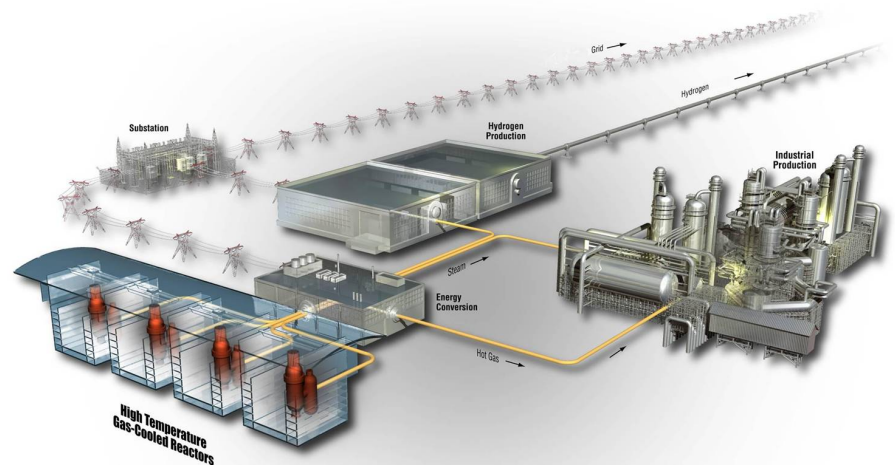**Technical Evaluation Study**

Project No. 23843

Integration of HTGRs and an Ex Situ Oil Shale Retort
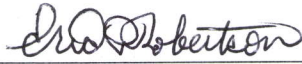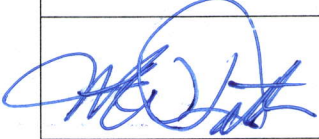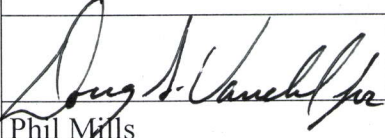
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NGNP Project	Technical Evaluation Study (TEV)	eCR Number: 587004

Signatures

Signature and Typed or Printed Name	Signature Code	Date (mm/dd/yyyy)	Organization/Discipline
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Rev.	Date	Affected Pages	Revision Description
0	12/13/10	All	Newly issued document

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1. Acronyms

API	American Petroleum Institute
ATP	Alberta Taciuk Processor
Btu	British thermal unit
CO	carbon monoxide
CO_2	carbon dioxide
DOE	Department of Energy
FA	Fischer assay
H_2	hydrogen
HTGR	high-temperature gas reactor
H_2S	hydrogen sulfide
MMSCFD	million standard cubic feet per day
MWe	megawatt (electric)
MWth	megawatt (thermal)
scf	standard cubic foot
SO_2	sulfur dioxide
TEV	technical evaluation
tonne	metric tonne (1000 kg)
ton	U.S. short ton (2000 lb)

2. INTRODUCTION

This technical evaluation (TEV) addresses potential integration opportunities for single or multiple high temperature gas-cooled reactor (HTGR) modules with production of oil from an ex situ oil shale retorting process. It has been prepared as part of a study for the Next Generation Nuclear Plant (NGNP) Project to evaluate integration of HTGR technology with conventional chemical processes. The NGNP Project is being conducted under U.S. Department of Energy (DOE) direction to meet a national strategic need identified in the *Energy Policy Act of 2005* to promote reliance on safe, clean, economic nuclear energy and to establish a greenhouse-gas-free technology for the production of hydrogen. The NGNP represents an integration of high-temperature reactor technology with advanced hydrogen, electricity, and process heat production capabilities, thereby meeting the mission need identified by DOE. The strategic goal of the NGNP Project is to broaden the environmental and economic benefits of nuclear energy in the U.S. economy by demonstrating its applicability to market sectors not being served by light water reactors.

An HTGR module produces process heat (steam or high-temperature helium), electricity, and/or hydrogen. An HTGR outlet temperature of 750°C for the primary fluid loop is assumed for this study, which reflects the initial HTGR design and assumes a conservative outlet temperature; temperatures of 950°C are anticipated for advanced HTGR designs. The output from a single HTGR module is assumed to be 600 MWth. A 25°C temperature approach is also assumed for the heat exchanger between the primary and secondary fluid loops.

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In conventional chemical processes, process heat, electricity, and hydrogen are generated by the combustion of fossil fuels such as coal and natural gas, resulting in significant emissions of greenhouse gases such as carbon dioxide (CO_2). An HTGR could produce and supply these products to conventional chemical processes without generating any greenhouse gases. The use of an HTGR to supply process heat, electricity, or hydrogen to conventional processes is referred to as an HTGR-integrated process.

2.1 Integration of HTGRs with an Ex Situ Oil Shale Operation

This report describes how an HTGR could be integrated into an ex situ oil shale production operation. A future report will provide a preliminary economic analysis, comparing the HTGR-integrated process with the base concept of an ex situ oil shale production process.

Two fluids, high temperature helium and steam, were considered as working fluids in the secondary flow loop that supplies heat to the ex situ retort. Other heat transfer fluids are possible, but because this report relies on completed assessments by the NGNP working group, considering new heat transfer fluids is beyond the scope of this report. For this TEV, the HTGR module(s) is assumed to be physically located near the oil shale operation such that the heat lost during surface transport of the heating fluid is negligible. This TEV does not offer an assessment of the optimal siting of an HTGR battery with respect to an in situ oil shale retort operation facility. If an optimal siting assessment is desired, a separate study will be conducted that balances the distance between the two facilities to consider safety, heat loss, and licensing concerns.

2.2 Oil Shale Background

The oil resource within the Green River Formation oil shale deposits in Colorado, Utah, and Wyoming is over 3 trillion barrels (Johnson et al. 2010a; Johnson et al. 2010b; Bartis et al. 2005). The total recoverable oil from this resource is estimated to be about 1.4 trillion barrels (Bartis et al. 2005), which greater than the 1.1 trillion barrels of total historical world oil production (BP, 2010). Comparing these historical and potential oil recoveries shows that the oil shale recoverable resource is very, very large and that commercial oil production from oil shale will likely continue for many decades and perhaps centuries due to the huge quantity of the resource.

