GA-A24237

DIRECT ENERGY CONVERSION FISSION REACTOR

**ANNUAL REPORT FOR THE PERIOD
OCTOBER 1, 2001 THROUGH DECEMBER 31, 2002**

**by
L.C. BROWN**

**Work supported by
Nuclear Energy Research Initiative (NERI)
Program No. DE-FG03-99SF21893 for
the U.S. Department of Energy**

MARCH 2003

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**GENERAL ATOMICS PROJECT 30052
MARCH 2003**

EXECUTIVE SUMMARY

Sandia National Laboratories (SNL), Los Alamos National Laboratories (LANL), the University of Florida (UF), Texas A&M University (TAMU) and General Atomics (GA) have undertaken a joint project to explore the possibilities of exploiting direct energy conversion (DEC) to increase the efficiency of electricity production from fission nuclear reactors. This report describes only the work performed at GA during Phase 3 of this three-year project. SNL leads the overall project and provides overall project reporting.

During Phase 1, the number of DEC concepts under investigation was reduced to three: Magnetic Collimator Fission Reactor (MCFR), Quasi-Spherical Magnetically Isolated Fission Electric Cell Reactor (QSMIFECR, or FECR for short), and Fission Enhanced MHD Gas Core Reactor (GCR). During Phases 2 and 3, each of the concepts has been further refined. Each of the concepts was championed by a particular laboratory:

1. Magnetic Collimator Fission Reactor — TAMU.
2. Quasi-Spherical Magnetically Isolated Fission Electric Cell Reactor — SNL.
3. Fission Enhanced MHD Gaseous Core Reactor — UF.

LANL and GA provided support to all three concepts in areas where they have specific expertise.

Toward the end of Phase 3, the FECR was selected to form the basis of a new NERI proposal in which magnetic isolation would be experimentally verified. The University of Florida chose to submit a separate new NERI proposal based on the gaseous core reactor.

In the intervening period, GA supported the Phase 3 effort in two areas:

1. Design and fabrication of the cathode for the FECR.
2. Design of the fuel recycle loop, including fission product removal, for the GCR.

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1. INTRODUCTION

Direct energy conversion (DEC) for fission may be defined, in a broad sense, as the production of electrical energy from a fission nuclear reactor without the use of a mechanical energy conversion device. In its purest form, DEC directly converts the kinetic energy of fission fragments into electrical energy and is the only potential means for producing electrical energy from a fission reactor without the Carnot efficiency limitations. This project was undertaken by Sandia National Laboratories (SNL), Los Alamos National Laboratories (LANL), the University of Florida (UF), Texas A&M University (TAMU) and General Atomics (GA) to explore the possibilities of exploiting DEC. In the initial scoping studies, a number of DEC techniques were explored as well as techniques that use direct fission energy to augment a more traditional energy recovery scheme. Phase 1 ended with the selection of two pure DEC techniques and one hybrid scheme: (1) the pure DEC techniques, Quasi-Spherical Magnetically Isolated Fission Electric Cell Reactor (QSMIFECR, or FECR for short) and; (2) Magnetic Collimator Fission Reactor (MCFR) were proposed by SNL. The University of Florida proposed the Gas Core Nuclear Reactor (GCR), which makes peripheral use of the direct fission product energy. SNL leads the overall project and provides overall project reporting and documentation.

Both the FECR and the MCFR directly convert the kinetic energy of the fission products into electrical energy by slowing the positively charged fission products with an electric field. The electric field, on the order of 2 MV, is self-generated by the transport of the fission products from the fuel cathode to the anode. The electric energy is extracted from the flow of electrons from the cathode to the anode through an external electric circuit. Since any kinetic energy lost through collisions of fission products within the fuel results in heat deposited in the cathode instead of electrical energy extracted from the particles, the fuel must be thin so that all the fission products can escape with minimal collisions. The fuel thickness must be on the order of a micron or less for significant DEC to take place. Moreover, if the fuel is supported by any thickness of inert material, the efficiency will be decreased by the thermal energy of the fission product deposited in the support.

The FECR is composed of many individual cells (Fig. 1), each composed of a fuel cathode and a moderator anode. Ideally, the cathode would be a point of fuel at the center of the anode, so that all fission products would travel along radii of the anode, always normal to the electric field. Since the volume of the fuel would be zero for this idealized geometry, the concept under investigation has the fuel in the form of a thin spherical shell and the cathode radius is a significant fraction of the anode radius. As the cathode radius approaches the anode radius, the reactor can contain more fuel but a larger fraction of the fission product kinetic energy is not directed normal to the electric field and thus becomes heat. Since the cathode must be connected

to the anode through an external electric circuit, there must be a penetration through the anode for the cathode lead wire. To minimize the number of connections, many cathodes are spaced along each support wire, which also serves as the electrical lead. The anode, which surrounds each cathode, has two axial penetrations somewhat larger than the diameter of the cathode so that a cathode assembly can be inserted into each anode. To prevent direct flow of electrons across the gap between the electrodes, the cathodes are insulated from the anodes by two separate mechanisms: each individual cell is insulated by an axial magnetic field provided by a superconducting magnetic solenoid wound around the entire reactor; and a sufficient length of insulator is placed at both ends of each cathode assembly to prevent electrical breakdown on the surface of the insulator.

Fig. 1. Cross section of FECR.

The MCFR is similar to the FECR in that the entire reactor is within a superconducting solenoid. The fuel for the MCFR is in the form of fine wires or thin tubes that are aligned along the magnetic field lines. Fission fragments exiting the fuel are constrained to a spiral path along the magnetic field line. After exiting the reactor, the fission fragments are retarded by an electric field and collected at the cathode. Any electron accompanying the fission fragments is repelled by a grid located between the reactor and the anode.

The GCR is only marginally a DEC concept as the majority of the fission energy is converted to heat and recovered by means subject to the Carnot limitations but the reactor temperature is very high so the theoretical efficiency is quite high. The reactor consists of a core of uranium tetrafluoride vapor and helium gas operating at 2500 K with a beryllium reflector. The gaseous core temperature is high but the structural and containment materials are cooled to more reasonable temperatures. The temperature of the gas exiting the reactor is too high for conventional turbines so the high temperature energy is extracted using magnetohydrodynamics (MHD). The uranium is still undergoing delayed fission as it passes through the MHD generator, providing the needed ionization. This ionization energy is the DEC component of the concept. A helium turbine-generator and a steam turbine-generator are used to extract additional energy at lower temperatures from the gas exiting the MHD generator.

This report documents the progress of GA in support of the overall project. The work was done in two areas:

1. Design of the Cathode for the FECR.
2. Design of the fuel recycle loop of the GCR.

These areas are independent. What follows are independent reports on the two topics. Much of the detailed information is presented in the Appendix.

2. POM-POM CATHODE FOR THE QUASI-SPHERICAL MAGNETICALLY ISOLATED FISSION ELECTRIC CELL REACTOR

Fuel design is a major concern of the FECR. As explained above, the original fuel concept was that a series of thin, electrically conductive spherical shell of fissionable material would be equally spaced along an electrically conductive wire or rod. Each spherical fuel shell would be centered within an electrically conductive spherically bounded space. Positively charged fission fragments exiting the shell would leave the shell negatively charged (cathode) and render the outer sphere positively charged (anode). When charged to the maximum extent, the voltage between anode and cathode would be over 2 million volts at which point electrons would be transferred from the cathode to the anode through an external circuit, generating electrical power.

Only fission fragments arising from fission events taking place within a micron or so of the outer surface of the spherical shell will retain most of their initial kinetic energy and make it to the anode so high efficiency requires that the fuel be restricted to a very thin layer. There is equal probability that a fission fragment will be directed toward the interior of the shell instead of outward toward the anode. There will be a 50% reduction in efficiency unless the interior-directed fragments traverse across the shell to the anode on the other side. This means that the sphere must be hollow and if any support material is used, it must also be very thin.

A cathode design, the “pom-pom” cathode, is proposed which eliminates some of the fabricability and structural concerns of the thin shell cathode. A conductive cathode consisting of a thin ($\sim 1\ \mu\text{m}$) conductive shell of fissile material will be very difficult to fabricate and very difficult to mount on the central support rod. An even more serious problem is the high electric field between the cathode and anode, which results in an outward electric force that must be balanced by a hoop stress in the shell. This hoop stress exceeds the tensile strength of most materials. The pom-pom cathode avoids the hoop stress problem by replacing the thin shell with strong fibers that are bound to the central support as shown in Fig. 2. The ends of the fibers repel each other in the electric field and the fissile material, which is coated on the tips of the fibers, effectively forms a dilute spherical shell. The hoop stress in a thin membrane is replaced by a pure tensile stress in the fiber.

Fig. 2. Pom-pom cathode and detail of interior structure.

The pom-pom cathode does add additional material, the fiber, which can attenuate fission products. The distribution of mass in the pom-pom cathode is shown in Fig. 3. The case shown assumed that a 5.4 mm diameter, 1 micron shell of uranium metal was replaced by a bundle of $0.5\ \mu\text{m}$ fibers 5.44 mm long with a $1\ \mu\text{m}$ coating of uranium metal on the outer 1 mm length of each fiber. The central core is modeled as a spherical region of close packed fibers and the fibers are assumed to be radial outside the core. For this case, the central core is $64\ \mu\text{m}$ in diameter, which is small compared with the center support fiber, as it will be for any case of interest.

The Pom-Pom cathode design appears to solve the basic fabricability question of FECR cathodes. The structure is strong enough to resist the electric forces that would destroy a thin shell structure. Carbon fibers of the desired size have been fabricated. The coating technique will have to be developed but there are several techniques that could be effective. The fuel is distributed within a rather thick spherical shell. The fuel constitutes 99.5% of the material in the fuel region.

Fig. 3. Radial density of pom-pom cathode.

3. SIMULATION OF THE GAS RECYCLE LOOP OF A GAS CORE REACTOR

3.1. INTRODUCTION

Dr. S. Anghaie of the University of Florida proposed that a MHD topping cycle be added to a GCR as a means of extracting a portion of the fission energy directly from the fission products. In this case, delayed fission within the MHD generator provides the requisite gaseous electrical conductivity, at relatively low temperatures, without seeding the stream with a low ionization potential materials such as cesium. The MHD-GCR, as originally conceived, is presented in Fig. 4. The University of Florida has overall responsibility for the GCR in this study. In particular, they are responsible for engineering of the reactor and power systems. Our efforts were associated with modeling the fuel/coolant recycle loop.

The GCR has the potential for very high thermal efficiencies due to the high operating temperature. A stated advantage of the GCR is the small amount of fuel that is subject to release in an accident. This advantage is only realized if the fission products are continuously removed from the fuel. In fact, the GCR cannot remain critical unless the fission product poisons are removed. The goal of our effort was to investigate means to minimize the circulating fission product activity without introducing a large energy penalty.

