Underground Coal Thermal Treatment as a Potential Low-Carbon Energy Source

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20 **ABSTRACT**

21 We evaluate a novel energy strategy, underground coal thermal treatment (UCTT); it involves
22 slowly pyrolyzing coal in-situ, transforming it to synthetic gas stream containing hydrogen and
23 low molecular-weight hydrocarbons, liquid fuel and char. This evaluation assesses the life-cycle
24 energy and greenhouse gas (GHG) impacts of UCTT for all process stages. It is based on
25 experimental results at two scales, a simple heat-transfer model and literature results. The results
26 show that UCTT can produce a high-quality liquid product and a gas mixture. UCTT's GHG
27 emissions are in the range of those reported for in situ processing of oil shale. Net energy returns
28 (NERs) of 0.48– 4.7 are in the range reported oil sands (2.8) and oil shale (0.48 – 2.6). Product
29 yield at low temperatures, heater temperature, the number of heaters and the moisture content of
30 the coal are key factors in determining the feasibility of the UCTT process.

31

1. INTRODUCTION

With current coal mining technologies and production rates, the US has approximately 270 years of coal reserves.¹ In addition to recoverable coal reserves, the US has vast coal resources, which are currently unrecoverable due to their depth, access, and other factors.² This provides an opportunity for an in situ technology to recover otherwise unrecoverable energy from coal. Although natural gas prices are at historic lows in the United States, price increases are projected, and prices will increase more rapidly with US natural gas exports.³ Furthermore, methane recovery from coal seams is common, but coalbed methane (CBM) produces less than 1% of a coal bed's energy content.⁴ In situ pyrolysis offers the possibility of substantially more energy recovery from the resource and the potential to convert the high-carbon content fuel into a lower carbon content, higher heating value syngas or liquid fuel.

Figure 1 shows an example of the UCTT concept. This novel in situ pyrolysis process, UCTT is proposed and evaluated. By slowly heating coal in-situ, the coal is transformed from long chain geopolymers to a synthetic gas stream containing gas and liquid products, and char. The coal contains native moisture as well as mineral matter, and these components are also heated but do not transform into valuable products. This process has the potential to leave large portions of the carbon from the coal in the ground in the form of char. Although UCTT requires additional energy input compared to CBM, the added resource utilization and carbon management may make this process worthwhile and motivates its evaluation.

UCTT differs significantly from underground coal gasification (UCG); it indirectly heats the coal to pyrolysis temperatures (200 - 600°C) rather than injecting air/oxygen mixtures to directly gasify the coal. UCTT offers several potential advantages over UCG including an improved ability to discontinue operations if needed and a reduced risk of subsidence. Several

organizations have investigated UCG⁵, and pilot studies have been performed in China⁶, Australia⁵, the US^{5,7}, and South Africa⁵. Although UCG research appears to be active in some countries, low oil prices have led to a decreased interest in UCG.

Although peer-reviewed studies of UCTT-type processes are limited, studies evaluating other in situ fossil fuel processes report life-cycle GHG emissions for the production of transportation fuels. These studies include thermal treatment of heavy oil, in situ production from oil sands and the Shell in situ conversion process (ICP) for oil shale conversion. As conventional sources of crude oil become scarce, transportation fuels are increasingly being produced from lower quality resources, like heavy oil and oil sands, and potentially oil shale. Brandt and Unnsach⁸ examined the energy intensity of thermally enhanced (steam injection) oil recovery of heavy oils in California. They report well-to-pump (WTP) greenhouse gas (GHG) emissions of 32 – 47g CO₂ e/MJ for gasoline produced from this resource (lower heating value, LHV). In comparison, well-to-wheels GHG emissions from conventional petroleum sources in the US are 18.1 g CO₂ e/MJ (US EPA 2009).⁹ Brandt and Unnsach⁸ found that the GHG emissions vary with energy demand of the heavy oil treatment (i.e., steam to oil ratio), choice of fuel used for steam generation, co-generation of electric power, and the electricity mix.

Brandt¹⁰ evaluated GHG emissions from the production of gasoline using the Shell ICP. This process heats an oil-shale field in situ, releasing liquid- and gas-phase fuels. Concerns over potential groundwater contamination led to the installation of a freeze wall to isolate the processing area from the water table. First, heater and producer wells are drilled. In the heating wells, electrical heaters heat the oil shale to 340 – 370°C over a period of several years. The liquid and gas fuels flow to the production wells for recovery. These products are then upgraded, transported, and refined into gasoline. The study reports GHG emissions of 38 – 63 g CO₂ e/MJ

gasoline. Work began on ICP in western Colorado in the 1980s, but activities in the US have ceased. However, work on this process continues in Jordan¹¹ and Israel¹².