The basis for this evaluation is an ex situ oil shale production project producing 50,000 bbl/day of shale oil, the product being ready for transport via pipeline to a local refinery. This analysis assumes that refining capacity exists in the region to accept the shale oil produced from the operation.

There are commercial ex situ oil shale operations internationally, but none in the United States. The current state of the ex situ oil shale industry is the commercial

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stage in Estonia, China, and Brazil, but new and more advanced methods and technologies are being considered for deployment in the United States, Jordan, and Australia. Numerous reports and analyses have been written and performed from which to draw the parameters necessary to perform an analysis of an ex situ oil shale production operation and its integration with an HTGR. A large-scale, commercial ex situ oil shale industry in the U.S. may emerge within the next 10 to 15 years at the earliest, depending on energy prices, regulatory climate, and public support. Development and deployment of a commercial HTGR may also require 10 to 15 years. Thus, this conceptual study of integrating an HTGR with an ex situ oil operation is timely.

3. PROCESS MODELING

For the purposes of this evaluation, production from an ex situ oil shale operation is assumed to be located in the western U.S. within the boundaries of the Piceance, Uinta, or Green River basins in areas where favorable stripping ratios exist and open pit mining methods can be used. Two cases were identified for modeling:

1.   A base case assumes the oil shale ore is mined in open pit mines, retorted using Alberta Taciuk Processor (ATP) technology with heat being provided by the combustion of the spent shale and produced hydrocarbon gas, and then upgraded. All electricity and hydrogen needs are supplied by outside sources.

2.   An HTGR-integrated case, which is the same as the base case except all heat, electricity, and hydrogen are supplied by an HTGR.

3.1 Base Case Process Model

Oil shale ore is mined from open pit mines located near the retort kiln. All mining equipment and machinery is powered by electricity purchased from the grid.

The rotating, horizontally-oriented ATP kiln is an advanced retorting process and is currently being commercially employed in China and demonstrated in Australia (Johnson et al. 2004; Li et al. 2010). The ATP kiln is illustrated in Figure 1.

Mined ore is fed into the ATP kiln by conveyor. The shale enters a preheat zone where the ore is heated from ambient temperature to about 250°C where water is vaporized and extracted from the process and condensed. The preheated shale enters the retort zone at 250°C and is heated to 500°C where the kerogen is pyrolyzed to form a mixture of hydrocarbon vapors and char. The hydrocarbon vapor stream consists of noncondensable gases and condensable raw shale oil. The char remains on the solid retorted shale particles and passes into the combustion zone where it is mixed with air and recycled hydrocarbon gases and is burned to a temperature of about 750°C. The calcite and dolomite in the shale substrate decompose between 600 and 700°C, releasing additional CO_2 in the flue

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gas stream. The combustion of the char and hydrocarbon gases provides the heat for the retort zone and the preheat zone. The hot spent shale (shale that has been retorted and combusted) cools as it transfers its heat to the incoming ore and is further cooled by water spray as it exits the processor (BLM 2007).
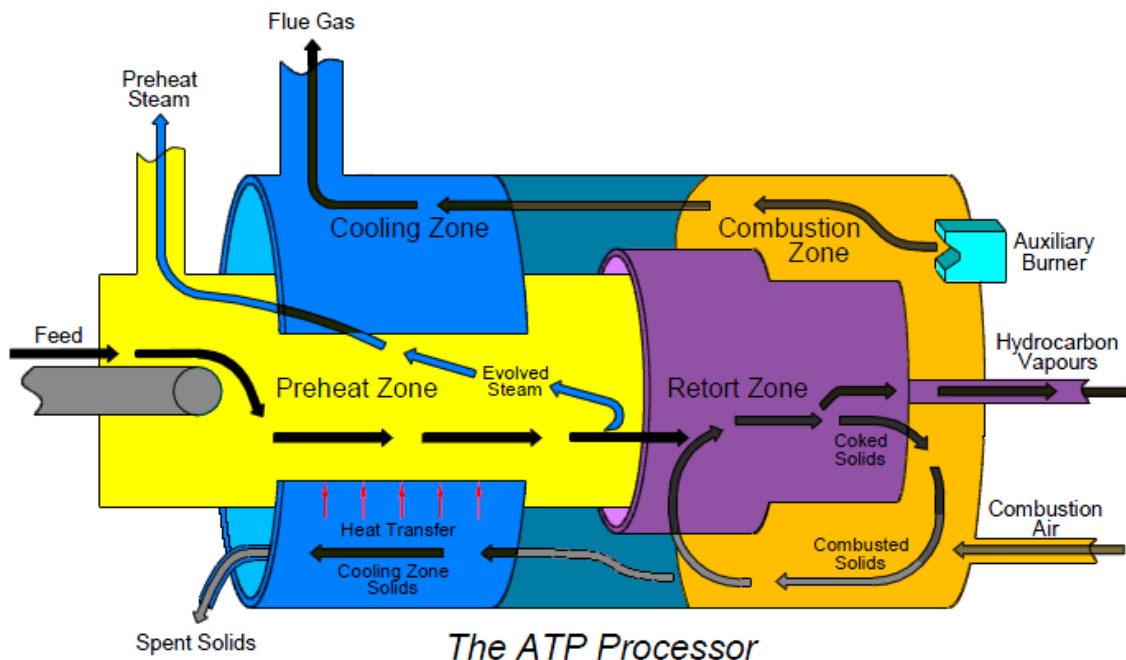

Figure 1. Base case ex situ retort process schematic employing an ATP retort (UMATAC 2008).

The condensable raw shale oil product leaves the ATP with a density of about 19 degrees API[a] (Vinegar 2006) and must be upgraded by hydrotreating to stabilize it and improve its quality before transport via pipeline to a refinery (Brandt 2007). For clarity, this raw shale oil, before hydrotreating, is called ATP-oil and the upgraded oil after hydrotreating is called refinery-ready oil. Hydrotreating the ATP-oil increases the API gravity to about 38 degrees and lowers its pour point to acceptable pipeline limits as well as reduces the nitrogen and sulfur concentrations (Utah 2007).