The fuel/coolant loop, which is the subject of this work, is outlined in Fig. 4. During Phase 3 of this effort, some of the parameters indicated on Fig. 4 were modified. The final values of the parameters used in this work are given in Table 1.

Table 1
MHD-GCR Design Parameters Provided by the University of Florida

Gas core inlet/outlet temperature	1550 K/2500 K
Gas core outlet pressure	197 atm
Gas core power output	100 MW
MHD generator outlet temperature	1800 K
MHD generator power output	18 MW
Ultrasafe heat ex. outlet temperature	1600 K
Helium compressor outlet temperature	1400 K
UF ₄ concentration in helium	10 mole percent

Fig. 4. Schematic utilized for the GCR simulation.

3.2. FLOW LOOP MODELING

We modeled the fuel/coolant recycle loop of a MHD-GCR based on the parameters given in Table 1. The original concept, Fig. 4, did not recognize that a significant amount of UF_4 would plate out in the heat exchanger that cooled helium to 1000°C and that 1000°C is still too hot to economically compress helium. Moreover, the helium purification system was not located so as to make use of the fact that certain fission products will be concentrated within certain portions of the recycle loop. The modeling effort allowed us to find a scheme that both recycled the helium (coolant) and UF_4 (fuel) using a minimum amount of energy and removed the fission products to reasonably low levels while, again, minimizing energy utilization.

The modeling was done using Aspen Plus®, available from Aspen Technology, Inc. Aspen Plus® is one of the foremost simulators used in the chemical industry for rigorous thermodynamic simulations of chemical processes. Using the simulator, the model can be easily and rapidly varied to investigate the effects of process permutations on process energy consumption and on the circulating activity.

Figure 5 is a simplified process flow diagram (PFD) showing the final configuration and the major units modeled. The major changes from the scheme shown in Fig. 4 are the reduction in compressor inlet temperature to near ambient and the incorporation of much of the fission product removal into the mainline flows.

Fig. 5. Simplified PFD of GCR fuel/coolant loop.

Modeling the flow loop requires thermodynamic properties of the species. Only helium and UF_4 are important in the heat and energy balance as the concentrations of fission products are negligible from a thermal standpoint. The properties of helium are available in the Aspen Plus® database but the properties of UF_4 were only available for the solid and vapor at low temperatures. High temperature, UF_4 fluid thermodynamic properties obtained from the literature (Anghaie 1992) were used in place of those in the Aspen database. The properties used in the simulation are given in Tables A.1 and A.2 of the Appendix.

The MHD generator was simulated as an isentropic turbine with an efficiency of 55% (Welch 1990). Given the outlet temperature, an energy balance over the MHD generator yields the outlet pressure of 15.6 atm. The MHD generator has a net electrical output of approximately 42 MW.

The ultrasafe heat exchanger of Fig. 4 is replaced by two heat exchangers and a gas-liquid separator as shown in Fig. 5. The first exchanger is operated as a partial condenser in which 3% of the UF_4 is condensed. This initial condensate is removed and processed to remove the low volatility fission products. The second heat exchanger cools the stream to 1600 K whereupon most of the remaining UF_4 condenses. Heat from both exchangers (~48.5 MW) is transported to a conventional Brayton/Rankine combined cycle power plant. The conventional power plant was not modeled in this effort.

The liquid UF_4 is pumped back to the reactor inlet and the helium is compressed for return to the reactor inlet. To reduce pumping costs, it is necessary to cool the helium before compressing it. Cooling also provides a means of removing the more volatile fission products from the stream. The helium compressor is modeled as an 88% efficient isentropic multistage compressor combined with interstage cooling. This is comparable to the efficiency used in the GT-HTGR. Temperature inlet reduction, multiple stages, and interstage cooling reduce the required work of compression for the compressors by 50%. Recuperation is employed to minimize the heat lost to the low temperature sink and an additional 8.9 MW is transferred to the combined cycle power plant.

During Phase 2, the work concentrated on modeling the various units present in the gas recycle loop such as the GCR and MHD Generator. Focus then shifted to the separation of the helium carrier gas from UF_4 . Phase 3 dealt with the more difficult separation of the fission products from the UF_4 . Various methods of separation were investigated and a separation scheme was modeled. Heat recuperation and integration were added and the model was varied to simultaneously investigate the tradeoff between reduction in circulating activity and increasing energy efficiency of the power plant.

3.3. CLEANUP OF REPRESENTATIVE FISSION PRODUCTS

It was not practical to model all of the 90 different fission products of uranium comprising 27 different elements (see Table A.3 in the Appendix). Even modeling the 27 elements is not warranted at this time. The fission products for each element were summed and the fluorides of six prominent elements were chosen for the model. Figure 6 indicates the yields of the most common fission product elements

Fig. 6. UF_4 fission product element with yields greater than 1% of total.

The six species: Xe, MoF_6 , ZrF_4 , SrF_2 , CeF_3 , and NdF_3 were chosen to represent the fission products in this simulation. These six particular elements were chosen for a variety of reasons. The fact that these elements represent the majority (74%) fission products is important but equally important is that the volatilities of the fluorides of these elements cover a wide range. Xe, MoF_6 and ZrF_4 have volatilities intermediate between UF_4 and helium and NdF_3 , CeF_3 and SrF_2 are less volatile than UF_4 . Moreover, thermodynamic data was available for these species. For most of these elements, the choice of fluoride was unambiguous but MoF_6 is stable at low temperatures, whereas, MoF_3 is stable at high temperatures. Ultimately MoF_6 was chosen, both because it represents the high volatility fission products and because we were unable to find experimental data on the vapor pressure of MoF_3 . Data on the elements chosen for inclusion are listed in Table 2. Tables A.1 and A.2. of the Appendix present additional data.

When a uranium atom fissions, the fluorine atoms to which it was bound will be liberated in a very chemically active state from which they will readily react with the fission products. The fluorine required to form the fission product fluorides is significantly less than that liberated from the fissioned uranium. The ratio of required fluorine to liberated fluorine is 1.15 at the reactor temperature and at room temperature it is 1.45. We have assumed that enough fluorine is added to the loop to give the indicated products. In practice, it may be necessary to limit fluorine addition to minimize corrosion. In any case, the ultimate model will have to include all the fission products in their correct temperature-dependent oxidation state. This model includes the full range of fission product volatilities expected and will be qualitatively correct.

Table 2
Compounds Chosen for Inclusion as Fission Products in the GCR Simulation

Element	% Yield	Coordination Number	Compound Formed	Vapor pressure, (atm) at 1600 K
Xe	15.93	0	Xe	na, all vapor
Mo	15.55	6	MoF ₆	209, essentially all vapor
Zr	15.06	4	ZrF ₄	609, essentially all vapor
Nd	11.33	3	NdF ₃	0.000212
Ce	9.18	3	CeF ₃	0.000261
Sr	7.09	2	SrF ₂	0.00208
Total %	74.14			

We would have liked to use a real gas model of the gas phase thermodynamics, such as the Redlich-Kwong thermodynamic equation-of-state, but were unable to find the critical properties of the fission product fluorides. The critical properties presented in Table A.2 were calculated using the critical property estimation methods of Joback, Wilson/Jasperson, Klerk, and Hakuta/Hirata found in (Poling 2001) and (Hakuta 1970). These methods provided rough estimates that varied as much as 30% between methods. Given the uncertainties in critical properties, we chose to use the ideal equation-of-state as the required data, vapor pressure, was available in the form of parameters for the Antoine equation. The ideal equation-of-state model should provide adequate results. The ideal equation-of-state adequately represents high temperature systems and where the temperature is low, the helium is the predominant species and helium acts as an ideal gas except at temperatures close to absolute zero.

No attempt was made to predict the actual concentrations of the various fission products used in the simulation. The actual concentrations of fission products expected are so low that they would be lost in the round off errors. The fission products were given the same arbitrary initial concentrations that is large compared with the actual value but small compared with the concentrations of helium and UF₄. All fission products are then expressed in terms of the circulating activity ratio or the flow rate of the fission product relative to the rate of generation of the fission product.

The fission products are separated from the main flow in three different locations. The low vapor pressure fission products: SrF₂, CeF₃, and NdF₃ are condensed out of the main flow in a partial condenser along with a small portion of the UF₄. The UF₄ is stripped from the low volatility fission product fluorides in a series of five wetted wall columns using recycled helium. High vapor pressure fission products: Xe, MoF₆, and ZrF₄ remain with the helium stream after condensing most of the liquid UF₄. The ZrF₄ plates out in the recuperator heat exchanger system and the very high volatility fission products continue with the helium. Multiple parallel exchangers are used so that a subset of the exchangers can be taken offline, heated and purged to

remove the condensed ZrF_4 . After the compressor, a 10% side stream of the helium is processed through a pressure swing adsorption (PSA) system to remove the Xe and MoF_6 . The recuperated helium is used to cool the walls of the MHD generator and the reactor before returning to the reactor inlet. The wall cooling amounts to about 5 MW, almost all of it from the MHD generator.

The circulating activity ratios for the representative fission products are all approximately 10, except for ZrF_4 . The circulating activity ratio for ZrF_4 is significantly less, around 1. Almost all of the ZrF_4 can be removed in the recuperation system with little energy penalty. The circulating activities of the other fission products can be reduced below 10 but with an increased energy penalty. Ultimately, the circulating activity can be increased or decreased depending upon energy considerations as well as safety requirements.

3.4. MODEL DETAILS

3.4.1. PFD and Primary Unit Design

The GCR PFD is presented in the Appendix as Fig. A.1, with accompanying stream information in Table A.4, and unit information in Table A.5. The PFD is divided into three sections. Section 100 includes the power generation units and primary UF_4 flow streams, located around the outside edge of the PFD. Section 200, located in the center of the PFD, contains the helium compressor unit, equipment for both helium/ UF_4 and fission product separations, and the primary helium flow streams. Section 300 contains low volatility fission product separation equipment, located in the upper right part of the PFD. Note the dual heat exchanger and fission product separation systems located in the equipment of Section 200. The stream path designated with a dashed line represents the main flow of helium. The solid line stream paths depict flows for fission product separations. Detailed discussion of the online/offline units and associated flow paths are discussed in the fission product separation section later in this report. Preliminary unit design focused on three main aspects: the power generation units (GCR, MHD generator, and ultrasafe heat exchangers), separation of UF_4 from helium to below detectable limits, and design of the helium compressor system.