In addition to studies of in situ processes to provide transportation fuels, researchers have proposed electricity production from oil shale with in situ carbon capture (EPICC). This method employs a solid fuel cell underground to heat a shale formation.¹³ The produced gas from this process flows back to the fuel cell to provide additional energy to generate electricity and to heat the formation. They report that EPICC's GHG emissions are 51 – 99 kg CO₂/MWh compared to 92-145 kg CO₂/MWhr for pulverized coal with carbon capture. This work is in the conceptual stages, and the authors cite EPICC's potential drawbacks including uncertain operation of subsurface fuel cells, potential geologic impacts without pressure management, and economic concerns associated with the value of stranded energy left in the formation and the long time period for retorting.

The goal of this study is to begin to understand the feasibility of a UCTT process, specifically by estimating UCTT's cradle-to-gate, life-cycle energy and greenhouse gas (GHG) emissions. The analysis includes the impacts of well drilling, heating the formation, recovery, cleanup, and transportation of the UCTT products. The energy required and product yields are based on experimental results and simulations that rely on the properties from the experiments.

2. MATERIALS AND METHODS

This study uses a simplified process model life-cycle assessment approach to determine energy and GHG emissions associated with UCTT. All results are presented on a LHV basis of the coal and products. Figure 2 shows the processes considered in the UCTT analysis. It is envisioned as a cradle-to-gate analysis with final products being transportation fuel (conventional gasoline) and electricity generated from the gas-phase products. The evaluation does not include the energy

and GHG emissions associated with the construction of the refineries and power plant or the manufacture of the drilling rig, the well casing, the well cement, or the associated fittings and equipment. The UCTT process transforms coal in the ground into char and two product streams: a two-phase liquid and a gas stream containing hydrogen and low molecular-weight hydrocarbons (typically less than C₄). While several options for heating a candidate formation exist, this analysis focuses on electrical heating of the formation. The gas-phase products are burned to reduce the purchased electricity needed to heat the formation. The liquid products are refined into a transportation fuel, conventional gasoline. As discussed in Section 3.2, UCTT will not likely produce sufficient gas-phase products to permit the sale of excess electricity.

The following subsections describe the resource, life-cycle stages, and other related processes.

2.1 Resource

This evaluation, including the experimental and simulation studies, is based on a Utah Sufco coal, a high-volatile, low-moisture bituminous coal. Table 1 shows the coal properties. The Sufco coal mine is located in Sevier County, UT in the Blackhawk Formation of the Wasatch Plateau coalfield; it is one of the longest continuously running underground long-wall mines in the US. It has approximately 126 million tons of recoverable resource and its annual production in 2012 was 5.7 million tons.¹⁴ Its average thickness is approximately, 3.5 m, although thicker portions of the seam exist, and the overburden depth ranges from 100 – 600 m.¹⁵

The evaluation assumes a 10 m thick seam of coal at a depth of 333 m; this hypothetical coal seam is sufficiently contiguous in the radial direction for the heat to be completely absorbed by the coal over the time period of interest. The seam is heated with a 10 m long, 0.25 m diameter heater. Only one well is drilled for the analysis; the heating well is also assumed to be the

producing well. The analysis assumes a formation pressure of 30 bar and a formation temperature of 20°C.

2.2 Drilling

For drilling the vertical well (a heating and producing well), diesel fuel consumption and well depth come from the Utah Division of Oil Gas and Mining Well Reports,¹⁶ and the average diesel consumption of 12.4 l/m for wells less than 3300 m deep is used. This value is in the range of reported fuel consumption of 18.6 l/m for well drilling.¹⁷

2.3 Heating the Formation

A preliminary analysis revealed that the energy needed to heat the formation and product yield are critical to the feasibility of UCTT, and these depend on the coal, char, and product properties. Consequently, much of this study focused on gathering experimental results to understand these key parameters. As discussed in the following sections, literature data provided energy requirements and GHG emissions for the other life cycle stages.

UCTT experiments were performed at two scales: scoping studies in a high-temperature, high-pressure, 1.9-cm diameter, fixed-bed reactor and larger scale studies in a 15-cm diameter, high-pressure, high-temperature rubblized-bed reactor.¹⁸ The scoping studies identified the most promising conditions as well as data for development of a yield model. The larger scale studies allowed for more representative product generation.