The noncondensable gases produced in the process vary in composition, depending on the oil shale, but are approximately 35% hydrocarbons, 18% H_2, with the remainder consisting of CO_2, CO, and H_2S (Brandt 2007). This gas stream is recycled into the ATP as needed for retorting heat. Any remaining gas will be sold as a commodity.

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[a] API (American Petroleum Institute) gravity is a common measure of the density of refinery feed stocks or crude oil and has units of degrees API. It is related to specific gravity: $°API = 141.5/\gamma - 131.5$, where γ is the specific gravity of the oil.

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A block flow diagram for the base case (ATP) ex situ oil shale operation is shown in Figure 2. Inputs include electric power, air, natural gas, and hydrogen. Outputs include flue gas, water, natural gas, spent shale, and refinery-ready oil. Electricity use for other processes is minor and is not shown in the figure, but is included in the analysis for electricity needs. Even though not all ore mining activities will be powered by electricity, all energy inputs for the mining portion are converted to electrical power in order to cleanly account for total energy inputs.
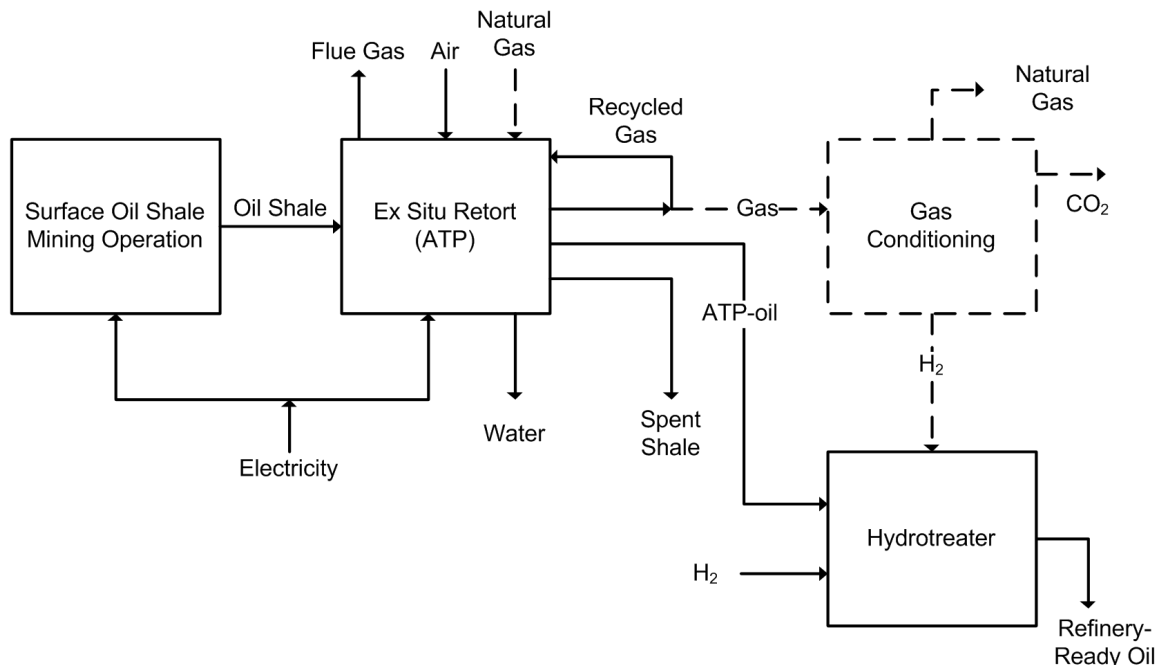

Figure 2. Block flow diagram for the base case ex situ retort using the ATP retort.

The dashed lines in Figure 2 represent equipment and flow lines that may or may not be required depending on the grade of the oil shale. If the oil shale ore is not rich enough in kerogen, not enough char and combustible gas will be generated to provide sufficient heat for the retort. The richness of the oil shale is indicated by its Fischer Assay (FA)[b] grade. If the FA grade is too low, then excess gas is not produced, the gas conditioning plant would not be needed, and additional natural gas (combusted to provide heat) and hydrogen (for the hydrotreater) would need to be purchased. The oil shale grade that results in excess heat and gas will be discussed in greater detail in Section 5.

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[b] The Fischer Assay, or FA, grade is commonly used in the oil shale industry to represent the richness or energy density of a given oil shale deposit. The FA grade when combined with a production efficiency specific to a particular retorting technology results in an estimate of the performance of a full scale retort (see process assumptions in Table 1).

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3.2 HTGR-Integrated Case Process Model