The GCR is simulated as a heat source with total duty of 100 MW, an outlet temperature of 2500 K, and a constant pressure of 197 atm. The effects of wall heat loss and the use of helium as a coolant is discussed in the heat integration loops and power balance section found later in this report. A design specification, created in AspenPlus, varies the flowrate through the reactor to keep the heat input at the designated 100 MW. Currently, this flowrate is at 2.04 kmol/s composed of 10% UF_4 in helium. As mentioned previously, the MHD generator is simulated as in an isentropic turbine with an efficiency of 55%. The outlet pressure is varied with the use of a design specification to keep the outlet temperature fixed at 1800 K. Currently, with the previously determined molar flowrate of the gas stream at 2.04 kmol/s, the outlet pressure is

reduced from 197 atm to 15.6 atm. The reduction in pressure results in a power output of approximately 42 MW. The ultrasafe heat exchanger is simulated as two separate units with a separator between them. The first exchanger reduces the temperature to 1772 K in order to condense 3 mol% of the UF₄ from which the low volatile fission product are separated in the columns of Section 300. The second exchanger reduces the remaining stream temperature to the designated 1600 K. The pressure drop over the exchangers was neglected. The total heat transferred to the power generation system from the two units is approximately 48.5 MW. Further details of the overall power output of the simulation are presented in the heat integration and power balance section later in this report.

Initially, with the outlet temperature from the second ultrasafe heat exchanger set to 1600 K, 28% of the UF₄ remained with the helium stream after the following separator. Another heat exchanger cools the gas stream to 1310 K, just above the melting point of UF₄, condensing virtually all of the UF₄. The liquid UF₄ is separated and pumped back to the reactor inlet. The negligible amount of UF₄ remaining with the helium is plated out when the stream is cooled for the helium compressor.

The helium compressor is simulated as a multistage compressor combined with interstage cooling. Without interstage cooling, the helium compressor outlet temperature was over 1800 K, too high to cool the walls of the MHD generator and GCR. In between and after the last stage of the helium compressor (three stages total), the internal stream temperature was reduced to 323 K, in order to reduce the work of compression to increase the pressure of the helium to 197 atmospheres. Work of compression can be represented by the equation

$$W_S = \frac{n\gamma RT_{in}}{\eta(\gamma-1)} \left[\left(\frac{P_{out}}{P_{in}} \right)^{\frac{(\gamma-1)}{n\gamma}} - 1 \right],$$

where n is the number of compression stages, γ is the ratio of heat capacities, T_{in} is the inlet temperature, P_{out}/P_{in} is the pressure ratio (Green 1999, Smith 1996), and η is the compressor efficiency (0.88 in this case). The combination of reduced inlet temperature, three stage compressor and interstage cooling reduced compression work by 50%, compared with the high temperature compression of the original concept (Fig. 4). Most of the heat removed while cooling to ambient temperatures is recovered in the recuperator. The helium passes through one side of the recuperator before passing through a water-cooled heat exchanger and then to the compressor. After the compressor system, the helium flows through the other side of the recuperator. The recuperator was specified to have an approach temperature of 20 K. The recuperator cold outlet stream temperature is 830 K at 197 atm. A more detailed discussion on the recuperator can be found in the heat integration loops and energy balance section of this report.

3.4.2. Fission Product Separations

Simulation of fission product separation in the gas recycle loop is broken down into different sections of the PFD. The simplified PFD shown in Fig. 5 indicates the location of the fission product separation equipment.

The low vapor pressure fission products, SrF_2 , CeF_3 , and NdF_3 are stripped from the UF_4 separated after the initial ultrasafe heat exchanger using a small amount of high pressure helium from the recuperator outlet. The amount of UF_4 condensed and processed through this system was selected so as to reduce the circulating activity ratio to approximately 10. The stripping takes place in a series of five wetted wall columns located in Section 300 of the PFD. Details of the stripping system are shown Fig. 7 along with pertinent process conditions. The first column achieves adequate separation of the fission products from the UF_4 , and the subsequent columns reduce UF_4 losses. The liquid outlet stream containing over 99.5% of the inlet fission products is sent to waste.

Fig. 7. Detail of low vapor pressure fission product separation.

High vapor pressure fission products, Xe , MoF_6 , and ZrF_4 , are separated from the helium stream after separation from the UF_4 liquid. The ZrF_4 plates out in a dual recuperator heat exchanger system. While one recuperator is online, reducing the helium temperature for compression and plating out ZrF_4 , the other is being treated with a bypass stream of 1% of the total hot purified helium to vaporize the plated ZrF_4 and send it through a packed bed adsorber for waste collection. Virtually all of the ZrF_4 is removed by this means resulting in a circulating activity ratio of 1.

Both Xe and MoF_6 are separated from a helium side stream after the compressor using pressure swing absorption (PSA). The size of the stream is the result of a compromise between low circulating activity and low processing cost and capital costs. Treating 10% of the helium results in a circulating activity ratio of approximately 10. PSA consists of two (or more) columns in parallel, each one packed with an appropriate fixed-bed adsorbent. It is based on the principle that adsorbents are capable of selectively adsorbing impurities (Xe and MoF_6 in this case) under higher pressure and desorbing them under lower pressure. The impurities are first adsorbed in

one column under the higher feed-gas pressure until the adsorbent nears saturation. The feed gas is then shifted to the other column and the impurities are desorbed from the offline unit by switching it to a lower tail-gas pressure. The impurities are removed continuously by switching the feed-gas flow back and forth between the two columns and “swinging” the pressure level up and down in each column. Typically the desired component (helium in this case) is not adsorbed and is recovered at high purity.

Once the online adsorber has achieved breakthrough, defined to be the point at which Xe and MoF₆ in the online adsorber reaches saturation, it will be switched to offline and the waste Xe and MoF₆ removed as described above. The Xe, MoF₆, and helium from the offline adsorber will be directed into a turbine expander, which enables separation of MoF₆ by taking advantage of the different vapor pressures of the two fission products. The remaining Xe and helium will then be separated using cryogenic distillation to separate Xe, which is then collected for waste.

The circulating activity results have been presented in terms of the circulating activity ratio, which is defined as the ratio of the fission product flow rate in the reactor outlet to the instantaneous fission product generation rate. The actual fission product flowrates are too small for Aspen Plus® to handle as they would be lost in the round off noise. For the purpose of the simulation, the rate of each fission product was set to 0.001 moles per second or approximately 0.5 ppm of the total flow. Table A.4 in the Appendix gives the relative circulating activity achieved for the fission products in each stream of the PFD. The maximum value of circulating activity ratio for each fission product are given in Table 3.

Table 3
Maximum Circulating Activity Ratios for Fission Products

Xe	ZrF ₄	MoF ₆	NdF ₃	CeF ₃	SrF ₂
9.86	1.10	9.90	10.6	11.0	10.1

Almost all of the ZrF₄ is removed while cooling the helium prior to the helium compressor. The other fission product's circulating activities can be modified as desired by changing the flow rates through the fission product separation sections. Decreasing the circulating activity ratio will require increased energy losses and capital equipment costs.

3.4.3. Heat Integration Loops and Energy Balance

The main opportunities for heat integration in the GCR-PFD are located in the heat exchangers of Section 200, where the helium stream is cooled for UF₄ and fission product separations, as well as for compression back up to 197 atm. In a minor role, the wall cooling effects of the GCR and MHD generator are also taken into consideration.

Each point in the helium recycle stream where temperature is reduced, 1600 to 1310 K, 1310 to 850 K, and finally 850 to 343 K, is an opportunity to place a recuperating heat exchanger. For the GCR PFD, all the recuperators are defined to have an approach temperature of 20 K. Heat exchanger pressure drop was neglected in this simulation. The 20 K approach temperature is generally the minimum accepted approach temperature for commercial heat exchange. Lower approach temperatures require large surface areas and results in expensive heat exchangers. The recuperator, where the temperature is reduced to 850 and 343 K is a dual system that has online and offline functions for fission product separation. The heat recuperation takes place in the online unit and is depicted in Fig. 8.

Fig. 8. Recuperator loops.

Additional recuperation takes place in the first ultrasafe heat exchanger. Some of the heat from this unit is used to heat the helium used for fission product separation in Section 300.

The effect of wall cooling in the GCR and MHD Generator was simulated with the use of a calculator block in Aspen Plus® that, through an iterative calculation, determined the heat loss. The equation utilized for the heat loss was:

$$Q = uA\Delta T_{lm} \quad ,$$

with $u = 13 \text{ W/m}^2 \text{ }^\circ\text{C}$, $A = 4.3 \text{ m}^2$ for the GCR, and $u = 30 \text{ W/m}^2 \text{ }^\circ\text{C}$, $A = 14 \text{ m}^2$ for the MHD generator. The heat transfer coefficients and areas were estimated, respectively, using chemical engineering heuristics and reactor size estimation from literature articles (Turton 1998, Welch 1990). When the heat loss was applied to the simulation, the resultant temperature increase of the helium cooling stream was negligible for the GCR and approximately 5 K for the MHD generator. This was due to the larger heat transfer coefficient and area used for the MHD generator.

A simplified energy balance over the complete loop is shown in Fig. 9. A more detailed balance is given in Table A.9.

Fig. 9. Energy balance.

4. CONCLUSIONS

We have shown chemical plant simulators are an important tool for the investigation of fission product removal from the fuel/coolant loop of the gaseous core reactor.

A key factor identified for UF₄/helium separations was that multiple coolers and separators are required if one wishes to recycle the UF₄ at high temperatures while minimizing the amount of solid UF₄ formed. Unless the helium is maintained above the melting point of UF₄, there is no way of eliminating the use of parallel heat exchanger systems, the online system removing UF₄ by plate-out while the offline system is heated to recover the plated-out UF₄. The parallel heat exchanger systems are required to remove fission products with volatilities similar to UF₄. They are especially effective in removing fission products such as ZrF₄, which are slightly more volatile than UF₄. The system removed almost all of the ZrF₄ from the loop.

The high vapor pressure fission products (Xe, MoF₆) must be removed from a side stream of the helium flow. All of these fission products can be removed at the cost of processing the whole helium stream for fission product removal. This can be very expensive as the PSA equipment has a significant pressure drop and large volumes. We assumed that 10% of the helium flow was processed, which resulted in a relative circulating activity of 10. We did not determine the pressure drop required for PSA: some additional work will be required in the PSA system to provide this pressure loss.

The low volatility fission products were easily removed using the partial condenser and wetted wall column system. The low volatility fission products are concentrated in the first condensate. Increasing the fractional condensation would decrease circulating activity at the expense of processing more material through the wetted wall column system. Condensing 3% of the UF₄ resulted in relative circulating activities of 10 for the low volatility fission products.

We did not locate data for fission products only slightly less volatile than UF₄. If such fission products exist, they will have much higher circulating activities than the fission products we used in this simulation.

We did not optimize the direct power from the loop but we did establish the means for evaluating MHD efficiency. Lowering the temperature at the compressor significantly lowered the compressor power by 50% but the interstage cooling load was a loss to the system.

5. FUTURE CONSIDERATIONS

There are still issues that can be addressed by modeling with Aspen Plus®. We did not address the separation of Xe and MoF₆ from the accompanying helium, but these separations will be easy. The MoF₆ can be adsorbed on a packed bed and the Xe can be separated from helium using cryogenic distillation. The remainder of the fission products should be included in the simulation: this will require laboratory data. Alternatively, quantum mechanical calculations are fast reaching the point that they may be used to calculate vapor pressures. When the full compliment of fission products are included, it is likely that it will be found that MoF₄ is more stable than MoF₆, if so it should replace the MoF₆ in the calculations.