The composition of the gas- and liquid-phase products comes from GC and GC/MS analysis, respectively, of the products from the larger scale reactor. Although additional species are present in limited amounts, in the baseline case the gas-phase products are represented by: H₂ (3%, 25%), H₂O (7%, 7%), CO (10%, 6%), CH₄, (35%, 39%), C₂H₄ (7%, 4%), C₂H₆ (10%, 6%), and CO₂ (28%, 12%) (by weight and mole %, respectively).

For the uncertainty evaluation, the experimental ranges for the gas-phase species vary from H₂ (0.83 – 3.5%), CO (4.5 - 15%), CH₄, (25 - 39%), C₂H₄ (1.1 – 7.1%), C₂H₆ (7.2 - 11%), and CO₂ (29 - 49%) (by weight), and the ratio of liquid to total product ranges from 0.30 to 0.58 (by weight). Consequently, the LHV of the product mixture ranges from 1.22 x 10⁴ to 1.93 x 10⁴ kJ/kg.

The liquid products contain approximately 85% carbon, 11% hydrogen, 0.5% nitrogen and 2% sulfur (by weight, ranges not available). The elemental composition of the liquid is in the range of that reported for conventional crude oil.¹⁹ Figures A.2 - A.4 show the product's simulated distillation profile, crude oil's simulation profile, and the products single carbon number profile, respectively, and illustrate that the UCTT product is "light-crude like".

Additional measurements were performed to determine the heat capacity (C_p) and thermal conductivity of the coal and char. These properties are used in the simulations and discussed in the following subsection. Heat capacity for the coal and char were measured with a TA DSC-Q20 differential scanning calorimeter. The measured C_p values were 1.25 ± 0.04 J/g°C for the coal and 1.41 ± 0.36 J/g°C for the char. Details of the heat capacity measurements and uncertainty can be found in the Appendix. Thermal conductivity was inferred from the larger scale experimental results as described in the Appendix. As a function of temperature, the thermal conductivity of the aggregate char, product mixture is:

$$k = 3.37 \times 10^{-4} T + 0.19$$

where,

T= temperature, K.

k = thermal conductivity, W/m K.

All properties of interest – density, heat capacity, thermal conductivity and thermal diffusivity – change as a function of temperature and coal conversion, which is also a function of temperature. The temperature simulation and yield estimates assume that properties remain constant until 234°C, one degree above the temperature at which water boils at 30 bar. As coal is converted to char and liquid and gas products, the properties in the temperature simulation changed as a weighted average of the aggregate composition. The difficulty in obtaining properties for all product species at UCTT temperatures and the formation pressure led us to the assumption of a simplified product mixture of 30% CH₄, 30% CO₂, 30% C₂H₆, and 10% water (by weight). The liquid properties were based on the single-carbon number analysis of the liquid product (Figure A.4). The Peng-Robinson Polar properties in the ProMaxTM process simulator provided the liquid and gas properties as a function of temperature at 30 bar. The coal and char properties are based on the experimental measurements for heat capacity and thermal conductivity, described above. The coal and char specific gravities are 1.31 and 0.99, respectively.²⁰ Relationships for each of the properties and their uncertainties as a function of temperature can be found in the Appendix (Figure A.5 – A.8).

Thermal diffusivity was calculated using:

$$\alpha = \frac{k}{\rho C_p}$$

where,

k = thermal conductivity, W/m K.

ρ = density, kg/m³.

C_p = heat capacity, J/kg K.

The thermal diffusivity for coal is 1.76 x 10⁻⁷ m²/s at temperatures below 234°C when it begins to transform into char. The thermal diffusivity of the coal, char, and product aggregate at 600°C

is $1.14 \times 10^{-6} \text{ m}^2/\text{s}$. Literature values for thermal diffusivity of coal and char vary widely. Clendenin et al.²¹ summarize the effect of coal treatment temperature on coal/char properties and report the diffusivity of raw coal, approximately $1 \times 10^{-7} \text{ m}^2/\text{s}$, and char treated to 600°C , $3.5 \times 10^{-7} \text{ m}^2/\text{s}$. They also report that coal/char thermal diffusivity is constant until approximately 300°C . It then increases with temperature in the range of temperatures of interest to a UCTT process ($200 - 600^\circ\text{C}$). Figure A.8 shows the coal, char, and product aggregate thermal diffusivity and uncertainty estimates as a function of temperature.