A block flow diagram for the HTGR-integrated ex situ oil shale operation is shown in Figure 3. Inputs include raw oil shale, electricity from the HTGR, and hydrogen from the HTGR via high temperature steam electrolysis. Outputs include water, natural gas, spent shale plus char, and refinery-ready stabilized shale oil. Items in red represent components associated/supplied by an HTGR. Electricity use for the gas conditioning plant and other processes is minor and is not shown in the figure, but is included in the analysis for electricity needs.
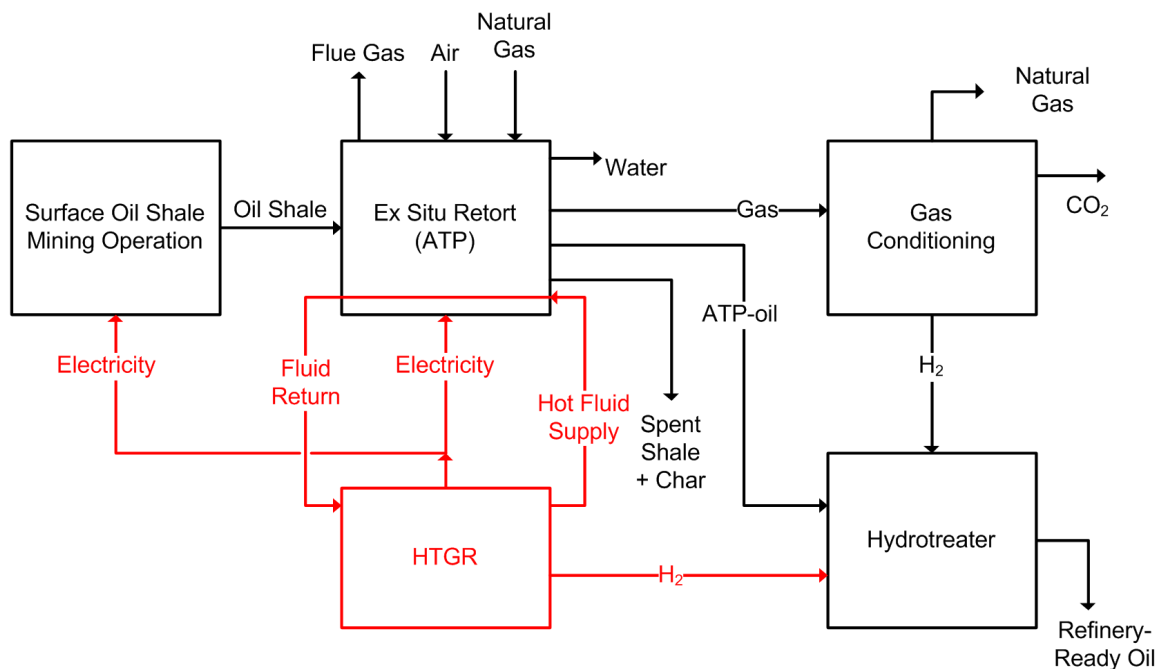

Figure 3. Block flow diagram for an HTGR-integrated ex situ oil shale retort operation.

For the HTGR-integrated case, the retorting heat is supplied by the HTGR to the ATP retort kiln in the form of hot gas. Specific heat transfer gases are discussed in Section 6.3.

The ATP technology would be modified in the HTGR-integrated case. High-temperature helium produced by the HTGR would replace the combustion of char and combustible gases to produce the heat necessary for the retort. In this case, the spent shale, coated with char, would be ejected from the retort as an output stream at 500°C (the retort temperature). CO_2 resulting from the decomposition nahcolite is included in the analysis, but CO_2 resulting from the decomposition of the carbonate material in the oil shale ore is not included because the temperature remains below the carbonate decomposition temperature of 600°C.

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4.   PROCESS ASSUMPTIONS

Assumptions used in ex situ oil shale retorting process calculations are shown in Table 1. An Excel™ spreadsheet was used to calculate the process results based on the inputs shown in the table. Calculations used in the spreadsheet are described in Appendix A.

Table 1. Major process assumptions for ex situ oil shale retort operation.

Model Input	Value	Units	Reference
Refinery oil rate	50,000	bbl/day	Assumed
Upgrading Yield	1.022	vol/vol	Bunger, 2004
Hydrogen requirement	1,350	scf/bbl	Fenton et al., 1981
Fischer Assay (FA) Grade	30.0	gal/ton	BLM, 2007
FA efficiency	0.92	vol/vol	BLM, 2007
Oil fraction	0.531	g/g kerogen	Schmidt, 2003
Gas fraction	0.176	g/g kerogen	Schmidt, 2003
Char fraction	0.209	g/g kerogen	Schmidt, 2003
Heat Content in Oil	5,900,000	Btu/bbl	TEV-1029, 2010
Heat Content in Gas	686	Btu/scf	Brandt, 2007
Heat Content in Char	4,354,121	Btu/ton	Yan, 2009
Water density	5.714	bbl/ton	Assumed
ATP oil density	0.940	g/mL	Vinegar, 2006

5.   PROCESS RESULTS

The two cases of an ex situ oil shale retort operation described Section 3 were modeled and results are described in this section. Both cases require 915 MWth to retort (718 MWth) and upgrade (197 MWth) the 74,444 ton/day of raw oil shale ore feed, and each case produces 50,000 bbl/day of refinery ready, 38° API crude oil. Assuming a commercial size for the ATP retort kiln of 500 tonne/hr (UMATAC 2008), 5.6 ATP kilns are required to process the ore.

In addition to the thermal requirements, the base case requires 289 MWe of equivalent electric power for mining, retorting, and other miscellaneous operations and the HTGR-integrated case requires 362 MWe or 73 MWe more than the base case to circulate heat transfer fluids. In the base case, electric power is purchased from the grid and in the HTGR case, the electricity is supplied by the HTGR.

Total hydrogen requirement for both cases is 66,000,000 scf/day. All the hydrogen in the base case is combusted to generate retorting heat using the input values in Table 1 and all

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the hydrogen needed for the upgrader is purchased from an outside source. In the HTGR case, 14,800,000 scf/day is available from the produced gas stream with the remainder (51,200,000 scf/day) being produced from a high-temperature steam electrolysis unit.

Carbon dioxide emissions for the base case are quite a bit higher than the HTGR case. The base case emits 19,700 ton/day of CO_2, while the HTGR case emits only 1,600 ton/day of CO_2.

Results for the two cases are compared and listed in Table 2.

Table 2. Major output results for the two cases considered in this evaluation for ex situ oil shale retorting.