The thermodynamic model for the MHD generator needs to be verified. Once there is confidence in the MHD thermodynamic model, the best operating conditions for the compressor can be determined.

Finally, the model can be expanded to include the complete power production system, including the Brayton and Rankine systems. This will permit the entire process to be optimized.

6. ACKNOWLEDGMENT

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APPENDIX ADDITIONAL DATA

Table A.1
Fuel and Fission Product Properties

Component	MW	T _{nbp} (K)	T _{mp}	T _{crit}	P _{crit} (atm)	GCR _{it} (cc/mol)	V _b	—	Z _{crit}
UF ₄ , (Winter 2002, Anghaie 2001)	314.0	1723	1309	2415	208.2	162.5	56.28	na	0.1170
Xe	131.3	165.0	161.4	289.7	57.64	118.0	na	0	0.286
MoF ₆	209.9	307.2	290.6	431.0	35.50	237.9	87.95	0.6490	0.286
ZrF ₄	167.2	1185.	1205.	1665.	161.1	156.0	40.17	1.338	0.1839
NdF ₃	201.2	2573.	1647.	3591.	379.3	114.6	87.95	1.794	0.1475
CeF ₃	197.1	2600.	1703.	3251.	342.0	118.6	34.07	1.735	0.1522
SrF ₂	125.6	2733.	1746.	3823.	379.0	123.6	31.53	1.772	0.1493

Table A.2
Vapor Pressure of Fuel and Fission Product Properties

Component	Extended Antoine's Equation in Aspen Plus
UF ₄ , (Anghaie 2001)	$\ln P(\text{atm}) = 74.217 + (-37977)/T(\text{K}) - 7.0 \ln T$, (1000-2500 K), Aspen Plus extrapolates $\ln P$ vs. $1/T$ outside temperature range
Xe	$\ln P(\text{atm}) = 29.4089115 - (1865.9/T) - 3.9013 \ln T + 0.011049T$, (161–290K)
MoF ₆ , (Canterford 1968)	$\ln P(\text{mmHg}) = 46.49734 - (4703.74/T) - 4.28004 \ln T$, (290–400K)
ZrF ₄ , (Sense 1963)	$\ln P(\text{mmHg}) = 30.859 - (28501.9/T)$, (889 – 1154K)
NdF ₃ , (Brown 1968-69)	$\ln P(\text{atm}) = 18.5 - (43135/T)$, (1383–1520K)
CeF ₃ , (Lim 1966)	$\ln P(\text{atm}) = 21.2 - (47120/T)$, (1373–1534K)
SrF ₂ , (Zaitsev 1990)	$\ln P(\text{atm}) = 23.49 - (47466/T)$, (1381–1720K)

Table A.3
Tabulated Fission Fragment Calculations

A	Z (e)	Isotope Yield	Isotope	Element	Element Yield ^(a)	Fluoride No. @ 2500°C	Fluorine Requirement
134	54	7.89	Xe-134	Xe	31.72	0	0
138	56	6.69	Ba-138	Ba	13.15	2	0.1344
133	54	6.67	Xe-133	Xe	31.72	0	0
139	56	6.46	Ba-139	Ba	13.15	2	0.1297
136	54	6.44	Xe-136	Xe	31.72	0	0
94	40	6.42	Zr-94	Zr	30	4	0.2579
100	42	6.42	Mo-100	Mo	30.98	3	0.1934
135	54	6.41	Xe-135	Xe	31.72	0	0
95	42	6.39	Mo-95	Mo	30.98	3	0.1925
93	40	6.37	Zr-93	Zr	30	4	0.2559
140	58	6.32	Ce-140	Ce	18.28	3	0.1904
96	40	6.27	Zr-96	Zr	30	4	0.2519
97	42	6.19	Mo-97	Mo	30.98	3	0.1865
137	55	6.16	Cs-137	Cs	6.16	1	0.0619
99	42	6.14	Mo-99	Mo	30.98	3	0.1850
141	58	6.08	Ce-141	Ce	18.28	3	0.1832
143	60	5.89	Nd-143	Nd	22.567	3	0.1774
91	40	5.88	Zr-91	Zr	30	4	0.2362
142	58	5.88	Ce-142	Ce	18.28	3	0.1771
98	42	5.84	Mo-98	Mo	30.98	3	0.1759
90	38	5.81	Sr-90	Sr	14.12	2	0.1167
144	60	5.38	Nd-144	Nd	22.567	3	0.1621
92	40	5.06	Zr-92	Zr	30	4	0.2032
101	44	5	Ru-101	Ru	15.245	3	0.1506
89	38	4.74	Sr-89	Sr	14.12	2	0.0952
132	54	4.31	Xe-132	Xe	31.72	0	0
102	44	4.16	Ru-102	Ru	15.245	3	0.1253
145	60	3.87	Nd-145	Nd	22.567	3	0.1166
88	38	3.57	Sr-88	Sr	14.12	2	0.0717
103	44	2.99	Ru-103	Ru	15.245	3	0.0901
146	60	2.94	Nd-146	Nd	22.567	3	0.0886
131	53	2.92	I-131	I	2.92	0	0
87	37	2.52	Rb-87	Rb	3.84	2	0.0506
147	60	2.18	Nd-147	Nd	22.567	3	0.0657
130	51	1.99	Sb-130	Sb	3.216	0	0
86	36	1.88	Kr-86	Kr	3.389	0	0
104	44	1.8	Ru-104	Ru	15.245	3	0.0542
148	60	1.66	Nd-148	Nd	22.567	3	0.0500
85	37	1.32	Rb-85	Rb	3.84	2	0.0265
149	61	1.04	Pm-149	Pm	1.04	3	0.0313
129	51	0.996	Sb-129	Sb	3.216	0	0
84	36	0.967	Kr-84	Kr	3.389	0	0
105	44	0.897	Ru-105	Ru	15.245	3	0.0270
150	60	0.647	Nd-150	Nd	22.567	3	0.0195
83	36	0.542	Kr-83	Kr	3.389	0	0
128	50	0.458	Sn-128	Sn	0.517	0	0
151	62	0.418	Sm-151	Sm	0.878	3	0.0126
106	44	0.398	Ru-106	Ru	15.245	3	0.0120

Table A.3 (Cont.)

A	Z (e)	Isotope Yield	Isotope	Element	Element Yield ^(a)	Fluoride No. @ 2500°C	Fluorine Requirement
82	34	0.319	Se-82	Se	0.569	0	0
152	62	0.239	Sm-152	Sm	0.878	3	0.0072
107	45	0.189	Rh-107	Rh	0.189	3	0.0057
153	62	0.157	Sm-153	Sm	0.878	3	0.0047
81	34	0.147	Se-81	Se	0.569	0	0
127	51	0.137	Sb-127	Sb	3.216	0	0
80	34	0.103	Se-80	Se	0.569	0	0
108	46	0.075	Pd-108	Pd	0.115	0	0
154	62	0.064	Sm-154	Sm	0.878	3	0.0019
126	51	0.064	Sb-126	Sb	3.216	0	0
79	33	0.056	As-79	As	0.084	0	0
155	63	0.031	Eu-155	Eu	0.055	3	0.0009
109	46	0.03	Pd-109	Pd	0.115	0	0
125	51	0.029	Sb-125	Sb	3.216	0	0
78	33	0.02	As-78	As	0.084	0	0
110	47	0.02	Ag-110	Ag	0.051	0	0
111	47	0.019	Ag-111	Ag	0.051	0	0
124	50	0.017	Sn-124	Sn	0.517	0	0
123	50	0.015	Sn-123	Sn	0.517	0	0
121	50	0.014	Sn-121	Sn	0.517	0	0
122	50	0.013	Sn-122	Sn	0.517	0	0
156	63	0.013	Eu-156	Eu	0.055	3	0.0004
113	47	0.012	Ag-113	Ag	0.051	0	0
120	49	0.011	In-120	In	0.033	0	0
119	49	0.011	In-119	In	0.033	0	0
118	49	0.011	In-118	In	0.033	0	0
117	48	0.011	Cd-117	Cd	0.042	0	0
114	48	0.011	Cd-114	Cd	0.042	0	0
112	46	0.01	Pd-112	Pd	0.115	0	0
116	48	0.01	Cd-116	Cd	0.042	0	0
115	48	0.01	Cd-115	Cd	0.042	0	0
77	33	0.008	As-77	As	0.084	0	0
157	63	0.007	Eu-157	Eu	0.055	3	0.0002
158	63	0.004	Eu-158	Eu	0.055	3	0.0001
76	32	0.002	Ge-76	Ge	0.003	0	0
160	65	0.001	Tb-160	Tb	0.001	3	0
75	32	0.001	Ge-75	Ge	0.003	0	0
159	64	0.001	Gd-159	Gd	0.001	3	0
72	30	0	Zn-72	Zn	0	0	0
161	65	0	Tb-161	Tb	0.001	3	0
74	31	0	Ga-74	Ga	0	0	0
73	31	0	Ga-73	Ga	0	0	0

^(a)Uranium fission fragment fractional yields by Ron Lipinski, SNL, adapted from (Gorur 1989, Vandenbosch 1973). Since each fission results in two fission fragments, yield per uranium atom sums to 2.