The evaluation also considers an enhanced thermal conductivity case, in which the coal thermal conductivity is 0.87 W/m K^{22} and the char thermal conductivity is 1.7 W/m K^{23} . Wellington et al.²² reported that coal in situ had a higher conductivity than pulverized coal. This results in a coal diffusivity of $5.31 \times 10^{-7} \text{ m}^2/\text{s}$ and a weighted average coal, char, product diffusivity of $1.64 \times 10^{-6} \text{ m}^2/\text{s}$ at 600°C .

Temperatures were predicted as a function of time and distance from the heater using a one-dimensional unsteady heat conduction in cylindrical coordinates, given by:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) = \frac{1}{\alpha} \frac{\partial T}{\partial t}$$

Where:

r = radius, m, with radial steps of 0.25 m.

t = time, s. The time step for the baseline case is 4750 s.

T = temperature, $^\circ\text{C}$.

α = thermal diffusivity, m^2/s . See Figure A.8.

The equation was solved using an explicit finite-difference method where the initial temperature of the outside surface of the 0.25 radius heater was 800°C . This was consistent with the larger scale experimental studies. The far-field background temperature of the formation was

20°C. The initial temperatures of the system were: the heater at 800°C and the coal formation at 20°C. Each cylindrical element occurred at intervals of 0.25 m away from the heater and the elements extended 17.25 m from the heater, and each time step was 4750 s. The single-well configuration's temperature prediction did not include the energy needed to heat and evaporate the water, but the multiple-well configuration did include water heating and evaporation. For both configurations, the energy needed to heat and evaporate was considered, as discussed below. The energy needed to vaporize the pyrolysis products was neglected. Above 233°C (the boiling temperature of water at 30 bar), the thermal diffusivity changed as a function of temperature (Figure A.8). These predicted temperatures were used in the yield model and in estimating the energy required to heat the coal, char and product mixture.

The energy requirement was calculated for the coal and water separately. For the coal, the energy required for each element at each time step in the simulation was calculated using:

$$Q = m C_p (T - T_{(t-\Delta t)})$$

where,

m= mass of material remaining within each element, kg. Above a temperature of 233 °C, coal transforms into the product mixture, and the product leaves the system.

C_p = heat capacity of coal at the average temperature of the element. Above a temperature of 233°C, C_p changes, see Figure A.7.

$T_{(t-\Delta t)}$ = average temperature at the previous time step at the midpoint of the element, °C.

T = midpoint temperature at time t , °C.

The cumulative energy required to heat the coal was calculated by summing the required energy at each time step.

The cumulative energy required to heat the water is given by:

235
$$Q = m\Delta H_{\text{vap, H}_2\text{O}} + mC_p (T - T_o)$$

236 where,

237 Q = energy, kJ.

238 m = mass of water in each element.

239 T_o = 20°C, background temperature.

240 T = Final midpoint temperature at each element, °C. If the final temperature exceeded the
241 boiling point of water at the formation pressure, the temperature was 233°C (boiling point of
242 water @ 30 bar).

243 C_p = 4.18 kJ/kg.

244 $\Delta H_{\text{vap, H}_2\text{O}} (@30 \text{ bar}) = 1,794 \text{ kJ/kg}$. This was included only if the final temperature of the element
245 exceeded 233 °C. At the end of the evaluation period if the element exceeded a temperature of
246 233 °C, all of the water in the element was assumed to evaporate and leave the system

247 The energy requirements for heating the water in each element to its final temperature were
248 then summed.

249 During the UCTT process, an operator might choose to heat the formation for a given time
250 period and then collect the product, or he could choose to produce continually. If products are
251 collected continually, energy leaves the system continually. It is unclear how such a process
252 would actually operate; consequently this energy leaving the system is included because it is
253 considered more conservative, i.e., requiring more energy. This energy is given by:

254
$$Q = m C_p (T - T_o)$$

255 where,

256 m = cumulative mass of material leaving the system from each element, kg.

257 C_p = heat capacity of product mixture, kJ/kg.

258 T_o = initial temperature of the element, °C.

259 T = midpoint temperature at time t , °C.

260

261 An additional simulation was performed using STAR-CCM+ to investigate the effect of multiple
262 wells and heat loss to the over/underburden using the same physical properties for the coal seam
263 and heater temperature as the baseline case. Figure A.9 shows the STAR-CCM+ simulation
264 domain, which included wells spaced 12.5 m apart and a 10-m thick coal seam with 25 m of
265 overburden and underburden. The overburden and underburden were assumed to have a
266 moisture content of zero.