Model Output	Base Case	HTGR-Integrated Case
Total heat required	915 MWth	915 MWth
Electricity required	289 MWe	362 MWe
Make-up hydrogen needed	66 MMSCFD	51 MMSCFD
Carbon dioxide emitted	19,700 ton/day	1,600 ton/day

6. DISCUSSION OF RESULTS

This section discusses how the richness of the shale ore (FA grade) affects the selection of surface equipment, and the integration of an HTGR

6.1 Richness (Fischer Assay Grade) of oil shale deposit

The assumed FA grade of 30 gal/ton produces nearly enough combustion products to supply the required combined retort and upgrading heat (94%). The remaining heat requirement (6%) is supplied by combusting purchased natural gas. Because no surplus gas is produced, the gas conditioning facility shown in Figure 2 (with dashed lines) is not necessary. A grade of 32 gal/ton or above is needed to supply the total required thermal energy. Mineable oil shale deposits range in grade up to 50 gal/ton (Dyni 2006). Even though the oil shale grade can change significantly on a small scale, the average oil shale grade taken from a large mine is not expected to be significantly higher than 32 gal/ton. Thus, the probability for needing a gas conditioning facility to process surplus gas for sale is expected to be small and the gas conditioning facility is not included in the final design of the base case ex situ oil shale retort operation. A gas conditioning plant is required for the HTGR-integrated case to remove impurities and separate hydrogen for use in the upgrading process.

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6.2 Flue gas (base case only)

The gas produced from the retort is composed mainly of light hydrocarbons, hydrogen, carbon monoxide, carbon dioxide, and hydrogen sulfide. The flue gas exiting the ex situ retort is the result of combusting produced gas and char plus supplemental natural gas. Combustion of these gases results in a flue gas rich in N_2, H_2O, CO_2, and SO_2. Treatment of the flue gas stream before atmospheric release to remove SO_2 and CO_2 is assumed, but not included in this evaluation.

6.3 Integration of HTGR technology to ex situ oil shale retort operations

The HTGR-integrated case uses heat in the form of hot gas produced from an HTGR as a substitute for the heat derived from combusting purchased and produced gas and char. A gas conditioning plant is necessary in this case because the produced gas will be sold after removing non-hydrocarbon impurities such as H_2, CO, CO_2, and H_2S. The hydrogen produced from the retort and separated in the gas conditioning plant is used to meet some of the requirement for the hydrotreating facility, thus reducing the amount required from the HTGR. The char coating the spent shale is assumed to be buried along with the spent shale as mine fill.

An HTGR-integrated case is composed of two heat transfer loops. The primary loop, containing helium, removes heat from the HTGR and transfers it to a secondary loop containing helium, steam, or other appropriate fluid. This secondary loop feeds into a modified ATP retort kiln where it transfers it heat to the oil shale ore such that it is pyrolyzed and forms oil, gas, and char.

Helium, steam, and nitrogen were analyzed for fluids in the secondary loop. The temperature of each fluid as it enters the retort kiln was 500°C and the pressure drop through the retort kiln was small. Results are shown in Table 3.

Table 3. Analysis of secondary loop fluids for HTGR integration with a modified APT retort operation.

Secondary Loop Fluid	T_{out} (°C)[a]	P_{ave} (psia)[b]	Flow rate (lbm/hr)	HTGR output (MWth)[c]
Helium	60	1,150	3.2E6	833
Steam	285	2,300	3.7E6	889
Nitrogen	60	830	14.8E6	840

[a] Fluid temperature as it come out of ATP retort kiln.

[b] Average fluid pressure in the kiln.

[c] HTGR output necessary to supply 915 MWth to retort operation.

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The HTGR output required for the thermal needs of an ex situ retort operation is roughly the same regardless of which fluid is selected for the secondary heat transfer loop. For each case the HTGR output is less than the 915 MWth needed because the circulators used to compress the gases add heat to the system, reducing the thermal required thermal output of the HTGR.

There may be some operational concerns, however, with the use of any of these gases and especially with steam in the secondary loop. The ATP kiln as currently designed, is run a slightly below atmospheric pressure and it would need to be redesigned in order to handle the much higher pressures anticipated when integrating an HTGR. Additionally, if steam were the secondary loop fluid, it comes out of the retort kiln as a condensed, sub-cooled liquid and flow through the kiln would need to be augmented by inclining the kiln such that the ore feed and steam outlet end is lower than the spent shale outlet and steam inlet end. The ATP retort kiln is currently configured to be strictly horizontal and it is unknown whether modifying its inclination in this manner would impede the retort process or lower its efficiency.

The total thermal output required from an HTGR in an integrated system is obtained by summing the thermal energy, electricity, and hydrogen needs of the ex situ oil shale retort operation. Table 4 lists the retort needs and the corresponding HTGR output necessary to supply those needs. Because of the uncertainty in the analysis and to be conservative, the reactor heat required is set equal to the process heat needed instead of using the HTGR output shown in Table 3.

Table 4. Process needs for a 50,000 bbl/day ex situ oil shale retort operation and the corresponding reactor heat required to meed those needs.

Operational Need	**Quantity Needed**	**Reactor Heat Required, MWth**	**Number of HTGR Modules**
Process Heat	915 MWth	915	1.53
Electricity	362 MWe	815[a]	1.35
Hydrogen	51.2 MMSCFD	466[b]	0.78
Total		2,196	3.66

[a]Assuming 44.4% Rankine cycle efficiency (INL 2010a).

[b]Assuming 65.9 MMSCFD per 600 MWth Reactor Heat (INL 2010a).

The total reactor heat required to supply the process heat, electricity, and hydrogen needs for a 50,000 bbl/day ex situ retort operation is 2,196 MWth or 3.66 HTGR modules with capacities of 600 MWth each.