Table A.4. Stream Table for GCR-PFD

Stream	He	UF ₄	Xe	ZrF ₄	MoF ₆	NdF ₃	CeF ₃	SrF ₂	Total Molar Flow (kmol/s)	Total Mass Flow (kg/s)	P (atm)	Fraction	Fraction
10A	1.84	0.204	8.86	0.0959	8.90	9.63	9.98	9.08	2.04	71.4	1580	197	0.11
102A	1.84	0.204	9.86	1.10	9.90	10.6	11.0	10.1	2.04	71.4	2500	197	1
102B	1.84	0.204	9.86	1.10	9.90	10.6	11.0	10.1	2.04	71.4	1800	15.6	1
103A	1.84	0.198	9.86	1.10	9.90	0.615	0.965	0.0773	2.03	69.5	1772	15.6	0
105B	1.84	0.203	9.86	1.10	9.90	9.63	9.98	9.08	2.04	71.2	1600	15.6	0.08
106A	1.87	0.204	10.00	1.10	10.0	9.63	9.98	9.08	2.07	71.6	1600	15.6	0.08
107A	0	0.166	0	3.25E-06	0.00431	9.63	9.98	9.08	0.166	52.2	1600	15.6	0
107B	0	0.166	0	3.25E-06	0.00431	9.63	9.98	9.08	0.166	52.2	1604	197	0
108A	0	0.0370	0	0.0000381	0.00148	0.00148	0.00190	0.000136	0.0370	11.6	1310	15.6	1
108B	0	0.0370	0	0.0000381	0.00148	0.00148	0.00190	0.000136	0.0370	11.6	1314	197	0
110A	0	0.204	0	0.0959	0.00590	9.63	9.98	9.08	0.204	64.1	1553	197	0
111A	0	0.204	0	0.0959	0.00590	9.63	9.98	9.08	0.204	64.1	1586	197	0
201A	1.87	0.0378	10.0	1.10	10.0	0.00148	0.00190	0.000136	1.90	19.3	1600	15.6	1
201B	1.87	0.0378	10.0	1.10	10.0	0.00148	0.00190	0.000136	1.90	19.3	1310	15.6	0.98
202A	1.87	0.000786	10.0	1.10	10.0	0	0	0	1.87	7.72	1310	15.6	1
202C	1.87	2.75E-09	10.0	1.00	10.0	0	0	0	1.87	7.47	850	15.6	1
202D	1.87	0	10.0	0	10.0	0	0	0	1.87	7.47	343	15.6	1
202F	1.87	0	10.0	0	10.0	0	0	0	1.87	7.47	323	197	1
202G	1.68	0	9.00	0	9.04	0	0	0	1.68	6.72	323	197	1
202K	0.187	0	1.00	0	1.00	0	0	0	0.187	0.747	323	197	1
203C	0.187	0	0	0	0.00	0	0	0	0.187	0.747	323	197	1
204A	1.87	0	9.00	0	9.04	0	0	0	1.87	7.47	323	197	1
205B	1.87	0	9.00	0	9.04	0	0	0	1.87	7.47	830	197	1
205C	1.87	0	9.00	0	9.04	0	0	0	1.87	7.47	1290	197	1
205E	1.87	0	9.00	0	9.04	0	0	0	1.87	7.47	1580	197	1
205F	1.87	0	9.00	0	9.04	0	0	0	1.87	7.47	1585	197	1
205G	1.87	0	9.00	0	9.04	0	0	0	1.87	7.47	1586	197	1
205H	1.84	0	8.86	0	8.89	0	0	0	1.84	7.35	1586	197	1
205I	0.0295	0	0.142	0	0.143	0	0	0	0.0295	0.118	1586	197	1
205J	0.0295	0	0.142	0	0.143	0	0	0	0.0295	0.118	1780	197	1
220A	1.87	0.000786	9.00	0	9.04	0	0	0	1.87	7.72	1580	197	1
221A	0.0187	7.86E-06	0.0900	0	0.0904	0	0	0	0.0187	0.0772	1580	197	1
221B	0.0187	7.86E-06	0.0900	1.00	0.0904	0	0	0	0.0187	0.000305	1441	197	1
221C	0	0	0	1.00	0	0	0	0	0.09E-07	0	1441	197	1
223A	negligible	negligible	1.00	0	1.00	0	0	0	2.04E-07	3.50E-05	323	197	1
223B	negligible	negligible	1.00	0	1.00	0	0	0	2.04E-07	3.50E-05	323	15.6	1
223C	negligible	negligible	0.00	0	1.00	0	0	0	1.03E-07	2.17E-05	323	15.6	1
223D	negligible	negligible	1.00	0	0	0	0	0	0.0000132	77	15.6	1	0
223E	negligible	negligible	1.00	0	0	0	0	0	LOIE-07	0.0000132	77	15.6	1
301A	3.51 E-06	0.000611	6.64E-06	9.97E-09	0.0000122	1.00	1.00	1.00	0.000615	0.192	1772	15.6	0
312A	0.0295	0.000598	0.142	9.97E-09	0.143	0.00167	0.00205	0.000161	0.0301	0.306	1600	15.6	1
320A	2.95E-06	0.0000129	0	0	0	1.00	1.00	1.00	0.0000162	0.00413	1657	15.6	0.18

Table A.5
Unit Design by PFD Section**SECTION 100**

Unit	RXR	MHD	UHX1	UHX2	URH
Hot Inlet Temperature, K	1580	2500	1800	1772	1553
Hot Outlet Temperature, K	2500	1800	1772	1600	1586
Cold Inlet Temperature, K	—	—	1586	—	—
Cold Outlet Temperature, K	—	—	1780	—	—
Inlet Pressure, atm	197	197	15.6	15.6	197
Outlet Pressure, atm	197	15.6	15.6	15.6	197
Power, MW	100	-41.95	-2.9	-45.6	1.4
Efficiency	—	55%	—	—	—

SECTION 200

Unit	HX1	HX2a	HX2b	HX3a	HX3b	HEC	PSA1	PSA2	EX1	HX4
Hot Inlet Temp, K	1600	1310	1580	850	1580	343	323	—	323	323
Hot Out Temp, K	1310	850	1580	343	1441	323	323	323	323	77
Cold Inlet Temperature, K	1290	830	—	323	—	—	—	—	—	—
Cold Out Temp, K	1580	1290	—	830	—	—	—	—	—	—
Inlet Pressure, atm	15.6	15.6	197	15.6	197	15.6	197	—	197	15.6
Outlet Press, atm	15.6	15.6	197	15.6	197	197	197	197	15.6	15.6
Power, MW	—	—	—	—	—	—	—	—	—	—
Efficiency	—	—	—	—	—	88%	—	—	—	—

SECTION 300

Unit	C1 x 5
Overhead Inlet Temperature, K	1772
helium Inlet Temperature, K	1780
Vapor Outlet Temperature, K	1600
Liquid Outlet Temperature, K	1657
Inlet Pressure, atm	—
Outlet Pressure, atm	—
Power, MW	—
Efficiency	—

Fig. A.2. Working simulation depicting heat streams.

Table A.6. Material Stream Table for Simulation

Stream	Mole Flow kmol/sec								Total Flow		T(K)	P(atm)	Vapor Fraction	Liquid Fraction
	He	UF4	Xe	ZrF4	MoF6	NdF3	CeF3	SrF2	(kmol/s)	(kg/s)				
101A	1.84	0.204	0	0	0	0	0	0	2.04	71.4	1580	197	0.89	0.11
101B	1.84	0.204	0	0	0	0	0	0	2.04	71.4	2500	197	1	0
102A	1.84	0.204	9.96E-07	9.96E-07	1.02E-06	9.96E-07	9.96E-07	9.96E-07	2.04	71.4	2500	197	1	0
102B	1.84	0.204	9.96E-07	9.96E-07	1.02E-06	9.96E-07	9.96E-07	9.96E-07	2.04	71.4	1800	15.6	1	0
102C	1.83	0.203	9.91E-07	9.91E-07	1.02E-06	9.91E-07	9.91E-07	9.91E-07	2.03	71.1	2500	197	1	0
102D	1.83	0.203	9.91E-07	9.91E-07	1.02E-06	9.91E-07	9.91E-07	9.91E-07	2.03	71.1	1800	15.6	1	0
102E	0.00892	0.000991	4.84E-09	4.84E-09	4.95E-09	4.84E-09	4.84E-09	4.84E-09	0.00991	0.347	2500	197	1	0
102F	0.00892	0.000991	4.84E-09	4.84E-09	4.95E-09	4.84E-09	4.84E-09	4.84E-09	0.00991	0.347	1800	15.6	1	0
103A	1.84	0.198	9.96E-07	9.96E-07	1.02E-06	5.76E-08	8.75E-08	7.64E-09	2.03	69.5	1772	15.6	1	0
104A	0.000035	0.00611	6.71E-12	9.06E-14	1.26E-11	9.38E-07	9.08E-07	9.88E-07	0.00615	1.92	1772	15.6	0	1
104B	0.000032	0.00550	6.04E-12	8.16E-14	1.13E-11	8.45E-07	8.18E-07	8.90E-07	0.00553	1.73	1772	15.6	0	1
105A	1.84	0.203	9.96E-07	9.96E-07	1.02E-06	9.02E-07	9.05E-07	8.97E-07	2.04	71.2	1772	15.6	1.00	0
105B	1.84	0.203	9.96E-07	9.96E-07	1.02E-06	9.02E-07	9.05E-07	8.97E-07	2.04	71.2	1600	15.6	0.92	0.08
106A	1.87	0.204	1.01E-06	9.96E-07	1.03E-06	9.02E-07	9.05E-07	8.97E-07	2.07	71.6	1600	15.6	0.92	0.08
107A	0	0.166	0	2.96E-12	4.44E-10	9.02E-07	9.05E-07	8.97E-07	0.166	52.2	1600	15.6	0	1
107B	0	0.166	0	2.96E-12	4.44E-10	9.02E-07	9.05E-07	8.97E-07	0.2	52.2	1604	197	0	1
108A	0	0.0370	0	3.46E-11	1.53E-10	1.39E-10	1.72E-10	1.34E-11	0.0370	11.6	1310	15.6	0	1
108B	0	0.0370	0	3.46E-11	1.53E-10	1.39E-10	1.72E-10	1.34E-11	0.0370	11.6	1314	197	0	1
109A	0	0.000786	0	8.72E-08	1.11E-11	0	0	0	0.000786	0.247	1310	15.6	0	1
109B	0	0.000786	0	8.72E-08	1.11E-11	0	0	0	0.000786	0.247	1314	197	0	1
110A	0	0.204	0	8.72E-08	6.08E-10	9.02E-07	9.05E-07	8.97E-07	0.204	64.1	1553	197	0	1
111A	0	0.204	0	8.72E-08	6.08E-10	9.02E-07	9.05E-07	8.97E-07	0.204	64.1	1586	197	0	1
112A	1.84	0.204	8.95E-07	8.72E-08	9.17E-07	9.02E-07	9.05E-07	8.97E-07	2.04	71.4	1580	197	0.89	0.11
201A	1.87	0.0378	1.01E-06	9.96E-07	1.03E-06	1.39E-10	1.72E-10	1.34E-11	1.90	19.3	1600	15.6	1	0
201B	1.87	0.0378	1.01E-06	9.96E-07	1.03E-06	1.39E-10	1.72E-10	1.34E-11	1.90	19.3	1310	15.6	0.98	0.02
202A	1.87	0.000786	1.01E-06	9.96E-07	1.03E-06	0	0	0	1.87	7.72	1310	15.6	1	0
202B	1.87	0.000786	1.01E-06	9.96E-07	1.03E-06	0	0	0	1.87	7.72	850	15.6	1.00	0
202C	1.87	2.75E-09	1.01E-06	9.09E-07	1.03E-06	0	0	0	1.87	7.47	850	15.6	1	0
202D	1.87	0	1.01E-06	0	1.03E-06	0	0	0	1.87	7.47	343	15.6	1	0
202F	1.87	0	1.01E-06	0	1.03E-06	0	0	0	1.87	7.47	323	197	1	0
202G	1.68	0	9.09E-07	0	9.31E-07	0	0	0	1.68	6.72	323	197	1	0
202K	0.187	0	1.01E-07	0	1.03E-07	0	0	0	0.187	0.747	323	197	1	0
203B	1.87	2.75E-09	1.01E-06	9.09E-07	1.03E-06	0	0	0	1.87	7.47	343	15.6	1	0
203C	0.187	0	0	0	0	0	0	0	0.187	0.747	323	197	1	0
204A	1.87	0	9.09E-07	0	9.31E-07	0	0	0	1.87	7.47	323	197	1	0
205B	1.87	0	9.09E-07	0	9.31E-07	0	0	0	1.87	7.47	830	197	1	0
205C	1.87	0	9.09E-07	0	9.31E-07	0	0	0	1.87	7.47	1290	197	1	0
205E	1.87	0	9.09E-07	0	9.31E-07	0	0	0	1.87	7.47	1580	197	1	0
205F	1.87	0	9.09E-07	0	9.31E-07	0	0	0	1.87	7.47	1585	197	1	0
205G	1.87	0	9.09E-07	0	9.31E-07	0	0	0	1.87	7.47	1586	197	1	0
205H	1.84	0	8.95E-07	0	9.16E-07	0	0	0	1.84	7.35	1586	197	1	0
205I	0.0295	0	1.44E-08	0	1.47E-08	0	0	0	0.0295	0.118	1586	197	1	0
205J	0.0295	0	1.44E-08	0	1.47E-08	0	0	0	0.0295	0.118	1780	197	1	0
221B	0	2.75E-09	0	9.09E-07	2.48E-12	0	0	0	9.12E-07	0.000153	343	15.6	0	1
221C	0	2.75E-09	0	9.09E-07	2.48E-12	0	0	0	9.12E-07	0.000153	1441	15.6	1	0
223C	0	0	1.01E-07	0	1.03E-07	0	0	0	2.04E-07	0.000035	323	197	0	1
301A	3.51E-06	0.000611	6.71E-13	9.06E-15	1.26E-12	9.38E-08	9.08E-08	9.88E-08	0.000615	0.192	1772	15.6	0	1
312A	0.0295	0.000598	1.44E-08	9.06E-15	1.47E-08	1.57E-10	1.86E-10	1.59E-11	0.0301	0.306	1600	15.6	1.00	0
320A	2.95E-06	0.000013	0	0	0	9.37E-08	9.07E-08	9.88E-08	0.000016	0.00413	1657	15.6	0.18	0.82
Fiss-In	0	0	9.96E-07	9.96E-07	1.02E-06	9.96E-07	9.96E-07	9.96E-07	6.00E-06	0.00103	2500	197	0.49	0.51
M201A	0.00104	0.166	2.19E-10	2.96E-12	4.44E-10	9.02E-07	9.05E-07	8.97E-07	0.167	52.2	1600	15.6	0	1
M201B	0.00104	0	2.19E-10	0	0	0	0	0	0.00104	0.00415	1600	15.6	1	0
M201C	1.87	0.0378	1.01E-06	9.96E-07	1.03E-06	1.39E-10	1.72E-10	1.34E-11	1.90	19.3	1600	15.6	1	0
M202A	0.000235	0.0370	6.26E-11	3.46E-11	1.53E-10	1.39E-10	1.72E-10	1.34E-11	0.0373	11.6	1310	15.6	0	1
M202B	0.000235	0	6.26E-11	0	0	0	0	0	0.000235	0.000943	1310	15.6	1	0
M202C	1.87	0.000786	1.01E-06	9.96E-07	1.03E-06	0	0	0	1.87	7.72	1310	15.6	1	0
M203A	5.00E-06	0.000786	2.64E-12	8.72E-08	1.11E-11	0	0	0	0.000791	0.247	850	15.6	0	1
M203B	5.00E-06	0	2.64E-12	0	0	0	0	0	5.00E-06	0.000020	850	15.6	1	0
M203C	1.87	2.75E-09	1.01E-06	9.09E-07	1.03E-06	0	0	0	1.87	7.47	850	15.6	1	0
M204A	5.80E-09	2.75E-09	5.53E-14	9.09E-07	2.48E-12	0	0	0	9.17E-07	0.000153	343	15.6	0	1
M204B	5.80E-09	0	5.53E-14	0	0	0	0	0	5.80E-09	2.32E-08	343	15.6	1	0
M204C	1.87	0	1.01E-06	0	1.03E-06	0	0	0	1.87	7.47	343	15.6	1	0
UF4-3B	0	0.000786	0	8.72E-08	1.11E-11	0	0	0	0.000786	0.247	850	15.6	0	1

