and measured HF partial pressures for boiling HF solutions.

B-7. QUALIFICATIONS ON PARAMETER USAGE

The ASPEN parameters tabulated in this appendix should be considered as sets of parameters suitable for conservative calculations of vapor pressures but not necessarily anything else. Essentially all the parameters, including the acid hydrolysis stoichiometry coefficients, were regressed from vapor pressure data and no other data.

The equilibrium coefficient of the nitric acid hydrolysis calculated with the K-STOIC parameters of Table B1 are roughly 100-fold higher than those obtained[23,24,25] by direct measurement of nitrate ion concentration (i. e., the K-STOIC parameters of Table B1 overestimate nitric acid hydrolysis). The K-STOIC and activity coefficient parameters used as a set probably calculate the correct activity of molecular nitric acid in solution, but could error if used for calculations of nitrate ion concentration (e. g., for solubility calculations).

Another unresolved question is whether there are significant ion-pair interactions between chloride ions and ions of sodium nitrate or aluminum nitrate. The vapor pressure data for mixtures needed for a resolution of this question are not available.

The data regression for the HF-H_2O parameters of Table B7 was first done using enthalphy and heat capacity data (at 25°C) as well as vapor composition data. Calculations with the parameters obtained fit the data for boiling solutions but were about a factor of two low at 25°C because the regression favored the enthalphy data at 25°C. It was decided that this approach provided a "warped" activity correlation being based on enthalphy and heat capacity at 25°C and on vapor composition at higher temperatures. The regression was then repeated using only vapor composition (TPXY) data to obtain the parameters of Table B7. One factor contributing to the discrepancy is that the HF vapor pressure correlation errs in neglecting the presence of H_2F_2 in the vapor over "100 %" HF. Warren[26] observed H_2F_2 in concentrated HF solutions and determined an equilibrium coefficient (at 25°C) of

$$[H_2F_2]/[HF]^2 = 2.7$$

which would indicate that "100 %" HF is mostly H_2F_2 rather than HF. A vapor pressure correlation for HF based on the (total) vapor pressure of "100 %" HF (the normal procedure) would then error significantly on the low side. This suggests that the correlation using the parameters of Table 1 is one with compensating errors (of perhaps a factor of two) in HF activity and vapor pressure.

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