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7.   SUMMARY

Results of major inputs and outputs are shown in Figure 4 for both cases. The main differences between the two cases is the usage of the combustible gases and char and the amount of CO_2 produced. The base case uses the produced gases and char to generate the retort heat, which increases the emissions of CO_2. The HTGR-integrated case sells the conditioned gas and greatly reduces the CO_2 emissions by supplying heat from the HTGR modules and eliminating fossil fuel combustion and carbonate mineral decomposition. In this evaluation, hydrogen and electricity used by the retort are assumed to be supplied by the HTGR modules.
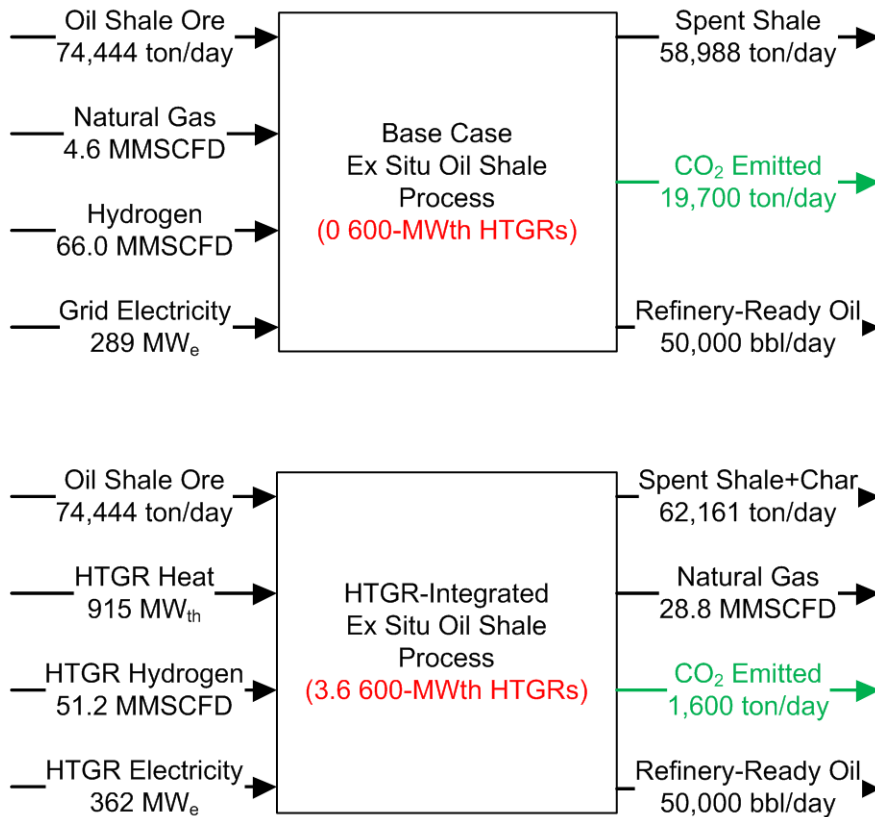
Figure 4. Major inputs and outputs for the two ex situ oil shale retort cases evaluated.

A steady source of heat will be needed for the ex situ retort process. If the HTGR and the oil shale retort operation are linked, one would have to be shut down if the other was taken off line for repairs, refueling, etc. Redundancy and planning for scheduled or unscheduled down time would be an important part of designing an integrated operation.

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8.   FUTURE WORK AND RECOMMENDATIONS

Future work will consist of incorporating an economic analysis to both of the cases considered in this document.

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10. APPENDIX A – Documentation of Calculations

This document lays out and explains the data required and calculations used to determine the amount of oil produced, heat required, electricity required, and carbon dioxide generated from an ex situ oil shale retorting operation employing the ATP technology and an alternative case where HTGR technology is used to supply heat, electricity and hydrogen to an ex situ ATP retort.

10.1 Required data

The required data are listed in this section. Table 5 lists some of the required data and their source.

Table 5. Data used as input for the Excel spreadsheet model.

Inputted values	Expression	Value	Units	Reference
Refinery-ready oil rate	q_o	5.0E4	bbl/day	Basis for evaluation
Upgrading Yield	Y_u	1.022	vol/vol oil	Bunger, 2004
Hydrogen Requirements	R_h	1.35E3	scf/bbl	Fenton, 1981
Fischer Assay Grade	G_{FA}	30.0	gal/ton shale	BLM, 2007
FA efficiency	η_{FA}	0.92	vol/vol FA	BLM, 2007
Oil fraction (mass basis)	F_o	0.531	g/g kerogen	Schmidt, 2003
Gas fraction (mass basis)	F_g	0.176	g/g kerogen	Schmidt, 2003
Char fraction (mass basis)	F_c	0.209	g/g kerogen	Schmidt, 2003
Heat Content in Oil	H_o	5.9E6	Btu/bbl oil	Value for generic crude oil
Heat Content in Char	H_c	4.354E6	Btu/ton char	Yan and Junwei, 2009
ATP oil API gravity	°API	19.0	°API	Vinegar, 2006

The molecular components of the gas and its composition are given in Table 6.

Table 6. The molar composition of the gas generated during the retorting of the oil shale using ATP technology.

Component	Mole fraction*	Gross heating value, Btu/scf
light HCs	0.3500	1100
H2	0.1800	292.2
CO	0.1567	242.3
H2S	0.1567	1346.9
CO2	0.1567	0
* Brandt, 2007		

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The composition of the retort product given as fractions of an original mass of raw oil shale is shown in Table 7.

Table 7. Mass fraction of retort products based on the mass of a given volume of raw oil shale using ATP technology.

Retort product	Mass fraction[a]
ATP oil	0.102
ATP gas	0.046
Spent shale	0.835
Water	0.016

[a] Utah, 2007

The energy requirements for the whole operation are listed in Table 8. These values were reported by Brandt (2009).

Table 8. Processes associated with ex situ retorting oil shale and their respective energy requirements

Process	Energy requirement (MJ/t raw shale)
Preliminary operations	1.0
Mining	318.5
Transportation from mine	16.5
Crushing	12.0
Startup	22.0
Retort - electricity	452.0
Retort - heat	918.5
Upgrading	251.5

10.2 Calculations section

The molecular weight and the gross heating value of the gas produced during the retort process are calculated from the data given in Table 6. The molecular weight is the sum of the products of the mole fraction and the molecular weight of each component:

$$M_g = \sum_{i=1}^{n} F_{m_i} M_i = 23.284 \frac{g}{mole} \; ;$$

where M_g is the molecular weight of the gas, F_{mi} is the molecular fraction of each component of the gas, M_i is the molecular weight of each component, n represents number of gas components, and I represents each component of the gas.

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The heat content of the gas produced during the retort process is the sum of the products of the mole fraction and the gross heating value of each component:

$$H_g = \sum_{i=1}^{n} F_{m_i} GHV_i = 686.571 \frac{Btu}{scf} \; ;$$

where H_g is the heat content of the gas and GHV_g is the gross heating value of the gas.