267 The STAR-CCM+ solves the conductive component of heat transfer:

$$\frac{\partial}{\partial t} \int_V \rho c_p T dV = - \oint_A \mathbf{q}'' \cdot d\mathbf{a}$$

268 where,

269 t = time, seconds.

270 ρ = the solid density,

271 c_p = specific heat,

272 T = the temperature,

273 $\mathbf{q}''$ = solid heat flux vector,

274 $\mathbf{a}$ = the normal area vector,

275 A = the area, and

276 V = the volume.

277 The solid heat flux vector is computed using Fourier's Law and is dictated by the fixed heater
278 temperature of 800°C. Second-order discretization for both temporal as well as spatial terms was

used along with an implicit iterative approach. A time step of 7,200 seconds was selected. On the surface of the heater, the mesh size was set to 2 cm. Therefore, the heating wells were sufficiently resolved to accurately capture the heat supplied by heaters into the coal seam. The very fine heater mesh slowly transitioned into a coarser mesh, with maximum cell size of 20 cm, for total of 21 million computation cells for the entire simulation domain.

2.4 Yield Model

A sigmoidal function was fit to the experimental scoping data (Figure 3), and this function was used to predict yield as a function (mass fraction of total coal utilized) of temperature in the UCTT simulations, discussed in the following subsection. The scoping data provided more consistent temperature profiles compared to the larger scale studies where measuring the internal temperature of the coal was challenging. The experimental data were fit by minimizing the least squares difference between the predicted and measured yields. For the baseline case, the yield was set at 0.4525 at temperatures of 950°C and above, from coal's proximate analysis and at less than 0.03 at a temperature of 340°C.

The baseline sigmoidal fit is given by:

$$Yield = \frac{Yield_{max}}{1 + e^{0.02096(k-Temp)}}$$

where,

Yield = the fraction of the coal that is volatilized on an as-received basis.

Yield_{max} = the maximum yield, from the proximate analysis, 0.4525, with a range of 0.446 (Umin) – 0.462 (Umax) (as received).

k = 472 °C (baseline), with a range of 567 – 357 °C (Umin – Umax).

Temp = temperature, °C.

The Appendix provides additional detail on the yield function and the associated uncertainty. Based on the experimental results, the model assumes a 50:50 split between liquid and gas-phase products for the baseline cases.

2.5 Liquid Products and Refining

Because the hydrogen and carbon content are similar to that of conventional crude, US average refining GHG emissions and energy requirement are selected. These are 3.2 MJ/kg crude and 8.69 g CO₂e/MJ crude, respectively.²⁴ The mass of crude oil moved into a refinery is slightly less than the mass of the product leaving the refinery and the heating value of the liquid product and crude oil differ. Consequently, the method outlined in Wang et al.²⁵ was used to adjust from a crude to gasoline basis.

2.6 Gas Products and Processing

The product gas contains approximately 30% CO₂, and removing this prior to combustion is relatively expensive. Consequently the gas product was presumed to be combusted in a 50% efficient natural-gas combined cycle (NGCC) turbine. This process generates 147 g CO₂ e/MJ of electricity.²⁶ Spath and Mann²⁶ report on a 53% efficient NGCC, and the emissions were adjusted to 50% efficiency. Because all of the gas is combusted in the NGCC to generate the electricity needed to heat the coal, no excess electricity is available for sale (see Section 3.2).

2.7 Liquid Product Transport

Energy and GHG emissions from transport of the liquid product are based on a US average of 6720 J/MJ product and 0.493 g CO₂ e/MJ product.²⁴

2.8 Electricity Generation and Fuel Combustion

Energy consumption and GHG emissions were assumed to be from a 50% efficient NGCC plant.²⁶ GHG emissions from combustion of gasoline were 75.2 g CO₂ e/MJ, and diesel emissions were 77.0 g CO₂ e/MJ. Natural gas combustion emits 56.6 g CO₂ e/MJ.

2.9 Net Energy Return

The net energy return (NER) and the net external energy return (NEER) are useful metrics for comparing fuel sources. The NER is the ratio of usable energy gained from an energy resource to the energy used (directly and indirectly) to obtain that resource. The NEER is the ratio of usable energy gained from an energy resource to the direct energy used (excluding e.g., any produced fuel consumed while producing the resource). For this analysis, the NER value assumes that the products are the refined liquid and gas product, and the NEER assumes that the gas is combusted to generate electricity to heat the formation. The NER and NEER presented are at the point of consumption, the fuel pump.

