LOCKHEED MARTIN

**PORTSMOUTH
GASEOUS
DIFFUSION
PLANT**

**Nuclear Criticality Safety Aspects of
Gaseous Uranium Hexafluoride (UF₆)
in the
Diffusion Cascade**

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April, 1997

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Executive Summary

Throughout the Gaseous Diffusion Plant Criticality Safety Documentation a recurring theme is that the process gas, UF_6 , is incapable of sustaining a nuclear chain reaction, or criticality. This infers a great deal of inherent safety in the process; such that strict nuclear criticality safety criteria need only be applied to upset conditions that result in deposition of enriched material in process equipment. These upset conditions are generally detectable and cause considerable operational problems as well.

However, two criticality experiments^{1,2} performed at the Los Alamos Criticality Laboratory have demonstrated that gaseous UF_6 can be brought to the critical condition and sustain a nuclear chain reaction. The experiments were conducted under ideal conditions and the implications on the safety aspect of the operating Gaseous Diffusion Plants were explored in a 1952 inter-company correspondence³. The correspondence was exploring design concepts and gives the critical conditions for a 30 ft. Sphere of UF_6 moderated by HF. Current safety considerations require that an in-depth analysis of the criticality potential of gaseous UF_6 be conducted for worst case plant operating conditions.

This paper determines the nuclear safety of gaseous UF_6 in the current Gaseous Diffusion Cascade and auxiliary systems. The actual plant safety system settings for pressure trip points are used to determine the maximum amount of HF moderation in the process gas, as well as the corresponding atomic number densities. These inputs are used in KENO V.a criticality safety models which are sized to the actual plant equipment. The KENO V.a calculation results confirm nuclear safety of gaseous UF_6 in plant operations.

ANS Transactions, Vol. 27, pp. 930-931, 1977

¹**A $\text{U}(95\%)\text{F}_6$ -Helium Circulating Gas Critical Assembly**
D. M. Barton, G.A. Jarvis, J.F. Davis III (LASL)

ANS Transactions, Vol. 27, pp. 934-935, 1977

²**Gas Core Reactors: Neutronics, SNM Proliferation, and Resource Utilization**
Thomas P. McLaughlin, Patick D. Soran, Gordon E. Hansen (LASL)

KS-316, Carbide and Carbon Chemicals, Oak Ridge, Tenn., 1952

³**Critical Conditions in Bare HF-Moderated Gaseous UF_6 Spheres**
A.D. Callihan, H.F. Henry, R.L. Macklin

1.0 INTRODUCTION

The Portsmouth Gaseous Diffusion Plant (PORTS) utilizes UF_6 in the gaseous phase to enrich the ^{235}U isotope. This report identifies the limiting process conditions of the PORTS Enrichment System and demonstrates that gaseous UF_6 is sub-critical under unlimited moderation conditions (e.g. HF).

2.0 PURPOSE

The purpose of this report is to verify the SAR statement:

" UF_6 in the gaseous phase, at pressures and temperatures existing in the enrichment cascade equipment, is incapable of supporting a nuclear chain reaction even when intermixed with hydrogenous material (e.g. HF)."

3.0 SCOPE

This report analyzes several conditions found in the enrichment system, determines the most reactive condition and demonstrates the gaseous phase as being sub-critical in all cases of loss of moderation control. This analysis covers current cascade operation which is limited up to a maximum of 10 wt% ^{235}U . Potential plant operations with enrichment up to 97.65 wt % ^{235}U are also investigated for completeness.

4.0 TECHNICAL JUSTIFICATION

Monte Carlo neutronics calculations for UF_6 gas in the cascade system are presented to demonstrate that the cascade system is sub-critical for all cases of gaseous UF_6 limited to 10 wt% ^{235}U enrichment.

5.0 EXAMPLE MATERIAL STUDY OF A TYPICAL POINT

The following typical cascade operating points were utilized to start the study.

- High side of cascade compressor -13 psia with a temperature range of 260-290 °F
(Some cells are operated above atmospheric pressure; 14.45 psia, but pressures are generally kept below atmospheric.)
- Low side of cascade compressor - 0.5-6 psia with a temperature range of 170-190 °F.

The method to convert a typical cascade point into isotopic densities was developed, and an average point for 10 psia with a temperature of 170 degrees °F was selected for the calculation.

5.1 Ideal Gas Law

The ideal gas law was selected for use due to it's simplicity; and the fact that little difference exists between the ideal law and a more sophisticated model such as a Van der Waals equation of state. Dr. E.J. Barber ⁷, states that the Ideal Gas Model is reasonable for UF₆ in the gaseous phase.

$$PV = nRT \quad \text{Ideal Gas Law}$$

$$n/V = P/RT \quad \text{Specific Volume}$$

w/ n = Number of Moles

$$R = \text{Gas constant} = 8.3143 \times 10^7 \text{ erg/K-Mol}$$

P = Pressure

T = Temperature

V = Volume

5.2 Unit Conversions

Pressure: Force per square area.

$$\text{lb}_f/\text{in}^2 * 4.4482 \text{ N/lb}_f * (\text{in}/2.54 \text{ cm})^2 = 0.689472 \text{ N/cm}^2 \text{ or } (\text{Kg-g/cm}^2)$$

with g = acceleration due to gravity equal to 9.80665 m/s²

$$(0.689472 \text{ Kg-a/cm}^2 * 1000 \text{ g/kg}) / 9.80665 \text{ m/s}^2$$

Therefore, the conversion is : 70.307 g/cm² per psia

$$10 \text{ psia} * 70.307 \text{ (g/cm}^2\text{)}/\text{psia} = 703.07 \text{ g/cm}^2$$

$$\text{Temperature: } (170 \text{ }^\circ\text{F} - 32) * (5/9) = 76.7 \text{ }^\circ\text{C} + 273.1 = 349.8 \text{ }^\circ\text{K}$$

$$\text{Gas Constant: } 8.3143\text{e}^7 \text{ erg/K-Mol} * 1.01972\text{e}^3 \text{ g-cm/erg}^1 = 84782.58 \text{ g-cm/K-Mol}$$

$$\text{Specific Volume} = P/RT = 703.07 / (84782.58 * 349.8) = 2.371\text{e-}5 \text{ Mol/cc}$$

$$\text{Atomic Weight of UF}_6 \text{ at 10 wt \% } ^{235}\text{U} = 351.8 \text{ g/Mol} \quad (\text{see page 5})$$

$$\text{UF}_6 \text{ Density} = 351.8 \text{ g/Mol} * 2.371\text{e-}5 \text{ Mol/cc} = 0.008341 \text{ gUF}_6\text{/cc}$$

5.3 Postulated HF Contamination

Generally, only part per million levels of HF are found in the cascade. However, for this example partial pressure due to HF concentration is assumed to be limited to atmospheric pressure.

Earlier work⁵ identifies equations of state and formulations for HF. See section nine for a discussion on the non-linear behavior of HF.

This example assumes the partial pressure of HF is 4.45 psia, making the system pressure equal to atmospheric pressure: (*The Portsmouth site conservatively defines atmospheric pressure as 14.45 psia.*)

- Pressure: $4.45 \text{ psia} * 70.307 \text{ (g/cm}^2\text{)}/\text{psia} = 312.87 \text{ g/cm}^2$
- Specific Volume = $P/RT = 312.87 / (84782.58 * 349.8) = 1.055 \times 10^{-5} \text{ Mol/cc}$
- Atomic Weight HF = 20 g/Mol
- HF Density = $20 \text{ g/Mol} * 1.055\text{e-}5 \text{ Mol/cc} = 2.11 \times 10^{-4} \text{ gHF/cc}$

¹F-288, CRC Handbook of Chemistry and Physics, 62nd ed.

5.4 CSAS Input Development

The Portsmouth Gaseous Diffusion site utilizes a validated CSAS module¹¹. The gas densities have to be translated into fractions of the theoretical density of the molecular form.