Table A.7
Heat Stream Table for Simulation

Stream	Q (MW)
Q101A	0.205
Q201A	21.5
Q201B	11.2
Q201C	10.3
Q201D	1.40
Q201E	8.87
Q202A	18.1
Q202B	17.8
Q202C	0.259
Q203A	-0.0132
Q203B	100.0
Q203C	99.987

Table A.8
Design Specifications and Calculation Blocks for Simulation

DESIGN SPECIFICATIONS

Name	3PERCENT	MHD-P	PRI1HT	PRI2HT
Specification	% liquid UF ₄ in bottoms of unit 3PU	Outlet stream of unit MHD	Heat (Q) of stream Q201B equals heat (Q) for RH2	Heat (Q) of stream Q202B equals heat (Q) for RH1
Value	0.03	1800	—	—
Manipulated Variable	3PU outlet temperature	MHD outlet pressure	Split of heat flow in unit QS1A	Split of heat flow in unit QS2A
Range	1000–1800	1 to 200	0.1 to 0.999	0.6 to 0.999

Name	TRXROUT	UREHEAT	WALHTMHD
Specification	Rxr net duty equals heat (Q) of stream Q203C	Heat (Q) of stream Q201D equals net duty of block URH	Net duty of block WHTO equals –30x14xDel_Tlm
Value	—	—	—
Manipulated Variable	Molar flowrate into unit RXR	Split of heat flow in block QS1B	Material flow split of unit B3
Range	1 to 2.5	0.1 to 0.9	0.001 to 0.03

CALCULATION BLOCKS

Name	HOT1	HOT2	UHOT	WLHTRXR
Variable name	PRI1OT	PRI2OT	HTPRI1	WHRXR
Variable description	Outlet temp of block RH2	Outlet temp of block RH1	Outlet temp of block URH	Duty of block RXRH
Variable name	O1BT	O2BT	TOV1B	TOUTH
Variable description	Temp of stream 201A	Temp of stream 202A	Temp of stream 205H	Temp of stream FISS-IN
Variable name	—	—	—	TINC
Variable description	—	—	—	Temp of stream 205F
Variable name	—	—	—	—
Variable description	—	—	—	—
Calculation	PRI1OT = O1BT–20	PRI2OT = O2BT–20	HTPRI1 = TOV1B	WHRXR = 13 * 4.34615 * ((20)-(TOUTH-TINC)) / (ALOG((20) / (TOUTH-TINC)))

Table A.9. Energy Balance for the GCR-PFD

System		Block	Stream	Power in, MW	Power out	Net
Gas	Core	Reactor	Power			
		100-RXR		100		
			Q 203A	0		100
MHD-Power		100-MHD			-42.0	42.0
Heat-to-Power		100-3PU			-2.91	
		100-UHX2			-45.6	
			Q 202C		-0.259	
			Q 201E		-8.87	
		200-HERH		0.119		
		100-HXRH		0.0657		
		200-HT1		0.000306		
						-57.4
Power-to-Turbines		200-HEC cooling			-18.3	
		200-HEC work		17.5		0.776
Power-to-Pumps		100-P1		0.151		
		100-P2		0.0299		
		100-P3		0.000634		
						0.181
Misc.			FISS-IN		0.00564	0.00564
			320A		-0.0221	-0.0221
Overall Balance		(Sum of net power)				0.0

Table A.10
Input File for Simulation

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DYNAPLUS
  DPLUS RESULTS=ON

TITLE 'VAPOR CORE REACTOR'

IN-UNITS SI PRESSURE=atm PDROP=atm

DEF-STREAMS CONVEN ALL

DESCRIPTION "
  General Simulation with Metric Units :
  C, bar, kg/hr, kmol/hr, MMKcal/hr, cum/hr.

  Property Method: None

  Flow basis for input: Mole

  Stream report composition: Mole flow "

DATABANKS PURE10 / SOLIDS / INORGANIC / PURE93 /
PURE856 &
  / ASPENPCD / COMBUST

PROP-SOURCES PURE10 / SOLIDS / INORGANIC / PURE93 /
&
  PURE856 / ASPENPCD / COMBUST

COMPONENTS
  HE-4 HE-4 /
  UF4 UF4 /
  XE XE /
  ZIRCO-01 ZRF4 /
  MOF6 /
  NEODY-01 NDF3 /
  CERIU-01 CEF3 /
  STRON-01 SRF2

FLOWSHEET
  BLOCK 100-SEP1 IN=106A OUT=M201C M201A
  BLOCK 100-P1 IN=107A OUT=107B
  BLOCK 200-HX1 IN=201A OUT=201B Q201A
  BLOCK 100-MIX4 IN=107B 109B 108B OUT=110A
  BLOCK 100-RXR IN=101A OUT=101B
  BLOCK 200-RXRH IN=205F OUT=205G Q203A
  BLOCK 200-SEP1 IN=201B OUT=M202C M202A
  BLOCK 100-P2 IN=108A OUT=108B
  BLOCK 100-MHD IN=102C OUT=102D
  BLOCK 200-HX2A IN=202A OUT=202B Q202A
  BLOCK 200-SEP2 IN=202B OUT=M203C M203A
  BLOCK 100-MIX5 IN=111A 205H OUT=112A
  BLOCK 100-HXRH IN=UF4-3B OUT=109A
  BLOCK 100-P3 IN=109A OUT=109B
  BLOCK 200-HX3A IN=202C 204A OUT=203B 205B
  BLOCK 200-MHDH IN=205E Q101A OUT=205F
  BLOCK 200-SEP4 IN=203B OUT=M204C M204A
  BLOCK 200-HEC IN=202D OUT=202F
  BLOCK 11-FPMIX IN=FISS-IN 101B OUT=102A
  BLOCK 200-M1A IN=M201A OUT=107A M201B
  BLOCK 200-M1B IN=M201B M201C OUT=201A
  BLOCK 200-M2A IN=M202A OUT=108A M202B
  BLOCK 200-M3A IN=M203A OUT=UF4-3B M203B
  BLOCK 200-M2B IN=M202B M202C OUT=202A
  BLOCK 200-M3B IN=M203B M203C OUT=202C
  BLOCK 200-M4A IN=M204A OUT=M204B 221B

  BLOCK 200-M4B IN=M204B M204C OUT=202D
  BLOCK 200-BP IN=202F OUT=202G 202K
  BLOCK 200-PSA IN=202K OUT=203C 223C
  BLOCK 100-B3 IN=102A OUT=102E 102C
  BLOCK 100-B4 IN=102D 102F OUT=102B
  BLOCK 100-WHTO IN=102E OUT=102F Q101A