The gas density (ρ_g) is calculated from the molecular weight:

$$\rho_g = 23.284 \frac{g}{mole} \left| \frac{lbm}{453.4 \, g} \right| \frac{mole}{22.4 \, L} \left| \frac{L}{1000 \, mL} \right| \frac{16.387 \, mL}{in^3} \left| \frac{1728 \, in^3}{ft^3} \right| = 0.065 \frac{lbm}{scf} .$$

Oil density is calculated from the API gravity that is given in Table 5.

$$\rho_o = \frac{141.5}{131.5 + °API} = \frac{141.5}{131.5 + 19} = 0.940 \frac{g}{mL} .$$

10.2.1 Heat from oil, gas, and char fractions

Kerogen in the oil shale is converted to oil, gas, and char during retorting. The heat contained in the kerogen that is converted to oil (H_{ko}) is calculated by:

$$H_{ko} = \frac{F_o H_o}{1.5899E5 \rho_o} = 20.959 \frac{Btu}{g} \; ;$$

where the constant 1.5899E5 is a conversion factor with units of mL/bbl. The heat contained in the kerogen that is converted to gas (H_{kg}) is calculated by:

$$H_{kg} = \frac{F_g H_g}{454.545 \rho_g} = 4.105 \frac{Btu}{g} \; ;$$

where the constant 453.6 is a conversion factor with units of g/lbm. The heat contained in the kerogen that is converted to char (H_{kc}) is calculated by:

$$H_{kc} = \frac{F_c H_c}{9.072E5} = 1.003 \frac{Btu}{g} \; ;$$

where the constant 9.072E5 is a conversion factor with units of g/ton. Total unit energy in the kerogen (H_{kt}) is the sum of the energy in the oil, gas, and char:

$$H_{kt} = H_{ko} + H_{kg} + H_{kc} = 26.067 \frac{Btu}{g} .$$

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Knowing the amount of energy (heat) created by the kerogen in the form of oil, gas, and char, the fractions of the total energy can be calculated. The fractions of heat as oil (F_{Ho}), gas (F_{Hg}), and char (F_{Hc}) are:

$$F_{Ho} = \frac{H_{ko}}{H_{kt}} = 0.804 \frac{Btu}{Btu} \; ;$$

$$F_{Hg} = \frac{H_{kg}}{H_{kt}} = 0.157 \frac{Btu}{Btu} \; ;$$

$$F_{Hc} = \frac{H_{kc}}{H_{kt}} = 0.038 \frac{Btu}{Btu} \; .$$

10.2.2 Production rates
The liquid oil as it is produced from the ATP retort is upgraded in a hydrotreater to create a liquid that is pipeline-quality and a high-quality refinery feedstock. To differentiate between the two liquids, the effluent oil from the ATP is called ATP oil, while the effluent from the hydrotreater is called refinery-ready oil. During the hydrotreating process, the volume of the oil increases slightly because of the addition of hydrogen and a reduction of its density. ___The basis for all production rates and heat requirements is 50,000 bbl/day of refinery-ready oil.___

10.2.2.1 ATP-Oil production rate
The ATP-oil production rate (q_{ATPo}) is calculated by:

$$q_{ATPo} = \frac{q_o}{Y_u} = 48,921 \frac{bbl}{day} \, .$$

10.2.2.2 Total gas produced during retort
The total gas production rate, which includes non-hydrocarbon gases, is calculated by:

$$q_g = q_{ATPo} \frac{H_o F_{Hg}}{H_g F_{Ho}} = 82,343,000 \frac{scf}{day} \, .$$

10.2.2.3 Natural gas production rate
The natural gas production rate (q_{ng}), which includes only the hydrocarbon portion of the produced gas stream is the product of the total gas rate (q_g) and the mole fraction of the produced gas that is hydrocarbons (F_{HC}, from Table 6):

$$q_{ng} = q_g F_{HC} = 28,820,000 \frac{scf}{day} \, .$$

10.2.2.4 Production of char
The amount of char produced per day is calculated by:

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$$q_c = q_{ATPo} \frac{H_o F_{Hc}}{H_c F_{Ho}} = 3{,}173 \frac{ton}{day}.$$

10.2.2.5 Raw oil shale ore required

The amount of raw oil shale ore per day (q_s) required for these production rates as feed into the ATP retort is:

$$q_s = 42 \frac{q_o}{Y_u \eta_{FA} G_{FA}} = 74{,}444 \frac{ton}{day}.$$

10.2.2.6 Spent shale produced

The amount of spent shale produced from the ATP retort (q_{ss}) is the product of the amount of raw oil shale ore per day (q_s) and the mass fraction of the spent shale (F_{ss}, from Table 7):

$$q_{ss} = q_s F_{ss} = 62{,}161 \frac{ton}{day}.$$

10.2.2.7 CO$_2$ produced

Brandt (2009) examined the amount of CO_2 emitted during operations associated with an ATP retort. He presented a low CO_2-producing scenario and a high CO_2-producing scenario. In this evaluation, the average of the two scenarios is used. This evaluation does not consider any CO_2 emitted after the product is refinery-ready oil, whereas Brandt considered the CO_2 emitted from during refining of the oil and during combustion of the final product is transportation vehicles. Additionally, Brandt uses the heat content of the refined product as the basis for his CO_2 analysis and this evaluation uses the heat content of the refinery-ready oil as the basis for the CO_2 analysis. The processes involved with retorting oil shale using ATP technology and their CO_2 emissions are shown in Table 9.

Table 9. Grams CO_2 emitted per megajoule (MJ) of refinery-ready oil for the four processes associated with retorting oil shale using ATP technology.