Table 5.4.1
Typical Cascade Point

<u>Compound</u>	<u>Theoretical Density</u>	<u>Gas Density</u>	<u>CSAS Input</u>
UF ₆	4.85 g/cc	0.008341 g/cc	0.00172
HF	1.00 g/cc	0.000211 g/cc	0.00021

Data: Assay = 10 wt % ²³⁵U, Moderation: H/X = 4.7 (see below)

Moderation Level

The moderation level of a system is given by the atomic ratio of hydrogen atoms to the fissile isotope, designated by X, the ratio is commonly denoted H/X. When dealing with low assay material H/U is usually used, however; this paper covers a large span of assays and will utilize the H/X ratio. Calculating H/X from the gas densities may be done by utilizing the Atomic Density Equation:

$$N = \rho * Na / At. Wt.$$

$$w / \rho = \text{Density [g/cc]}$$

$$Na = \text{Avogadro's Number}$$

$$At. Wt. = \text{Atomic Weight}$$

The gas densities above are given for the molecules HF and UF₆ so the atomic weights of the molecules have to be used in the equation. Since there is only one hydrogen atom per HF molecule and one uranium atom per UF₆ molecule the molecular ratio is equal to the atomic ratio H/U.

$$H/U = HF/UF_6 = (\rho(HF)*Na/At.Wt.(HF)) / (\rho(UF_6)*Na/At.Wt.(UF_6))$$

Simplified:

$$H/U = \rho(HF)/\rho(UF_6) * At.Wt.(UF_6)/At.Wt.(HF)$$

So the H/U ratio is just the ratio of the densities times the ratio of the atomic weights. The atomic weight of HF is always 20.0063, but the atomic weight of UF₆ varies slightly with assay, see the example below for 10 wt% ²³⁵U.

While weight percents are convenient for working with uranium, isotopic percents are more convenient for scientific applications, a method for converting weight percents to isotopic percents is given in Appendix E.

For 10 wt. % ^{235}U an isotopic % is equal to 10.011.

Four significant digits are used for the atomic calculations; however, for convenience a whole number representation is used in print. Please refer to the following Atomic Weight Table for the difference.

At. Wt. Table		Whole Number Representation
^{235}U	235.0439	235
^{238}U	238.0508	238
^{16}O	15.9994	16
^{19}F	18.9984	19
^1H	1.0079	1
HF	20.0063	20
Av. Num.	0.602205	#/b-mole

$$\text{Atomic Weight UF}_6 \text{ at 10 wt\% } ^{235}\text{U} = 235(.1011) + 238(.8989) + 20(6) = 357.8$$

For the above example of a typical cascade point the numerical evaluation becomes:

$$\text{H/U} = (0.000211/0.008341) * (357.8/20) = 0.452$$

To find the hydrogen to fissile isotope ratio divide by the isotopic assay which is found by:

$$\text{H/X} = 0.452 / 0.1011 = 4.515$$

Fissile Isotope Density

For the ^{235}U density multiply the UF_6 gas density by the U/UF_6 fraction, which varies slightly with assay; for 10 wt. % ^{235}U the fraction is 0.67586. The fissile isotope density is found by simply multiplying the uranium density by the assay:

$$0.008341 \text{ (gUF}_6\text{/cc)} * 0.67586 = 0.005637 \text{ (gU/cc)} * 0.10 \text{ [for 10 wt\% } ^{235}\text{U]} = 5.637 \times 10^{-4} \text{ g}^{235}\text{U/cc.}$$

6.0 CASE DEVELOPMENT

While the above example is worked out for a typical pressure in the cascade system, the maximum pressures are of interest. To be conservative, the densest gas possible is required for each case. The densest gas would exist at the highest pressure possible at the lowest possible temperature. Significant differences in operations were found between the Low Enrichment (Low E) and the Very High Enrichment (VHE); therefore, separate cases are presented.

6.1 Cascade Case

Low E Case: 330 Building limited to 10 wt% ^{235}U

Most of the 330 Building operates below atmospheric pressure (14.45 psia), thus avoiding UF_6 releases. The maximum pressure the cascade will attain is 25.0 psia per the Safety Analysis Report ³. The lowest possible temperature would be 170 °F in the Surge Drum Room.

VHE Case: 326 Building limited to 97.65 wt% ^{235}U (represents the HEU refeed)

The maximum pressure of this building is limited to 14.45 psia by the Operational Safety Report (OSR). This also allows a lower operating temperature of 140 °F.

6.2 Withdrawal Case

Low E Case: Low Assay Withdrawal (LAW) Station is limited to 10 wt% ^{235}U .

The highest UF_6 gas pressure in the cascade is at the discharge of the product withdrawal pumps, the Worthington Centrifugal Compressors. These compressors increase the pressure of the UF_6 gas to 30-35 psia. However, the pump curve, Fig. 1, indicates that the limiting pressure is 45 psia, when all flow stops. The Worthington compressors generally discharge just below 300 °F, with a range of 270-300 °F. Some cooling of the UF_6 occurs in the pipe before it reaches the condensers, which take the gas into a liquid phase. The cold side of the heat exchanger ranges from 150-160 °F; however, at this pressure the UF_6 will condense at about 195 °F. Therefore, 190 °F is used to calculate the densest possible gas during the withdrawal process.

In addition, the Worthington Centrifugal Compressors are incapable of compressing HF into a liquid phase (ref 3). Therefore, only the gas phase of HF is a potential moderator.

Figure 1. Worthington Centrifugal Compressor Curve

6.3 Autoclave/Refeed Case

Low E Case: Low Assay Withdrawal (LAW) Station is limited to 10 wt% ^{235}U .

The highest pressure the UF_6 gas will experience is while the UF_6 cylinder is heated to 235 °F in the autoclave. In some situations there are incompressible light gases contaminating the UF_6 , and these gases contribute to increasing the pressure. The light gasses in the cylinder are conservatively assumed to be HF because it is the most effective moderator and most common contaminate. Operators monitoring the autoclave process do not allow the pressure to exceed 100 psia so 110 psia is used in the calculations.

VHE Case: 326 Product Withdrawal (PW) Station is approved up to 100 wt% ^{235}U .

While large autoclaves are used at PORTS for Low E material, they are not used with the VHE material. While the VHE product has been suspended it is being investigated for completeness. The VHE cylinder refeeding does not use the high temperatures that are required for the large Low E cylinders. The VHE cylinders are evacuated directly into the cascade and could only see the maximum cascade pressure. Since the stopcock valve is open to the cascade, even if heat lamps were applied to the cylinders, the cylinder could only be the maximum cascade pressure of 14.45 psia. Therefore, for VHE the product refeed case is also covered by the cascade case.

6.4 Liquid Sampling at X-345

While pressurization is not used on VHE material for withdrawal or refeeding, it is pressurized in the sampling process; currently this is strictly a Department of Energy function and is not preformed by LMUS. Autoclaves are used for this process and the limiting Safety System Settings are 114.7 psia trip limit and 230 °F trip limit. This material is of course in the liquid phase and would be outside the scope of this report. However, both the liquid and gas phase of UF_6 exist during liquid sampling because a void space is always required to avoid mechanical failures.

The pressures and temperatures of liquid sampling were found to be outside the scope of the UF_6 Phase Diagram. Investigation revealed that the original equations are presented by J.L. Feuerbacher⁷. The Phase Relation equations are presented here:

Solid, Vapor : 0° to 64 °C.

$$\text{Log}_{10}P_{(\text{mm})} = 6.38353 + 0.0075377t - 942.76/(t + 183.416) \quad (82)$$

error = +/- 0.05% with 95% Confidence Level

Liquid, Vapor : 64° to 116 °C.

$$\text{Log}_{10}P_{(\text{mm})} = 6.99464 - 1126.288/(t + 221.963) \quad (83)$$

error = +/- 0.03% with 95% Confidence Level

Liquid, Vapor : 116 °C. to critical point

$$\text{Log}_{10}P_{(\text{mm})} = 7.69069 - 1683.165/(t + 302.148) \quad (84)$$

error = +/- 0.3% with 95% Confidence Level

The above set of equations were automated by program PHASE, given in Appendix C. The temperatures were converted to Fahrenheit and the pressures converted to psia.

With program PHASE, it was found that the solid-vapor transition for 114.5 psia is about 262 °F which is above the safety system cut off temperature. Therefore, the temperature limit of 230 °F is the limiting control, at 230 °F the corresponding condensation pressure is 78.2 psia.

6.5 Limiting UF₆ Density

The densest gas possible would be just as the vapor state was condensing. This is represented on the phase diagram, Fig. 2, as the line from the Triple Point raising to the right. A series of points along the line were checked for density, and the densest gas is at the highest pressure in spite of the higher temperature. Therefore, the densest UF₆ gas on the phase diagram is the point in at 100 psia and 250 °F.

The autoclave case for Low E cylinders generates a higher fissile isotope density due to the conservative assumptions (all UF₆) in the autoclave rupture scenario. There are no scenarios that would pressurize the VHE material to higher than liquid sampling.