  BLOCK 200-QS3A IN=Q203B Q203A OUT=Q203C
  BLOCK 200-RH1 IN=205B OUT=205C
  BLOCK 200-QS2A IN=Q202A OUT=Q202C Q202B
  BLOCK 200-QS1A IN=Q201A OUT=Q201C Q201B
  BLOCK 200-RH2 IN=205C OUT=205E
  BLOCK 200-MIX3 IN=202G 203C OUT=204A
  BLOCK 100-3PU IN=102B OUT=103A 104A
  BLOCK 100-B1 IN=104A OUT=301A 104B
  BLOCK 100-UHX2 IN=105A OUT=105B
  BLOCK 100-MIX1 IN=103A 104B OUT=105A
  BLOCK 100-MIX2 IN=105B 312A OUT=106A
  BLOCK 200-HS IN=205G OUT=205I 205H
  BLOCK 200-HERH IN=205I OUT=205J
  BLOCK 300-FSEP IN=301A 205J OUT=312A 320A
  BLOCK 200-HT1 IN=221B OUT=221C
  BLOCK 100-URH IN=110A OUT=111A
  BLOCK 200-QS1B IN=Q201C OUT=Q201D Q201E

PROPERTIES IDEAL
  PROPERTIES PENG-ROB / PSRK / RK-ASPEN / RK-SOAVE /
  VANL-2

ESTIMATE ONLY
  DHVL UF4 VETERE TOWER=300. TUPPER=2500.
  DHVL MOF6 VETERE TOWER=300. TUPPER=2500.
  DHVL NEODY-01 VETERE TOWER=300. TUPPER=2500.
  DHVL CERIU-01 VETERE TOWER=300. TUPPER=2500.
  DHVL STRON-01 VETERE TOWER=300. TUPPER=2500.

PROP-DATA PCES-1
  IN-UNITS SI PRESSURE=atm MOLE-VOLUME='cc/mol'
  PDROP=atm
  PROP-LIST VLSTD
  PVAL UF4 0.0
  PVAL ZIRCO-01 0
  PVAL MOF6 0.0
  PVAL NEODY-01 0.0
  PVAL CERIU-01 0.0
  PVAL STRON-01 0.0

PROP-DATA PURE-1
  IN-UNITS SI PRESSURE=atm MOLE-VOLUME='cc/mol'
  PDROP=atm
  PROP-LIST MW / OMEGA / PC / TB / TC / TFP / VB / &
  VC / ZC
  PVAL UF4 314.0225 / 1.504 / 208.2 / 1723 / 2415 / &
  1309 / 56.281 / 162.5 / 0.1707
  PVAL ZIRCO-01 167.218 / 1.338 / 161.1 / 1205.15 / 1665 &
  / 1185.15 / 40.17 / 156 / .1839
  PVAL MOF6 209.93 / 0.649 / 35.5 / 307.15 / 431 / &
  290.55 / 87.95 / 237.9 / 0.2391
  PVAL NEODY-01 201.235 / 1.794 / 379.3 / 2573.15 / 3251 &
  / 1647.15 / 32.95 / 114.6 / 0.1475
  PVAL CERIU-01 197.11 / 1.735 / 342.5 / 2600.15 / 3591 &
  / 1703.15 / 34.07 / 118.6 / 0.1522
  PVAL STRON-01 125.617 / 1.772 / 378.8 / 2733.15 / 3823 &
  / 1746.15 / 31.53 / 123.6 / 0.1493

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Table A.10 (Cont.)

PROP-DATA DHVLWT-1 IN-UNITS SI PRESSURE=atm TEMPERATURE=C & MOLE-ENTHALP='kcal/mol' PDROP=atm PROP-LIST DHVLWT PVAL UF4 49.06225494 1449.850000 .3800000000 0.0 & 1449.850000 PVAL ZIRCO-01 35.58699 932 .38 0 932 PVAL MOF6 6.604702876 34.00000000 .3800000000 0.0 & 34.00000000	STREAM 205E SUBSTREAM MIXED TEMP=881.851586 PRES=197 MOLE-FLOW HE-4 1.61296902 / XE 8.964E-007 / MOF6 & 9.174518E-007
PROP-DATA DHVLWT-1 IN-UNITS SI PRESSURE=atm MOLE-ENTHALP='cal/mol' PDROP=atm PROP-LIST DHVLWT PVAL NEODY-01 1.08177619E+5 2573.150000 .3800000000 0.0 & 2573.150000 PVAL CERIU-01 1.11302606E+5 2600.150000 .3800000000 0.0 & 2600.150000	STREAM 205F SUBSTREAM MIXED TEMP=842.920536 PRES=197 MOLE-FLOW HE-4 1.95111639 / XE 1.520426E-006 / MOF6 & 1.555735E-006
PROP-DATA DHVLWT-1 IN-UNITS SI PRESSURE=atm PDROP=atm PROP-LIST DHVLWT PVAL STRON-01 6.72304408E+8 2733.150000 .3800000000 0.0 & 2733.150000	STREAM 205G SUBSTREAM MIXED TEMP=900. PRES=197. MOLE-FLOW HE-4 1.95111639 / XE 1.5204E-006 / MOF6 & 1.5557E-006
PROP-DATA PLXANT-1 IN-UNITS SI PRESSURE=atm PDROP=atm PROP-LIST PLXANT PVAL UF4 74.217 -37977 0 0 -7 0 0 1000 2500 PVAL ZIRCO-01 30.859 -28501.9 0 0 0 0 889.75 1153.95 PVAL NEODY-01 18.5 -43135 0 0 0 0 1383 1520 PVAL CERIU-01 21.2 -47120 0 0 0 0 1373 1634	STREAM FISS-IN SUBSTREAM MIXED TEMP=2500. PRES=197. MOLE- FLOW=6E-006 MOLE-FRAC HE-4 0. / UF4 0. / XE 0.166 / ZIRCO-01 & 0.166 / MOF6 0.17 / NEODY-01 0.166 / CERIU-01 0.166 & / STRON-01 0.166
PROP-DATA PLXANT-1 IN-UNITS SI PRESSURE=mmHg PDROP=atm PROP-LIST PLXANT PVAL MOF6 46.49734 -4703.74 0 0 -4.28004 0 0 290 400	DEF-STREAMS HEAT Q101A STREAM Q101A INFO HEAT DUTY=1000.
PROP-DATA PLXANT-1 IN-UNITS SI PRESSURE=kPa PDROP=atm PROP-LIST PLXANT PVAL STRON-01 23.49 -47466 0 0 0 0 1381 1720	DEF-STREAMS HEAT Q201A DEF-STREAMS HEAT Q201B DEF-STREAMS HEAT Q201C DEF-STREAMS HEAT Q201D DEF-STREAMS HEAT Q201E DEF-STREAMS HEAT Q202A
STREAM 101A SUBSTREAM MIXED TEMP=1579.621 PRES=197. MOLE- FLOW=1.5 MOLE-FRAC HE-4 0.9 / UF4 0.1	STREAM Q202A INFO HEAT DUTY=1.
STREAM 101B SUBSTREAM MIXED TEMP=2500. PRES=197. MOLE- FLOW=1.5 MOLE-FRAC HE-4 0.9 / UF4 0.1	DEF-STREAMS HEAT Q202B DEF-STREAMS HEAT Q202C DEF-STREAMS HEAT Q203A
STREAM 102B SUBSTREAM MIXED TEMP=1800.00033 PRES=22.8919431 MOLE-FLOW HE-4 2.1679071 / UF4 0.240878567 / XE & 1.689362E-006 / ZIRCO-01 1.689362E-006 / MOF6 & 1.730070E-006 / NEODY-01 1.689362E-006 / CERIU-01 & 1.689362E-006 / STRON-01 1.689362E-006	STREAM Q203A INFO HEAT DUTY=1. DEF-STREAMS HEAT Q203B STREAM Q203B INFO HEAT DUTY=100000000. DEF-STREAMS HEAT Q203C
STREAM 205B SUBSTREAM MIXED TEMP=830 PRES=197 MOLE-FLOW HE-4 1.61272853 / XE 8.964E-007 / MOF6 & 9.174518E-007	STREAM Q203C INFO HEAT DUTY=100000000. BLOCK 11-FPMIX MIXER PARAM T-EST=2500.

Table A.10 (Cont.)

BLOCK 100-B4 MIXER PARAM T-EST=1800.	FRAC STREAM=M204B SUBSTREAM=MIXED COMPS=HE-4 UF4 XE & ZIRCO-01 MOF6 NEODY-01 CERIU-01 STRON-01 FRACS=1. 0. & 1. 0. 0. 0. 0. 0.
BLOCK 100-MIX1 MIXER	
BLOCK 100-MIX2 MIXER	
BLOCK 100-MIX4 MIXER PARAM T-EST=1550.	BLOCK 200-PSA SEP2 FRAC STREAM=223C SUBSTREAM=MIXED COMPS=HE-4 UF4 XE & ZIRCO-01 MOF6 NEODY-01 CERIU-01 STRON-01 FRACS=0. 0. & 1. 0. 1. 0. 0. 0.
BLOCK 100-MIX5 MIXER	
BLOCK 200-M1B MIXER	
BLOCK 200-M2B MIXER PARAM MAXIT=90 T-EST=1310.	BLOCK 300-FSEP SEP2 FRAC STREAM=312A SUBSTREAM=MIXED COMPS=HE-4 UF4 XE & ZIRCO-01 MOF6 NEODY-01 CERIU-01 STRON-01 FRACS=0.9999 & 0.9788 1. 1. 1. 0.001671 0.002045 0.000161 FLASH-SPECS 312A TEMP=1600. PRES=0. FLASH-SPECS 320A TEMP=1657. PRES=0.
BLOCK 200-M3B MIXER	
BLOCK 200-M4B MIXER PARAM MAXIT=100 T-EST=400.	
BLOCK 200-MIX3 MIXER	BLOCK 100-HXRH HEATER PARAM TEMP=1310. PRES=0.
BLOCK 200-QS3A MIXER	
BLOCK 100-B1 FSPLIT FRAC 301A 0.1	BLOCK 100-RXR HEATER PARAM TEMP=2500. PRES=0.
BLOCK 100-B3 FSPLIT FRAC 102E 0.008	BLOCK 100-UHX2 HEATER PARAM TEMP=1600. PRES=0.
BLOCK 200-BP FSPLIT FRAC 202K 0.1	BLOCK 100-URH HEATER PARAM TEMP=1580. PRES=0.
BLOCK 200-QS1A FSPLIT FRAC Q201B 0.5	BLOCK 100-WHTO HEATER PARAM TEMP=1800. PRES=0. MAXIT=90 TOL=0.1
BLOCK 200-QS1B FSPLIT FRAC Q201D 0.5	BLOCK 200-HERH HEATER PARAM TEMP=1780. PRES=0.
BLOCK 200-QS2A FSPLIT FRAC Q202B 0.7	BLOCK 200-HT1 HEATER PARAM PRES=0. VFRAC=1. MAXIT=100 T-EST=1500.
BLOCK 200-M1A SEP2 FRAC STREAM=M201B SUBSTREAM=MIXED COMPS=HE-4 UF4 XE & ZIRCO-01 MOF6 NEODY-01 CERIU-01 STRON-01 FRACS=1. 0. & 1. 0. 0. 0. 0. 0.	BLOCK 200-HX1 HEATER PARAM TEMP=1310. PRES=0.
BLOCK 200-M2A SEP2 FRAC STREAM=M202B SUBSTREAM=MIXED COMPS=HE-4 UF4 XE & ZIRCO-01 MOF6 NEODY-01 CERIU-01 STRON-01 FRACS=1. 0. & 1. 0. 0. 0. 0. 0.	BLOCK 200-HX2A HEATER PARAM TEMP=850. PRES=0.
BLOCK 200-M3A SEP2 FRAC STREAM=M203B SUBSTREAM=MIXED COMPS=HE-4 UF4 XE & ZIRCO-01 MOF6 NEODY-01 CERIU-01 STRON-01 FRACS=1. 0. & 1. 0. 0. 0. 0. 0.	BLOCK 200-MHDH HEATER PARAM PRES=0. T-EST=850.
BLOCK 200-M4A SEP2	BLOCK 200-RH1 HEATER PARAM TEMP=1200. PRES=0.
	BLOCK 200-RH2 HEATER PARAM TEMP=1550. PRES=0.
	BLOCK 200-RXRH HEATER PARAM PRES=0. DUTY=100.
	BLOCK 100-3PU FLASH2 PARAM TEMP=1770. PRES=0.
	BLOCK 100-SEP1 FLASH2 PARAM PRES=0. DUTY=0. MAXIT=90 T-EST=1600.