Process	CO$_2$ emitted (g/MJ of refinery-ready oil)	
	Base case[a]	HTGR-integrated case
Mining and miscellaneous energy use	7	3.5
Heating the oil shale to retort temperature	29	0
Mineral decomposition	20	1.3[b]
Upgrading the ATP-oil to refinery-ready oil	1.5[c]	0
Total	58	20

[a] Average values from Brandt (2009), Figure 2.
[c] Back calculated from formula given in INL (2010).
[b] Applies the upgrading/refining energy-required ratio (0.131) from Table 2 of Brandt (2007) to calculate the emissions for upgrading alone.

CO_2 emissions values for the base case as well as the HTGR-integrated case are shown in the table. The HTGR-integrated case is assumed to have ½ the CO_2 emissions from mining and

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miscellaneous energy use because half of the mining equipment is assumed to use electric power. The CO_2 emissions for the base case and the HTGR case are much different because the base case includes CO_2 emitted from nahcolite and carbonate decomposition, whereas the HTGR case includes only decomposition of the nahcolite. The HTGR case has no CO_2 emissions from heating the oil shale to retort temperature, no any resulting from the upgrading step because the heat, electricity, and hydrogen inputs are supplied by the CO_2-free HTGR.

has no, heating the oil shale to the retort temperature, or upgrading the ATP-oil to refinery-ready oil because all the energy and hydrogen supplied to these processes comes from the HTGR, not from fossil fuel-based energy. The total CO_2 emissions (E_c) for the base case are 58 g/MJ and emissions for the HTGR-integrated case are 20 g/MJ.

Brandt (2007) states that the heating value of the upgraded shale oil (refinery-ready oil) is nearly equal to that of raw shale oil (ATP-oil). The refinery-ready oil is assumed to have the same heat content as ATP-oil. The value for the heat content of the oil (H_o) is 5.9E6 Btu/bbl (see Table 5). The total rate of CO_2 emission (q_c) for the base case is calculated by:

$$q_c = \frac{E_c H_o q_o}{8.597E8} = 19{,}731 \frac{\text{ton}}{\text{day}} \;;$$

where the constant 8.597E8 is used to convert g-Btu/MJ to tons. The CO_2 emissions rate for the HTGR-integrated case is 1,647 ton/day.

10.2.3 Energy required
Both thermal energy and electrical energy are required for the ex situ retort operation. The thermal energy requirements are a combination of the retorting process and the upgrading process. The electrical energy requirements include all the mining processes as well as electricity used to operate the retort kiln.

10.2.3.1 Thermal energy
The thermal energy required to retort enough shale to produce 50,000 bbl/day of refinery-ready oil is calculated by multiplying the retort heat (see Table 8) by the mass of mined oil shale ore. Making this calculation, the thermal energy required for the retort is 718 MWth.

The thermal energy required by the upgrading process is calculated by multiplying the upgrading heat requirement listed in Table 8 by the mass of the mined oil shale ore. The energy required for upgrading the ATP-oil to refinery-ready oil is 197 MWth.

The total thermal energy required is the sum of the retort thermal energy and the upgrading thermal energy, or 915 MWth.

10.2.3.2 Electrical energy
Processes using electrical energy include mining, transporting the ore to the crushers and on to the retort kiln, crushing the ore, surface facility supply, and turning of the rotary retort kiln. Even though not all mining activities will be powered by electricity, Brandt (2009) converts all

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energy inputs for the mining portion to electrical power in Table 8 in order to cleanly account for total energy inputs. Accordingly, the electrical energy requirements were converted from thermal energy to electrical energy by multiplying each by a factor of 0.45, the efficiency assumed by Brandt (2009) to convert thermal energy to electrical energy.

The retort kiln requirement for a 50,000 bbl/day output of refinery-ready oil is calculated by multiplying the retort electricity requirement by the mass of the mined oil shale ore. The retort electricity requirement is 159 MWe.

The mining operation is calculated in the same manner resulting in an electric energy requirement of 112 MWe. Other processes are lumped together and include preliminary operations, transporting the ore, crushing the ore, and startup. Combining these items and multiplying by the ore production rate results in 18 MWe for the remaining electricity requirements.

The total electrical energy required is the sum of the needs of the retort kiln, mining, and other processes, or 289 MWe. For the base case, the electricity is purchased from the grid, while in the HTGR-integrated case, the electricity is supplied by the HTGR.

10.2.4 Hydrogen required
Hydrogen is needed for upgrading the raw ATP-oil to the refinery-ready oil before it leaves the ex situ oil shale retort operation site. The total hydrogen requirement (R_{ht}) is calculated by multiplying the hydrogen requirements (R_h) listed in Table 5 and the ATP-oil production rate (q_{ATPo}):

$$R_{ht} = R_h q_{ATPo} = 66{,}043{,}000 \, \frac{scf}{day} \; ;$$

10.2.4.1 Base case hydrogen requirements
In the base case, if enough hydrogen gas is generated from the retorting of the oil shale, it can be separated from that stream and used on site for the hydrotreating process to upgrade the ATP-oil. However, calculations show that the richness of the oil shale needs to be more than 35 gal/ton (the default value is 30 gal/ton) in order to produce enough hydrogen for use in the hydrotreating up grader. Therefore, for the base case all the hydrogen required for upgrading is purchased.

10.2.4.2 HTGR-integrated case hydrogen requirements
In the HTGR-integrated case, none of the hydrogen produced from retorting the oil shale is combusted to provide heat for the retort and all of it is available for use in upgrading. The amount of hydrogen produced during the retort is calculated by multiplying the total gas production rate (q_g) by the mole fraction of the gas that is hydrogen (see Table 6) or 0.18. Total hydrogen produced is calculated to be 14,822,000 scf/day, which is not enough to totally satisfy the hydrogen required by the upgrading process. The additional hydrogen requirement (total requirement minus produced hydrogen, or 51,221,000 scf/day) is supplied by the high temperature steam electrolysis associated with the HTGR.

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10.2.5 ATP trains

The largest ATP constructed or under plans for construction is a 500 tonne/hr kiln (UMATAC, 2008). Dividing the size of this operation by the 500 tonne/hr train size gives us the number of ATP kilns necessary for this operation, or 5.33 ATP kilns per 50,000 bbl/day output of refinery-ready oil.

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