Figure 2. UF_6 Phase Diagram

6.6 Case Summary

Table 6.6.1

Case Summary

<u>Cases</u>	<u>Pressures and Temperatures</u>
1. Typical Cascade Point	10 psia at 170 °F
2. Top Cascade Pressure	LowE - 25 psia at 170 °F VHE - 14.45 psia at 140 °F
3. Withdrawal Pressure	LowE only - 45 psia at 190 °F
4. Autoclave/Refeed	LowE only - 110 psia at 235 °F
5. Liquid Sampling	78.2 psia at 230 °F
6. Limiting UF ₆ Density	LowE only - 100 psia at 250 °F

Other equipment used in the Cascade also have characteristic limiting pressures, however they are conservative to the above cases. For example at the Portsmouth Plant:

A&B Booster Stations	25 psia
A-Booster Station to X-326 Bld.	14.3 psia
Emergency Booster Station (EBS)	12.5 psia (safe) 10.0 (low speed)
Holding Drums	12.5 psia

6.7 Case Evaluation

Table 6.7.1
Cases at 10 wt. % ^{235}U

Cases	Maximum UF_6 Pressure (psia)	Temperature ($^{\circ}\text{F}$)	Fissile Isotope Density ($\text{g}^{235}\text{U}/\text{cc}$)
1	10	170	5.64×10^{-4}
2	25	170	1.41×10^{-3}
3	45	190	2.46×10^{-3}
4	110	235	5.62×10^{-3}
5	78.2	230	4.02×10^{-3}
6	100	250	5.00×10^{-3}

Table 6.7.2

Cases at 97.65 wt. % ^{235}U

Cases	Maximum UF_6 Pressure (psia)	Temperature ($^{\circ}\text{F}$)	Fissile Isotope Density ($\text{g}^{235}\text{U}/\text{cc}$)
1	10	170	5.44×10^{-3}
2	14.45	140	8.26×10^{-3}
5	78.2	230	3.89×10^{-2}

See Appendix 1 for calculations.

The highly enriched UF_6 gas has been demonstrated to remain subcritical for cascade and withdrawal cases. The only case in question is the liquid sampling operation. Further analysis of this condition is required; however, the safety of the liquid sampling operation is based on safe geometry and moderation control. The safety of the operation is not in question, just if the original SAR statement can be verified.

It was also of interest to investigate a scenario to demonstrate the criticality safety aspects of withdrawing UF_6 gas with HF moderation. A scenario of an emergency withdrawal of VHE material to a 30B cylinder was chosen. Because, the 30B cylinder is larger than the accumulators and there are no physical barriers preventing the introduction of a large cylinder to the Extended Range Product (ERP) station.

7.0 CALCULATIONAL APPROACH

7.1 Calculational Method

The calculations were performed using the KENO V.a module in the Standardized Computer Analyses for Licensing Evaluation (SCALE), Version 4.2, to calculate the neutron multiplication factor, k_{eff} ¹⁰. The SCALE package used is located on a QA production version of the Battelle PSRM NS system at the Portsmouth Gaseous Diffusion Plant (PORTS). PSRM NS is loaded on a IBM 6000, workstation, and has a configuration control plan¹¹. ENDF/B-IV 27 energy group cross sections were used in the evaluation. The experimental data used in the validation describes the area of applicability of the computer code¹².

Production calculations may be performed for all enrichments of uranium systems with the CSAS25 sequence and the 27-group ENDF/B-IV cross sections only. This validation is considered to cover the majority of fissile systems that may be encountered at a gaseous diffusion plant.

7.2 Modeling Approach

7.2.1 Liquid Sampling

Per plant procedure: UF₆ Cylinder Fill, Temperature, Pressure and Assay Limits ¹⁴, only 5" diameter cylinders are allowed to be filled with VHE material. The 12" cylinders are limited to 40 wt % ²³⁵U. Table 7.2.1 demonstrates the use of the small cylinders on site under Liquid Sample conditions.

Table 7.2.1
Gas Phase of UF₆ Cylinders at Liquid Sample Conditions

Cylinders	Diameter	Limited Assay wt % ²³⁵ U
12A,12B,12MD, 12FN	12"	40
8H	8	70
8S	8	97.85
5A,5B	5	100

A 12" diameter cylinder was chosen to demonstrate that at 100 wt% ²³⁵U under the liquid sample conditions that UF₆ gas remains sub-critical under all possible moderation conditions. Although this situation would require several failures and violations of procedures it would demonstrate the nuclear safety of UF₆ under extreme circumstances.

7.2.2 Emergency VHE Withdrawal

The emergency VHE product withdrawal case was found to have a fissile isotope density of 0.00243 g²³⁵U/cc. This case will require evaluation based on postulated use in the enrichment cascade.

The three pieces of equipment after the withdrawal compressors are the condenser, the accumulator, and the UF_6 cylinder. Both the cylinders and accumulators are geometrically safe for this assay of equipment in the solid and liquid phase³. The optimum moderated gaseous mixture will have to be found for the condenser which is a 10" diameter cylinder approximately 8' long.

However, the ERP withdrawal station does not physically exclude the introduction of 2 ½-ton cylinders for loading. Since a 30B, 2 ½-ton cylinder, would be more than adequate to cover either the condenser or accumulator in size, it is conservative to use the 30B cylinder dimensions to represent this equipment. Since the thickness of the steel walls of the equipment cannot easily be verified and it is conservative not to use them, they will not be included in the model. The model will be fully reflected with a foot of water on all sides. See appendix 2 for the Keno V.a inputs of this model.

7.3 CSAS Model

7.3.1 Gas Phase during Liquid Sample Model at X-345

Table 7.3.1 was developed with the maximum allowed temperature to 230 °F and the maximum allowed pressure of 114.7 psia corresponding to the two Safety System trip points of the autoclave system. The temperature of 230 °F implies that only 78.2 psia of UF_6 could exist, and the remain pressure is conservatively assumed to be HF. The lower temperatures correspond to the condensation points of the selected pressures per program PHASE, appendix C.

Table 7.3.1

UF₆/HF Series at 100 wt.% ²³⁵U

CSAS File	UF ₆ (psia)	HF (psia)	Temp. °F °K	H/X	CSAS INPUT UF ₆	CSAS INPUT HF
LS-20	20	94.7	144 335.3	4.74	3.559×10^{-3}	4.684×10^{-3}
LS-30	30	84.7	166 347.6	2.82	5.151×10^{-3}	4.042×10^{-3}
LS-40	40	74.7	184 357.6	1.87	6.676×10^{-3}	3.456×10^{-3}
LS-50	50	64.7	199 365.9	1.29	8.155×10^{-3}	2.933×10^{-3}
LS-60	60	54.7	211 372.6	0.912	9.611×10^{-3}	2.435×10^{-3}
LS-70	70	44.7	222 378.7	0.639	1.103×10^{-2}	1.958×10^{-3}
LS-80	80	34.7	233 384.8	0.434	1.241×10^{-2}	1.496×10^{-3}

In fact, the conditions in Table 7.3.1 could only exist in the void volume of a 5" diameter cylinder during liquid sampling. However, for the calculations the above data was assumed to completely fill a 12" cylinder.

Data on the 12B cylinder indicates that the diameter is 30.5 cm and it is 126 cm. in length with 1/4 inch wall thickness. The 12A cylinder is constructed of nickel and the 12B cylinder is constructed of monel. However, a tolerance is not published with this information so the metals are left out of the model and it is conservative to all of the small series of UF₆ cylinders.

7.3.2 Emergency VHE Withdrawal Model

Data on the 30B Cylinder indicates that the diameter is 76 cm., the length is 206 cm. and it has 1/2" carbon steel walls. The published minimum volume is 736 Liters, using the above gross dimensions in a right cylinder yields a volume of 934 Liters. Therefore, the right cylinder model is a conservative representation of the 30B cylinder.

A series of runs were developed to investigate the effect of varying UF_6 and HF pressure. The total mixture pressure is limited to 45 psia. To conservatively represent all possible cases of UF_6 - HF combinations the UF_6 pressure is varied from 20 psia, to 45 psia. The remaining pressure is assumed to be due to HF gas, thus covering all possible HF contamination levels in the enrichment cascade.

Since 190°F was chosen because it was the condensation temperature for UF_6 at 45 psia, varying temperatures were selected off of the UF_6 phase diagram, Fig. 2, for each of the pressures. A series of condensation points are examined. The temperature is limited to 150°F, because of the cooling water temperature.

Since there can be variation in the enrichment of the UF_6 in the cascade, the KENO V.a inputs were conservatively developed at 100 wt. % ^{235}U instead of 97.65 wt. % ^{235}U . Please refer to Table 7.3.1 for the input data.