Table A.10 (Cont.)

BLOCK 200-SEP1 FLASH2 PARAM PRES=0. DUTY=0.	DEFINE PRIDH BLOCK-VAR BLOCK=200-RH2 VARIABLE=NET-DUTY & SENTENCE=RESULTS SPEC "PRID1" TO "PRIDH" TOL-SPEC "1" VARY BLOCK-VAR BLOCK=200-QS1A SENTENCE=FRAC VARIABLE=FRAC & ID1=Q201B LIMITS ".1" ".999"
BLOCK 200-SEP2 FLASH2 PARAM PRES=0. DUTY=0.	
BLOCK 200-SEP4 FLASH2 PARAM PRES=0. DUTY=0.	
BLOCK 200-HX3A HEATX PARAM DELT-COLD=20. U-OPTION=PHASE FEEDS HOT=202C COLD=204A PRODUCTS HOT=203B COLD=205B	DESIGN-SPEC PRI2HT DEFINE PRID2 INFO-VAR INFO=HEAT VARIABLE=DUTY STREAM=Q202B DEFINE PRIDHT BLOCK-VAR BLOCK=200-RH1 VARIABLE=NET-DUTY & SENTENCE=RESULTS SPEC "PRID2" TO "PRIDHT" TOL-SPEC ".1" VARY BLOCK-VAR BLOCK=200-QS2A SENTENCE=FRAC VARIABLE=FRAC & ID1=Q202B LIMITS ".6" ".999"
BLOCK 100-P1 PUMP PARAM PRES=197. EFF=0.9	
BLOCK 100-P2 PUMP PARAM PRES=197. EFF=0.9	
BLOCK 100-P3 PUMP PARAM PRES=197. EFF=0.9 NPHASE=2 BLOCK-OPTION FREE-WATER=NO	
BLOCK 100-MHD COMPR PARAM TYPE=ISENTROPIC PRES=100. SEFF=0.55 NPHASE=2 & SB-TOL=0.001 BLOCK-OPTION FREE-WATER=NO	DESIGN-SPEC TRXROUT DEFINE NETPOW INFO-VAR INFO=HEAT VARIABLE=DUTY STREAM=Q203C DEFINE RXRDUT BLOCK-VAR BLOCK=100-RXR VARIABLE=NET-DUTY & SENTENCE=RESULTS SPEC "RXRDUT" TO "NETPOW" TOL-SPEC "1" VARY STREAM-VAR STREAM=101A SUBSTREAM=MIXED & VARIABLE=MOLE-FLOW LIMITS "1" "2.5"
BLOCK 200-HEC MCOMPR PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=197. FEEDS 202D 1 PRODUCTS 202F 3 COMPR-SPECS 1 SEFF=0.88 / 2 SEFF=0.88 / 3 SEFF=0.88 COOLER-SPECS 1 TEMP=323. / 2 TEMP=323. / 3 TEMP=323.	
BLOCK 200-HS SSPLIT MOLE-FLOW MIXED 205I 0.0295 * DEF-KEY KEYNO=1 COMPS=HE-4	DESIGN-SPEC UREHEAT DEFINE UHEAT INFO-VAR INFO=HEAT VARIABLE=DUTY STREAM=Q201D DEFINE PRI2DH BLOCK-VAR BLOCK=100-URH VARIABLE=NET-DUTY & SENTENCE=RESULTS SPEC "UHEAT" TO "PRI2DH" TOL-SPEC ".1" VARY BLOCK-VAR BLOCK=200-QS1B SENTENCE=FRAC VARIABLE=FRAC & ID1=Q201D LIMITS ".1" ".9"
DESIGN-SPEC 3PERCENT DEFINE SPLIT MOLE-FLOW STREAM=104A SUBSTREAM=MIXED & COMPONENT=UF4 DEFINE INLET MOLE-FLOW STREAM=102B SUBSTREAM=MIXED & COMPONENT=UF4 SPEC " SPLIT/INLET" TO ".03" TOL-SPEC ".0001" VARY BLOCK-VAR BLOCK=100-3PU VARIABLE=TEMP SENTENCE=PARAM LIMITS "1000" "1800"	DESIGN-SPEC WALHTMHD DEFINE WDUTY BLOCK-VAR BLOCK=100-WHTO VARIABLE=NET-DUTY & SENTENCE=RESULTS DEFINE TCOUT STREAM-VAR STREAM=205F SUBSTREAM=MIXED & VARIABLE=TEMP DEFINE TCIN STREAM-VAR STREAM=205E SUBSTREAM=MIXED & VARIABLE=TEMP DEFINE THOUT STREAM-VAR STREAM=102B SUBSTREAM=MIXED & VARIABLE=TEMP DEFINE THIN STREAM-VAR STREAM=102A SUBSTREAM=MIXED & VARIABLE=TEMP
DESIGN-SPEC MHD-P DEFINE MHDT STREAM-VAR STREAM=102D SUBSTREAM=MIXED & VARIABLE=TEMP SPEC "MHDT" TO "1800" TOL-SPEC ".01" VARY BLOCK-VAR BLOCK=100-MHD VARIABLE=PRES SENTENCE=PARAM LIMITS "1" "200"	
DESIGN-SPEC PRI1HT DEFINE PRID1 INFO-VAR INFO=HEAT VARIABLE=DUTY STREAM=Q201B	

Table A.10 (Cont.)

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SPEC "WDUTY" TO &
  "-30*14 * ((THIN-TCOUT)-(THOUT-TCIN))/(ALOG((THIN-
TCOUT)/(THOUT-TCIN)))"
TOL-SPEC ".1"
VARY BLOCK-VAR BLOCK=100-B3 SENTENCE=FRAC
VARIABLE=FRAC &
  ID1=102E
LIMITS ".001" ".03"

CALCULATOR HOT1
  DEFINE PRI1OT BLOCK-VAR BLOCK=200-RH2
VARIABLE=TEMP &
  SENTENCE=PARAM
  DEFINE O1BT STREAM-VAR STREAM=201A
SUBSTREAM=MIXED &
  VARIABLE=TEMP
F  PRI1OT=O1BT-20
  READ-VARS O1BT
  WRITE-VARS PRI1OT

CALCULATOR HOT2
  DEFINE PRI2OT BLOCK-VAR BLOCK=200-RH1
VARIABLE=TEMP &
  SENTENCE=PARAM
  DEFINE O2BT STREAM-VAR STREAM=202A
SUBSTREAM=MIXED &
  VARIABLE=TEMP
F  PRI2OT=O2BT-20
  READ-VARS O2BT
  WRITE-VARS PRI2OT

CALCULATOR UHOT
  DEFINE HTPRI1 BLOCK-VAR BLOCK=100-URH
VARIABLE=TEMP &
  SENTENCE=PARAM
  DEFINE TOV1B STREAM-VAR STREAM=205H
SUBSTREAM=MIXED &
  VARIABLE=TEMP
F  HTPRI1=TOV1B
  READ-VARS TOV1B
  WRITE-VARS HTPRI1

CALCULATOR WLHTRXR
  DEFINE WHRXR BLOCK-VAR BLOCK=200-RXRH
VARIABLE=DUTY &
  SENTENCE=PARAM
  DEFINE TOUTH STREAM-VAR STREAM=FISS-IN
SUBSTREAM=MIXED &
  VARIABLE=TEMP
  DEFINE TINC STREAM-VAR STREAM=205F
SUBSTREAM=MIXED &
  VARIABLE=TEMP
F  WHRXR = 13*4.34615*((20)-(TOUTH-TINC))/
F  (ALOG((20)/(TOUTH-TINC)))
F
C  u=13
C  A=4.34615
C  20 was used for del_T1, to prevent taking log of a negative
number
C  the choice of del_T1 does not significantly alter the result for
C  Del_T log mena calc
  READ-VARS TOUTH TINC
  WRITE-VARS WHRXR

TRANSFER T-1

SET BLOCK-VAR BLOCK=100-WHTO VARIABLE=TEMP
SENTENCE=PARAM
EQUAL-TO STREAM-VAR STREAM=102D
SUBSTREAM=MIXED &
  VARIABLE=TEMP

TRANSFER T-2
  SET BLOCK-VAR BLOCK=100-WHTO VARIABLE=PRES
SENTENCE=PARAM
  EQUAL-TO STREAM-VAR STREAM=102D
SUBSTREAM=MIXED &
  VARIABLE=PRES

TRANSFER T-3
  SET STREAM-VAR STREAM=FISS-IN SUBSTREAM=MIXED
VARIABLE=TEMP
  EQUAL-TO BLOCK-VAR BLOCK=100-RXR
VARIABLE=TEMP &
  SENTENCE=PARAM

CONV-OPTIONS
  PARAM TEAR-METHOD=DIRECT TOL=0.001 SPEC-
METHOD=SECANT &
  COMB-METHOD=BROYDEN MSPEC-
METHOD=BROYDEN SPEC-LOOP=INSIDE &
  TEAR-VAR=YES
  SECANT BRACKET=YES

STREAM-REPOR MOLEFLOW

PROPERTY-REP PARAMS PCES PARAM-PLUS

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