Table 7.3.2

UF₆/HF Series at 100 wt.% ²³⁵U

CSAS File	UF ₆ (psia)	HF (psia)	Temp. °F °K	H/X	CSAS INPUT UF ₆	CSAS INPUT HF
VHE-20	20	25	150 338.7	1.25	3.524×10^{-3}	1.224×10^{-3}
VHE-25	25	20	155 341.4	0.80	4.369×10^{-3}	9.715×10^{-4}
VHE-30	30	15	168 348.7	0.50	5.135×10^{-3}	7.135×10^{-4}
VHE-35	35	10	175 352.5	0.286	5.924×10^{-3}	4.704×10^{-4}
VHE-40	40	5	188 359.8	0.125	6.635×10^{-3}	2.305×10^{-4}
VHE-45	45	0	190 360.9	0	7.441×10^{-3}	0

7.4 Calculational Results

7.4.1 Liquid Sampling Case Results

Table 7.4.1

Calculational Results for Liquid Sampling Case

CSAS File	Mass UF ₆ (Kg.)	Mass HF (Kg.)	Keff.	Sigma.	Keff + 2*Sigma
LS-20	1.59	0.431	0.32090	0.00355	0.32800
LS-30	2.31	0.374	0.35675	0.00338	0.36351
LS-40	2.99	0.320	0.38359	0.00373	0.39105
LS-50	3.65	0.271	0.39715	0.00372	0.40459
LS-60	4.30	0.225	0.41295	0.00365	0.42025
LS-70	4.93	0.181	0.41617	0.00365	0.42347
LS-80	5.55	0.135	0.42876	0.00449	0.43775

In the above Table 7.4.1, all of the calculations are below the acceptable margin of safety; Keff. plus two standard deviation are less than 0.95.

7.4.2 Emergency VHE Withdrawal Case Results

Table 7.4.2

Calculational Results for Emergency Withdrawal Case

CSAS File	Mass UF ₆ (Kg.)	Mass HF (Kg.)	Keff.	Sigma	Keff + 2*Sigma
VHE-20	15.972	1.144	0.43513	0.00351	0.44215
VHE-25	19.803	0.908	0.45417	0.00400	0.46217
VHE-30	23.271	0.667	0.46511	0.00389	0.47289
VHE-35	26.850	0.440	0.48474	0.00355	0.49184
VHE-40	30.070	0.215	0.48904	0.00394	0.49692
VHE-45	33.725	0	0.49445	0.00443	0.50331

In the above Table 7.4.2, all of the calculations are below the acceptable margin of safety; K_{eff} plus two standard deviation are less than 0.95. The VHE-45 case, apparently without moderation, still has a $K_{effective}$ of about 0.5 due to the conservative water reflector reflecting moderated neutrons back to the core.

7.5 Optimum Moderation Consideration

It was of interest to calculate the HF pressure required to meet optimum moderation conditions of H/X equal to 500⁸. Assuming 20 psia of UF_6 at 150°F and full enrichment, the HF pressure required for optimum moderation is 10,000 psia. Therefore, optimum moderation could not reasonably be achieved in the gas phase of UF_6 and HF. This analysis is limited to the maximum pressures of the cascade, those limited pressures result in very low H/X moderation levels. Please note that in the enrichment cascade HF usually only exists in the ppm range and to have any significant amounts of HF is a loss of control over the process.

Notice, that taking the ratio of the gross masses of UF_6 and HF and multiplying by the atomic mass ratio of 17.5 the H/X atomic ratio is approximately reproduced.

8.0 NON-LINEAR ASPECTS OF HF

For the purposes of this report, HF was taken as an ideal gas. However, studies have shown non-linear behavior of HF at high pressures and low temperatures. This report attempted to cover all possible ranges of HF pressures in the enrichment cascade to quantify the reactive effect on the fissile isotope. However, the results shown in Table 7.4; demonstrate that the highest reactivity is with low concentrations of HF and high concentrations of UF_6 . While non-linear properties of HF may be of a concern for liquid and solid phases of UF_6 and HF combinations, they do not have a significant effect at the high temperatures and low pressures found in the enrichment cascade.

The property that raises concern is that HF has a large electric dipole moment similar to water and it will form an HF-HF dimer. Also, both the monomer and dimer forms will cluster together and form straight and cyclic chains and, possibly (sources conflict) benzene ring type structures. Molecular weights of up to 80 have been measured, so molecules of four HF atoms are common and possibly up to $[HF]_6$, in the gaseous phase. The liquid and solid phases demonstrate infinite chains of HF atoms. However, the net affect on criticality safety in the gas phase is minor. This report is attempting to define the most reactive case of UF_6 -HF, not the highest concentration of HF. In fact this paper demonstrates that the most reactive case is at a high concentration of UF_6 and low concentrations of HF. A pressure of 2 psia HF translates to a molecular weight of about 22 (ref. 5, p. 55). So the average of all the $[HF]_x$ is barely above the 20 atomic weight of a single molecule of HF.

9.0 REFRIGERANT R-114

The refrigerant used in the enrichment cascade is a fluorocarbon (R-114). The chemical species is identified as Dichlorotetrafluoroethane, or $C_2Cl_2F_4$ with a molecular weight of 114. Since the refrigerant molecule does not contain hydrogen atoms it cannot be as effective a moderator as Hydrofluoric Acid (HF). It does contain carbon atoms which can be used as moderators, however the effectiveness of hydrogen over carbon as a moderator is about a factor of a thousand to one³. Also, R-114 contains two chlorine atoms, which are neutron absorbers or poisons to a nuclear chain reaction. Whether R-114 is a net moderator or net poison is not a concern because it could not be as effective a moderator as HF.

Other fluorocarbons that could be contaminants in the enrichment cascade would have the same argument for safety as the refrigerant, R-114.

10.0 ASSUMPTIONS AND CONCLUSIONS

10.1 Assumptions

The following assumptions were made in this evaluation. If these assumptions are later determined to be invalid, this evaluation may not be conservative and should be modified to take into account only the valid assumptions.

- 1) This report only deals with the gaseous state of Uranium Hexafluoride (UF_6). It does not address the contingent condition of losing the gaseous state.
- 2) A top pressure of 45 psia was based on the specific performance curve of the product withdrawal compressor, any change to the Worthington Centrifugal Compressors could change the curve. The Paducah facility utilizes a 350 cfm Normetex Pump which is a positive displacement pump for a withdrawal pump. The positive displacement pump could compress the UF_6 gas even higher; however, there is a dual set of pressure transmitters that will shut down the Normetex pump, and the setting assures that a limit of 42 psia is never reached.

- 3) A top autoclave pressure of 110 psia was based on rupture disk ratings. Changes in autoclave procedures or rupture disks would have to be analyzed.
- 4) The only moderating agents assumed to exist in the cascade system is gaseous Hydrofluoric Acid (HF) and the refrigerant R-114. Any new refrigerant would have to be analyzed.
- 5) Cylinder dimensions used in this report were conservatively taken from ref. 9 and 14. Larger equipment would have to be re-evaluated.
- 6) Changes in liquid sampling procedures, specifically safety system limit settings, would have to be reanalyzed.

The Ideal Gas Law was only used in calculating atomic densities at specific pressures and temperatures. Limiting temperatures or pressures were determined from physical limits or safety system trip points with the corresponding pressure/temperature determined from the UF_6 phase diagram or with the program PHASE developed from the original phase relation equations⁶.

10.2 Conclusions

UF_6 gas at the temperatures and pressures available in the Portsmouth Gaseous Diffusion Plant and the Paducah Gaseous Diffusion Plant will remain sub-critical under all conditions found in the facility.

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14. *UF₆ Cylinder, Fill, Temperature and Assay Limits, Portsmouth Plant Procedure*; 8.0-5; FV-5.4
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Appendix A. Computational Program: GAS II

This is an engineering assistance program presented in the BASIC programming language.

Input: Pressure, Temperature and Enrichment of UF_6 gas; Postulated HF pressure

Output: UF_6 density, HF density, Fissile Isotope Density and moderation levels.

Note: The program and the accompanying cases developed for the paper include a percent of the GAT-225 Single Parameter Limit for ^{235}U . However, this was dropped out of the paper when it was found that the single parameter limit was developed in aqueous conditions and was felt not to be applicable in gaseous UF_6 conditions.

Appendix A

Computational Program: GAS II

Originally, the calculations for this report were done on spreadsheets; however, it was found difficult to transfer spreadsheets from one engineer to another. Validation in any sense of the spreadsheet was found to be impractical due to having to change it for each problem. Therefore, a simple basic code was developed to facilitate the calculations in this paper. Also, this format allows readability and easy transformation to another platform.

Program : GAS II

```
10 CLS
20 SPV = 0
30 RHO = 0
40 LINE INPUT "What pressure (psia)?----->",P$
50 P=VAL(P$)
60 P=P*70.307
70 LINE INPUT "What temperature - degrees F?----->",T$
80 T = VAL(T$)
90 T = ((T-32)*5/9)+273.1
100 R = 84782.58
110 LINE INPUT "What enrichment?----->",E$
120 E = VAL(E$)
130 ATWT = (2.35*E + (1-(E/100))*238) + 6*19
140 ATWTU = (2.35*E + (1-(E/100))*238)
150 PRINT
160 PRINT
170 PRINT "Press          Temp          Gas Cons.   At. Wt."
180 PRINT P,T,R,ATWT
190 PRINT
200 SPV = P/(R*T)
210 RHO = ATWT*SPV
220 PRINT "Specific Volume          UF6 Density"
230 PRINT SPV,,RHO
240 PRINT
250 LINE INPUT "What HF Pressure are you using (psia)?----->",HFP$
260 HFP = HFP(HFP$)
270 HFP = HFP/(R*T)
280 PRINT
290 HFSPV = HFP/(R*T)
300 HFATWT = 20
310 HFRHO = HFATWT*HFSPV
320 PRINT " HFpres          HF At. Wt. Spec. Vol.          Density"
330 PRINT HFP,HFATWT,HFSPV,HFRHO
340 PRINT
350 PRINT
360 PRINT "Press Space Bar to Continue."
```

```

370 LOCATE,,0
380 IF INKEY$<> " " THEN GOTO 380
390 CLS
400 PRINT "Required Data for Selected Point :"
410 PRINT
420 PRINT "Comp.      Theo.Density      Gas Density
CSAS Input"
430 PRINT
440 PRINT "UF6          4.85 g/cc",RHO,RHO/4.85
450 PRINT
460 PRINT "HF           1.00 g/cc",HFRHO,HFRHO
470 PRINT
480 PRINT "Input Data :"
490 PRINT "UF6 Pressure = "P" g/cm^2",P/70.307"psia"
500 PRINT "Temperature = "T" Kelvin",((T-273.1)*9/5)+32" F"
510 PRINT
520 PRINT "Postulated HF (Acid) in gas phase:"
530 PRINT "HF Pressure = "HFP" g/cm^2,HFP/70.307" psia"
540 PRINT
550 PRINT "Uranium assay used was : "E: wt. % 235U."
560 PRINT
570 FRACTION = ATWTU/(ATWTU+(6*19))
580 URHO = RHO*FRACTION
590 U235RHO=URHO*(E/100)
600 AFRACTION = U235RHO/0.0115
610 PRINT "Precent of GAT-225 Single Parameter Limit:
AFRACTION*100%"
620 PRINT "Fissile Isotope Density : "U235RHO" (g235U/CC)"
630 M = (HFRHO/RHO)*(ATWT/20)
640 PRINT "Moderation Level: H/U ="M"      H/X = "M/(E/100)
650 PRINT "          UF6          HF          Net Wt. (All Kg.)
660 PRINT "30B",RHO*934.5,HFRHO*934.5,(HFRHO+RHO)*934.5
670 PRINT "12B",RHO*92.058,HFRHO*92.058,(HFRHO+RHO)*92.058

```

Variable Table

SPV UF_6 Specific Volume; HFSPV - HF Specific Volume
 RHO UF_6 Density; HFRHO - HF Density
 P UF_6 Pressure; HFP - HF Pressure
 T Temperature - Both Gases
 R Gas Constant
 E Enrichment
 ATWT - Atomic Weight UF_6 ; ATWTU - Atomic Weight
 HFATWT HF Atomic Weight (always 20)*
 FRACTION Fraction of U/ UF_6 weight at current assay
 URHO Uranium Density; U235RHO - Fissile Isotope Density
 M Moderation Level (H/U)
 MASS Total Mass of gas in 30B cyl. model

This Appendix is calculating the maximum fissile isotope density; therefore, it conservatively assumes the maximum pressure as being due to UF_6 .

* A further advancement in the calculation may be done if the atomic weight of HF were made variable with pressure per the graph in ref. 6, to account for the HF_x dimer effect. Then calculating the atomic densities of hydrogen would have to account for how many HF's in the average HF_x .

Attached to this appendix are the set of results for the 13 problems that KENO codes were preformed for.

For File	Pressure	Temperature
LS-20	20	144
LS-30	30	162
LS-40	40	181
LS-50	50	197
LS-60	60	210
LS-70	70	221
LS-80	80	232
VHE-20	20	150
VHE-25	25	155
VHE-30	30	168
VHE-35	35	175
VHE-40	40	188
VHE-45	45	190

Required Data for Selected Point : File: LS-40

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	3.252943E-02	.0067071
HF	1.00 g/cc	3.481302E-03	3.481302E-03

Input Data:

UF6 Pressure = 2812.28 g/cm² 40 psia
Temperature = 355.8778 Kelvin 181 F

Postulated HF (Acid) in gas phase:

HF Pressure = 5251.933 g/cm² 74.7 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 190.4676 %

Fissile Isotope Density : 2.190377E-02 (g235U/cc)

Moderation Level: H/U = 1.8675 H/X = 1.8675

	UF6	HF	Net Wt. (All Kg.)
30B	30.39876	3.253276	33.65203
12B	2:994594	.3204817	3.315076

Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File: LS-50

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	3.967092E-02	8.179571E-03
HF	1.00 g/cc	2.941786E-03	2.941786E-03

Input Data:

UF6 Pressure = 3515.35 g/cm² 50 psia
Temperature = 364.7667 Kelvin 197 F

Postulated HF (Acid) in gas phase:

HF Pressure = 4548.863 g/cm² 64.7 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 232.2827 %

Fissile Isotope Density : 2.671251E-02 (g235U/cc)

Moderation Level: H/U = 1.294 H/X = 1.294

	UF6	HF	Net Wt. (All Kg.)
30B	37.07247	2.749099	39.82157
12B	3.652025	.2708149	3.92284

Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : LS-20

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	1.726176E-02	3.559126E-03
HF	1.00 g/cc	4.683921E-03	4.683921E-03

Input Data:

UF6 Pressure = 1406.14 g/cm² 20 psia
 Temperature = 335.3222 Kelvin 144 F

Postulated HF (Acid) in gas phase:

HF Pressure = 6658.073 g/cm² 94.7 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 101.0717 %

Fissile Isotope Density : 1.162325E-02 (g235U/cc)

Moderation Level: H/U = 4.735 H/X = 4.735

	UF6	HF	Net Wt. (All Kg.)
30B	16.13111	4.377125	20.50824
12B	1.589083	.4311924	2.020275

Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : LS-30

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	2.514283E-02	5.184088E-03
HF	1.00 g/cc	4.067999E-03	4.067999E-03

Input Data:

UF6 Pressure = 2109.21 g/cm² 30 psia
 Temperature = 345.3222 Kelvin 162 F

Postulated HF (Acid) in gas phase:

HF Pressure = 5955.003 g/cm² 84.7 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 147.2172 %

Fissile Isotope Density : 1.692998E-02 (g235U/cc)

Moderation Level: H/U = 2.823333 H/X = 2.823333

	UF6	HF	Net Wt. (All Kg.)
30B	23.49597	3.801545	27.29752
12B	2.314598	.3744918	2.68909

Required Data for Selected Point : File : LS-60

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	4.668084E-02	9.624915E-03
HF	1.00 g/cc	2.438818E-03	2.438818E-03

Input Data:

UF6 Pressure = 4218.42 g/cm² 60 psia
 Temperature = 371.9889 Kelvin 210 F

Postulated HF (Acid) in gas phase:

HF Pressure = 3845.793 g/cm² 54.7 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 273.3274 %

Fissile Isotope Density : 3.143265E-02 (g235U/cc)

Moderation Level: H/U = .9116667 H/X = .9116667

	UF6	HF	Net Wt. (All Kg.)
30B	43.62324	2.279075	45.90232
12B	4:297345	.2245127	4.521858

Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : LS-70

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	5.358074E-02	1.104758E-02
HF	1.00 g/cc	1.960753E-03	1.960753E-03

Input Data:

UF6 Pressure = 4921.49 g/cm² 70 psia
 Temperature = 378.1 Kelvin 221 F

Postulated HF (Acid) in gas phase:

HF Pressure = 3142.723 g/cm² 44.7 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 313.728 %

Fissile Isotope Density : 3.607872E-02 (g235U/cc)

Moderation Level: H/U = .6385715 H/X = .6385715

	UF6	HF	Net Wt. (All Kg.)
30B	50.0712	1.832323	51.90353
12B	4.932536	.180503	5.113039

Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File :LS-80

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	6.026115E-02	1.242498E-02
HF	1.00 g/cc	1.497895E-03	1.497895E-03

Input Data:

UF6 Pressure = 5624.56 g/cm² 80 psia
Temperature = 384.2111 Kelvin 232 F

Postulated HF (Acid) in gas phase:

HF Pressure = 2439.653 g/cm² 34.7 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 352.8434 %

Fissile Isotope Density : 4.057699E-02 (g235U/cc)

Moderation Level: H/U = .43375 H/X = .43375.

	UF6	HF	Net Wt. (All Kg.)
30B	56.31405	1.399783	57.71383
12B	5.547521	.1378932	5.685414

Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : VHE-20

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	1.709185E-02	3.524094E-03
HF	1.00 g/cc	1.224345E-03	1.224345E-03

Input Data:

UF6 Pressure = 1406.14 g/cm² 20 psia
Temperature = 338.6556 Kelvin 150 F

Postulated HF (Acid) in gas phase:

HF Pressure = 1757.675 g/cm² 25 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 100.0769 %

Fissile Isotope Density : 1.150884E-02 (g235U/cc)

Moderation Level:

H/U = 1.25 H/X = 1.25

Net Weight of 30B UF6 cylinder: 17.11649 kg. Mass of UF6: 15.97234 kg.
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : VHE-25

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	.021191 4.369279E-03	
HF	1.00 g/cc	9.715071E-04 9.715071E-04	

Input Data:

UF6 Pressure = 1757.675 g/cm² 25 psia
Temperature = 341.4334 Kelvin 155 F

Postulated HF (Acid) in gas phase:

HF Pressure = 1406.14 g/cm² 20 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 124.0784 %

Fissile Isotope Density : 1.426901E-02 (g235U/cc)

Moderation Level:

H/U = .8 H/X = .8

Net Weight of 30B UF6 cylinder: 20.71086 kg. Mass of UF6: 19.80299 kg.
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : VHE-30

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	2.490245E-02	5.134525E-03
HF	1.00 g/cc	7.135372E-04	7.135372E-04

Input Data:

UF6 Pressure = 2109.21 g/cm² 30 psia
Temperature = 348.6556 Kelvin 168 F

Postulated HF (Acid) in gas phase:

HF Pressure = 1054.605 g/cm² 15 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 145.8098 %

Fissile Isotope Density : 1.676812E-02 (g235U/cc)

Moderation Level:

H/U = .5 H/X = .5

Net Weight of 30B UF6 cylinder: 23.93814 kg. Mass of UF6: 23.27134 kg.
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : VHE-35

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	2.873238E-02	5.924201E-03
HF	1.00 g/cc	4.704442E-04	4.704442E-04

Input Data:

UF6 Pressure = 2460.745 g/cm² 35 psia
Temperature = 352.5444 Kelvin 175 F

Postulated HF (Acid) in gas phase:

HF Pressure = 703.07 g/cm² 10 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 168.2349 %

Fissile Isotope Density : 1.934701E-02 (g235U/cc)

Moderation Level:

H/U = .2857143 H/X = .2857143

Net Weight of 30B UF6 cylinder: 27.29003 kg. Mass of UF6: 26.8504 kg.
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : VHE-40

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	3.217781E-02	.0066346
HF	1.00 g/cc	2.305001E-04	2.305001E-04

Input Data:

UF6 Pressure = 2812.28 g/cm² 40 psia
Temperature = 359.7667 Kelvin 188 F

Postulated HF (Acid) in gas phase:

HF Pressure = 351.535 g/cm² 5 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 188.4087 %

Fissile Isotope Density : .021667 (g235U/cc)

Moderation Level:

H/U = .125 H/X = .125

Net Weight of 30B UF6 cylinder: 30.28557 kg. Mass of UF6: 30.07016 kg.
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Required Data for Selected Point : File : VHE-45

Comp.	Theo.Density	Gas Density	CSAS Input
UF6	4.85 g/cc	3.608858E-02	7.440944E-03
HF	1.00 g/cc	0	0

Input Data:

UF6 Pressure = 3163.815 g/cm² 45 psia
Temperature = 360.8778 Kelvin 190 F

Postulated HF (Acid) in gas phase:

HF Pressure = 0 g/cm² 0 psia

Uranium Assay used was : 100 wt.% 235U.

Percent of GAT-225 Single Parameter Limit: 211.3072 %

Fissile Isotope Density : 2.430033E-02 (g235U/cc)

Moderation Level:

H/U = 0 H/X = 0

Net Weight of 30B UF6 cylinder: 33.72477 kg. Mass of UF6: 33.72477 kg.
Ok

1LIST 2RUN 3LOAD" 4SAVE" 5CONT 6,"LPT1 7TRON 8TROFF 9KEY 0SCREEN

Appendix B. KENO V.a Inputs with CSAS 25

Appendix B

Keno V.A Inputs with CSAS 25

FILE: LS-20

DATA: Material: 20 psia UF₆, 94.7 psia HF, 100% ²³⁵U

Geometry: 12B Cylinder w/o metal wall

Reflector: Full 1' Water Reflector

Mass UF₆ = 1.59 Kg. Mass HF = 0.431 H/X = 4.74

Results: Keff. = 0.32090 +/- 0.00355

#CSAS25

GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE LS-20

27GROUPNDF4 INFHOMMEDIUM

UF6 1 3.559E-3 335.6 92235 100.0 END

HFACID 1 4.684E-3 335.6 END

H2O 2 1.0000 293.0 END

END COMP

GAS STUDY, 12B CYLINDER, FULLY REFLECTED, FILE LS-20

READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM

READ GEOM

UNIT 1

COM='12B CYLINDER W/O SHELL'

ZCYLINDER 1 1 15.875 2P63

ZCYLINDER 2 1 46.355 2P93.48

CUBOID 0 1 2P50 2P50 2P95

END DATA

END

FILE: LS-30

DATA: Material: 30 psia UF₆, 84.7 psia HF, 100% ²³⁵U

Geometry: 12B Cylinder w/o metal wall

Reflector: Full 1' Water Reflector

Mass UF₆ = 2.31 Kg. Mass HF = 0.374 H/X = 2.82

Results: Keff. = 0.35675 +/- 0.00338

#CSAS25

GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE LS-30

27GROUPNDF4 INFHOMMEDIUM

UF6 1 5.151E-3 347.6 92235 100.0 END

HFACID 1 4.042E-3 347.6 END

H2O 2 1.0000 293.0 END

END COMP

GAS STUDY, 12B CYLINDER, FULLY REFLECTED, FILE LS-30

```

READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM
READ GEOM
UNIT 1
COM='12B CYLINDER W/O SHELL'
ZCYLINDER 1 1 15.875 2P63
ZCYLINDER 2 1 46.355 2P93.48
CUBOID 0 1 2P50 2P50 2P95
END DATA
END

```

```

FILE:          LS-40
DATA:   Material: 40 psia UF6, 74.7 psia HF, 100% 235U
        Geometry: 12B Cylinder w/o metal wall
        Reflector: Full 1' Water Reflector
        Mass UF6 = 2.99 Kg.    Mass HF = 0.320    H/X = 1.87
Results: Keff. = 0.38359 +/- 0.00373

```

```

#CSAS25
GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE LS-40
27GROUPNDF4          INFHOMMEDIUM
UF6  1 6.676E-3 357.6 92235 100.0 END
HFACID 1 3.456E-3 357.6          END
H2O   2 1.0000 293.0          END
END COMP
GAS STUDY, 12B CYLINDER, FULLY REFLECTED, FILE LS-40
READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM
READ GEOM
UNIT 1
COM='12B CYLINDER W/O SHELL'
ZCYLINDER 1 1 15.875 2P63
ZCYLINDER 2 1 46.355 2P93.48
CUBOID 0 1 2P50 2P50 2P95
END DATA
END

```

```

FILE:          LS-50
DATA:   Material: 50 psia UF6, 64.7 psia HF, 100% 235U
        Geometry: 12B Cylinder w/o metal wall
        Reflector: Full 1' Water Reflector
        Mass UF6 = 3.65 Kg.    Mass HF = 0.271    H/X = 1.29
Results: Keff. = 0.39715 +/- 0.00372

```

```

#CSAS25
GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE LS-50
27GROUPNDF4          INFHOMMEDIUM
UF6   1 8.155E-3 365.9 92235 100.0 END
HFACID 1 2.933E-3 365.9          END
H2O    2 1.0000   293.0          END
END COMP
GAS STUDY, 12B CYLINDER, FULLY REFLECTED, FILE LS-50
READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM
READ GEOM
UNIT 1
COM='12B CYLINDER W/O SHELL'
ZCYLINDER 1 1 15.875 2P63
ZCYLINDER 2 1 46.355 2P93.48
CUBOID    0 1 2P50 2P50 2P95
END DATA
END

```

```

FILE:          LS-60
DATA:   Material: 60 psia UF6, 54.7 psia HF, 100% 235U
        Geometry: 12B Cylinder w/o metal wall
        Reflector: Full 1' Water Reflector
        Mass UF6 = 4.30 Kg.   Mass HF = 0.225   H/X = 0.912
Results: Keff. = 0.41295 +/- 0.00365

```

```

#CSAS25
GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE LS-60
27GROUPNDF4          INFHOMMEDIUM
UF6   1 9.611E-3 372.6 92235 100.0 END
HFACID 1 2.435E-3 372.6          END
H2O    2 1.0000   293.0          END
END COMP
GAS STUDY, 12B CYLINDER, FULLY REFLECTED, FILE LS-60
READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM
READ GEOM
UNIT 1
COM='12B CYLINDER W/O SHELL'
ZCYLINDER 1 1 15.875 2P63
ZCYLINDER 2 1 46.355 2P93.48
CUBOID    0 1 2P50 2P50 2P95
END DATA
END

```


FILE: LS-70
 DATA: Material: 70 psia UF₆, 44.7 psia HF, 100% ²³⁵U
 Geometry: 12B Cylinder w/o metal wall
 Reflector: Full 1' Water Reflector
 Mass UF₆ = 4.93 Kg. Mass HF = 0.181 H/X = 0.639
 Results: Keff. = 0.41617 +/- 0.00365

#CSAS25
 GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE LS-70
 27GROUPNDF4 INFHOMMEDIUM
 UF6 1 1.103E-2 378.7 92235 100.0 END
 HFACID 1 1.958E-3 378.7 END
 H2O 2 1.0000 293.0 END
 END COMP
 GAS STUDY, 12B CYLINDER, FULLY REFLECTED, FILE LS-70
 READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM
 READ GEOM
 UNIT 1
 COM='12B CYLINDER W/O SHELL'
 ZCYLINDER 1 1 15.875 2P63
 ZCYLINDER 2 1 46.355 2P93.48
 CUBOID 0 1 2P50 2P50 2P95
 END DATA
 END

FILE: LS-80
 DATA: Material: 80 psia UF₆, 34.7 psia HF, 100% ²³⁵U
 Geometry: 12B Cylinder w/o metal wall
 Reflector: Full 1' Water Reflector
 Mass UF₆ = 5.55 Kg. Mass HF = 0.135 H/X = 0.434
 Results: Keff. = 0.42876 +/- 0.00449

#CSAS25
 GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE LS-80
 27GROUPNDF4 INFHOMMEDIUM
 UF6 1 1.241E-2 384.8 92235 100.0 END
 HFACID 1 1.496E-3 384.8 END
 H2O 2 1.0000 293.0 END
 END COMP
 GAS STUDY, 12B CYLINDER, FULLY REFLECTED, FILE LS-80
 READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM

READ GEOM
 UNIT 1
 COM='12B CYLINDER W/O SHELL'
 ZCYLINDER 1 1 15.875 2P63
 ZCYLINDER 2 1 46.355 2P93.48
 CUBOID 0 1 2P50 2P50 2P95
 END DATA
 END

FILE: VHE-20
 DATA: Material: 20 psia UF₆, 25 psia HF, 100% ²³⁵U
 Geometry: 30B Cylinder w/o metal wall
 Reflector: Full 1' Water Reflector
 Mass UF₆ = 15.972 Kg. Mass HF = 1.144 H/X = 1.25
 Results: Keff. = 0.43513 +/- 0.00351

#CSAS25
 GAS STUDY, UF₆ GAS, FULLY REFLECTED, FILE VHE-20
 27GROUPNDF4 INFHOMMEDIUM
 UF₆ 1 3.524E-3 338.6 92235 100.0 END
 HFACID 1 1.224E-3 338.6 END
 H₂O 2 1.0000 293.0 END
 END COMP
 GAS STUDY, 30B CYLINDER, FULLY REFLECTED, FILE VHE-20
 READ PARAM NPG=300 GEN=105 NSK=1 PLT=no END PARAM
 READ GEOM
 UNIT 1
 COM='30B CYLINDER W/O SHELL'
 ZCYLINDER 1 1 38 2P103
 ZCYLINDER 2 1 68.48 2P133.48
 CUBOID 0 1 2P70 2P70 2P135
 END DATA
 END

FILE: VHE-25
 DATA: Material: 25 psia UF₆, 20 psia HF, 100% ²³⁵U
 Geometry: 30B Cylinder w/o metal wall
 Reflector: Full 1' Water Reflector
 Mass UF₆ = 19.803 Kg. Mass HF = 0.908 H/X = 0.80
 Results: Keff. = 0.45417 +/- 0.00400

```

#CSAS25
GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE VHE-25
27GROUPNDF4          INFHOMMEDIUM
UF6   1 4.369E-3 341.4 92235 100.0 END
HFACID 1 9.715E-4 341.4      END
H2O    2 1.0000   293.0      END
END COMP
GAS STUDY, 30B CYLINDER, FULLY REFLECTED, FILE VHE-25
READ PARAM NPG=300 GEN=105 NSK=1 PLT=NO END PARAM
READ GEOM
UNIT 1
COM='30B CYLINDER W/O SHELL'
ZCYLINDER 1 1 38 2P103
ZCYLINDER 2 1 68.48 2P133.48
CUBOID     0 1 2P70 2P70 2P135
END DATA
END

```

```

FILE:          VHE-30
DATA:   Material: 30 psia UF6, 15 psia HF, 100% 235U
        Geometry: 30B Cylinder w/o metal wall
        Reflector: Full 1' Water Reflector
        Mass UF6 = 23.271 Kg.    Mass HF = 0.667      H/X = 0.50
Results: Keff. = 0.46511 +/- 0.00389

```

```

#CSAS25
GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE VHE-30
27GROUPNDF4          INFHOMMEDIUM
UF6   1 5.1345E-3 348.7 92235 100.0 END
HFACID 1 7.135E-4 348.7      END
H2O    2 1.0000   293.0      END
END COMP
GAS STUDY, 30B CYLINDER, FULLY REFLECTED, FILE VHE-30
READ PARAM NPG=300 GEN=105 NSK=1 PLT=NO END PARAM
READ GEOM
UNIT 1
COM='30B CYLINDER W/O SHELL'
ZCYLINDER 1 1 38 2P103
ZCYLINDER 2 1 68.48 2P133.48
CUBOID     0 1 2P70 2P70 2P135
END DATA
END

```

FILE: VHE-35
 DATA: Material: 35 psia UF₆, 10 psia HF, 100% ²³⁵U
 Geometry: 30B Cylinder w/o metal wall
 Reflector: Full 1' Water Reflector
 Mass UF₆ = 26.850 Kg. Mass HF = 0.440 H/X = 0.286
 Results: Keff. = 0.48474 +/- 0.00355

#CSAS25
 GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE VHE-35
 27GROUPNDF4 INFHOMMEDIUM
 UF6 1 5.924E-3 352.5 92235 100.0 END
 HFACID 1 4.704E-4 352.5 END
 H2O 2 1.0000 293.0 END
 END COMP
 GAS STUDY, 30B CYLINDER, FULLY REFLECTED, FILE VHE-35
 READ PARAM NPG=300 GEN=105 NSK=1 PLT=NO END PARAM
 READ GEOM
 UNIT 1
 COM='30B CYLINDER W/O SHELL'
 ZCYLINDER 1 1 38 2P103
 ZCYLINDER 2 1 68.48 2P133.48
 CUBOID 0 1 2P70 2P70 2P135
 END DATA
 END

FILE: VHE-40
 DATA: Material: 40 psia UF₆, 5 psia HF, 100% ²³⁵U
 Geometry: 30B Cylinder w/o metal wall
 Reflector: Full 1' Water Reflector
 Mass UF₆ = 30.070 Kg. Mass HF = 0.215 H/X = 0.125
 Results: Keff. = 0.48904 +/- 0.00394

#CSAS25
 GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE VHE-40
 27GROUPNDF4 INFHOMMEDIUM
 UF6 1 6.635E-3 359.8 92235 100.0 END
 HFACID 1 2.305E-4 359.8 END
 H2O 2 1.0000 293.0 END
 END COMP
 GAS STUDY, 30B CYLINDER, FULLY REFLECTED, FILE VHE-40
 READ PARAM NPG=300 GEN=105 NSK=1 PLT=NO END PARAM

READ GEOM
UNIT 1
COM='30B CYLINDER W/O SHELL'
ZCYLINDER 1 1 38 2P103
ZCYLINDER 2 1 68.48 2P133.48
CUBOID 0 1 2P70 2P70 2P135
END DATA
END

FILE: VHE-45
DATA: Material: 45 psia UF₆, 0 psia HF, 100% ²³⁵U
Geometry: 30B Cylinder w/o metal wall
Reflector: Full 1' Water Reflector
Mass UF₆ = 33.725 Kg. Mass HF = 0.000 H/X = 0.00
Results: Keff. = 0.49445 +/- 0.00443

#CSAS25
GAS STUDY, UF6 GAS, FULLY REFLECTED, FILE VHE-45
27GROUPNDF4 INFHOMMEDIUM
UF6 1 7.441E-3 360.9 92235 100.0 END
H2O 2 1.0000 293.0 END
END COMP
GAS STUDY, 30B CYLINDER, FULLY REFLECTED, FILE VHE-45
READ PARAM NPG=300 GEN=105 NSK=1 PLT=NO END PARAM
READ GEOM
UNIT 1
COM='30B CYLINDER W/O SHELL'
ZCYLINDER 1 1 38 2P103
ZCYLINDER 2 1 68.48 2P133.48
CUBOID 0 1 2P70 2P70 2P135
END DATA
END

Appendix C. Computational Program: PHASE

This is an engineering assistance program presented in the BASIC programming language.

Input: Temperature of UF₆ gas

Output: Corresponding pressure to the PHASE diagram, the appropriate phase of the UF₆ gas and the corresponding error given with the original equations.

Appendix C
Calculational Program : PHASE

```
10  CLS
20  LINE INPUT "What temperature is it <F> ? ", T$
30  PRINT
40  T=VAL(T$)
50  IF T<32 THEN GOTO 390
60  T = (T-32)/1.8
70  IF T>116 THEN GOTO 290
80  IF T>64 THEN GOTO 190
90  LOGP = 6.38353+.0075377*T-942.76/(T+183.416)
100 P=10^LOGP
110 P=P*.0193367
120 PRINT "Pressure = "P" psia +/- "P*.0005
130 PRINT
140 PRINT "For Temperature = "T*1.8+32" F  "T"  C"
150 PRINT
160 PRINT "Solid - Vapor Sublimation Line"
170 PRINT "Re: Equation 82 - range: 32-147.2 F"
180 GOTO 400
190 LOGP = 6.99464-1126.288/(T+221.963)
200 P=10^LOGP
210 P=P*.0193367
220 PRINT "Pressure = "P" psia +/- "P*.0003
230 PRINT
240 PRINT "For Temperature = "T*1.8+32" F  "T"  C"
250 PRINT
260 PRINT "Liquid - Vapor Condensation Line"
270 PRINT "Re: Equation 83 - range: 147.2-240.8 F"
280 GOTO 400
290 LOGP = 7.69069-1683.165/(T+302.148)
300 P=10^LOGP
310 P=P*.0193367
320 PRINT "Pressure = "P" psia +/- "P*.003
330 PRINT
340 PRINT "For Temperature = "T*1.8+32" F  "T"  C"
350 PRINT
360 PRINT "Liquid - Vapor Condensation Line"
370 PRINT "Re: Equation 84 - range: over 240.8 F"
380 GOTO 400
390 PRINT "Sorry, too cold!"
400 PRINT
410 PRINT "Uncertainties represent 95% Confidence Level"
420 PRINT
```

430 PRINT "***** Press F2 to run another case. *****"

Variable Table for Computational Program : PHASE

<u>Variable</u>	<u>Description</u>
T	Temperature (input in F and converted to C for calculations)
LOGP	The Log ₁₀ of the pressure in mm Hg.
P	The pressure (Originally in mm Hg converted to psia.)

Appendix D. Migration Area in Converters

Appendix D

Migration Area in Converters

The original safety calculations of the Gaseous Diffusion Cascades were based on Migration Area principles. Low density of the gas phase would allow a larger area for neutrons to migrate or travel before interacting. If the migration area is larger than half the equipment size, then generated neutrons are bound to leak out before an interaction can take place. The following technical discussion demonstrates how to calculate the migration Area and compares that to the physical converter sizes, calculating there cross-sectional areas.

However, instead of the laborious hand-calculations, the Keno code is used to directly calculate the multiplications involved and the Migration Area is simply back calculated.

The following tables contains all of the information needed to determine the Migration Area for each of the converter cases.

Table D.1
Material Study of the Cases.

Size	P(psia)	Temp (F)	Enrich	CSAS UF ₆	²³⁵ U	²³⁸ U	F
OOO	25	154	3.0	4.41e-03	8.84e-07	3.58e-05	2.20e-04
OO	25	154	15	4.41e-03	5.49e-06	3.11e-05	2.20e-04
O	25	154	15	4.41e-03	5.49e-06	3.11e-05	2.20e-04
27	14.45	133	50	2.64e-03	1.10e-05	1.10e-05	1.32e-04
25	14.45	133	100	2.64e-03	2.21e-05	0	1.32e-08

Pressures were based on maximum allowed in the Cascade and temperatures were determined to be the sublimation temperatures from program PHASE. The enrichment levels were found from the cascade gradient in the SAR, ref. 3; the resulting table, above, is a conservative representation of the historical use of the equipment. Both the CSAS 25 inputs and the traditional atomic densities are shown. No HF contamination was used in the calculations for Migration Area and all keffs. were ran with bare cylinders, so these tables in Appendix D do not represent a conservative model of cascade equipment.

Table D.2
Dimensions of the Converters

Size	Diam (in)	Radius (cm)	Area (cm ²)	Length (in)	½ Length (cm)
OOO	154.375	196.056	120756.7	291.25	369.8875
OO	105	133.35	55864.5	221	280.67
O	105	133.35	55864.5	215	273.05
27	47.5	60.325	11432.59	129	163.83
25	38.375	48.7462	7461.98	129	163.83

Dimensions were obtained from the SAR, ref 3. The calculated cross-sectional area is the largest cross-section of each converter model.

Geometric Buckling for cylinders is defined by:

$$B_g^2 = (2.405/R)^2 + (\pi/L)^2$$

(ref. 15)

Calculating the geometric buckling from the above equation and using KENO V.a with the CSAS package and the material in Table D.1 to calculate the Keff. and Kinf. values for the five cases. The Migration Area may be found by the relationship:

$$K_{eff} = K_{\infty} / (1 + M^2 B_g^2)$$

(ref. 15)

Solving for M² :

$$M^2 = (K_{\infty}/K_{eff} - 1) / B_g^2$$

Table D.3
Buckling, K's and Migration Area

Size	B_g^2	K_{∞}	K_{eff}	M^2
000	1.69e-04	.47203	0.00617	448095
00	3.57e-04	1.15453	0.00622	517711
0	3.58e-04	1.15453	0.00614	521858
27	1.68e-03	1.69664	0.00295	341481
25	2.55e-03	1.97209	0.00414	186215

A geometric system is inherently safe if the cross-sectional area is less than half of the Migration Area. In all of the converter cases the Migration Area in Table D.3 is much larger than the largest cross-sectional area of the equipment in Table D.2. Therefore, the above tables demonstrate the geometric safety of all the converters used in the gaseous diffusion plants.

Appendix E. Isotopic Conversions

Appendix E

For conversion from an enrichment given in weight percent of the uranium 235 isotope (Wt.%) to the scientific isotopic percent (Iso.%), a text book formula could be presented; however, a physical approach can quickly derive the answer.

From the Atomic Equation:

$$N = \rho Na / At. Wt.$$

While ρ is a density generally in (g/cc), in this case it is substitute with a Wt. % (g/g).

For:
$$N = Wt.\% Na / At. Wt.$$

For an atomic number per gram representation.

So:
$$N_{235} = Wt.\% Na / 235 \quad \text{And} \quad N_{238} = (1 - Wt.\%) Na / 238$$

Therefore we have a representation of the actual numbers of isotopes per gram in question, the isotopic percent (Iso.%) is simply:

$$Iso\% = N_{235} / (N_{235} + N_{238})$$

Installing our isotopic representations into the formula:

$$Iso.\% = (Wt.\% Na / 235) / \{ (Wt.\% Na / 235) + [(1 - Wt.\%) Na / 238] \}$$

Notice that Avogadro's Number (Na) is in every term, dropping it simplifies to :

$$Iso.\% = (Wt.\% / 235) / (Wt.\% / 235) + (1 - Wt.\%) / 238$$

Notice that the term (Wt.%/235) is in several places, dividing by it in each term:

$$Iso\% = 1 / \{ 1 + (235/238)[(1 - Wt.\%) / Wt.\%] \}$$

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