2.10 Sensitivity and Uncertainty

Table 2 summarizes selected emission factors, assumptions and properties investigated for the sensitivity and uncertainty analyses. The preliminary analysis of UCTT identified the energy required to heat the formation and product yield as being key to the feasibility of this process. Recognizing this, the sensitivity analysis focused on several factors affecting the yield and heating of the formation. These included coal moisture content, thermal conductivity, yield model, refining energy requirements, heater temperature and formation heating period. The uncertainty analysis explored how the range of experimental uncertainty affects the results, and it propagated all experimental uncertainty. For a single well, the results present the least and most favorable experimentally derived parameters (Umin - Umax). The analysis also included the

effect of multiple wells and heat loss to the overburden. This is denoted as “Multiple” in Table 2 and the subsequent results.

3 RESULTS AND DISCUSSION

Analysis of the products from the larger scale studies revealed that carbon tends to partition to the char, while hydrogen tends to partition to the gas and liquid products (Figure 4). Oxygen tends to be found in the water and gas products, while sulfur tends to partition to the char and liquid products. The mass balance shown in Figure 4 uses average coal composition; however inherent inhomogeneties in the coal exist. Consequently, the balance does not account for approximately 3% of the carbon and 6% of the hydrogen, and it slightly over-accounts for oxygen and sulfur. The experimental results show that UCTT can produce a high-quality liquid product and a lower energy content gas. This suggests that UCTT is worth further evaluation.

Figure 5 shows the energy required and the energy produced, and Figure 6 shows the simulated temperature profile for baseline conditions. In this figure for a 2.5-year heating period, the edge of the element located 17 m away from the heater, which is next to the simulation boundary (17.25 m away from the heater), is 0.04°C above the background temperature of 20°C; at 5 years this difference increases to 0.5°C. The temperature and yield profiles follow similar trends for all cases, with temperatures decreasing rapidly with distance from the heater. Figure 7 shows the temperature profile for the multiple heater configuration.

For all cases, the produced gas contains less energy than that required to heat the formation. For the baseline case, the produced gas contains approximately 45% of the energy needed to heat the formation, and 7% of the energy in the products is needed replace the energy leaving the system with the heated products (7%). For the 20% moisture case (Table 2), the produced gas contains only 23% of the energy needed to heat the formation (at 2.5 years). For the Umax case,

the produced gas contains 85% of the energy required to heat the formation (at 2.5 years). Considering all the life-cycle energy requirements, heating the formation requires the majority of the energy, greater than 80%, for all cases.

3.1 Net Energy Return

As time progresses, NER values decline since relatively small volumes of coal are treated to significant temperatures. Considering just the process of heating the formation, Figure 5 shows how NER declines over time. It also shows the energy required and the energy produced. For the baseline case, it shows that the NER declines from 1.4 at 2.5 years to approximately 1.2 at 5 years. Figure 5 also confirms that the energy leaving the system with the products is small compared to the energy required to heat the coal and moisture.

Figure 8 shows that NERs decrease as a function of time for heating the formation for all cases. The multiple-well case shows a slightly different trend than the single-well cases where NERs increase until approximately 1 year and then decline. The temperature profiles of the multiple-well case are retarded by the heating and evaporation of the water, which decreases the initial NERs. In addition, the multiple-well case NER looks slightly wavier than the single-well cases, which is due to the simulation mesh size away from the heater. The multiple well, Umax and maximum-yield cases exhibit the greatest NERs. Figure 8 illustrates the importance of yield model, liquid fraction of the product, heater temperature and configuration, and the initial moisture content. As moisture content increases NER decreases. At a 20% moisture content, heating the formation requires more energy than it produces in approximately 1 year, indicated by an NER of less than one. At 5 years, both the minimum yield and the 10% moisture case have process NERs of less than 1.

If the WTP lifecycle stages are considered, NER values are lower than those for just heating the formation. Table 3 summarizes the WTP NER and NEER values for each case. This suggests that the cases with a moisture content much greater than the baseline (3.2% moisture) or a heater temperature much lower than the baseline are unlikely to be feasible. However, coals that exhibit higher yields (>0.3) are more likely to be commercially viable.

The baseline NEER for gasoline produced from the UCTT process is 1.1 (range of 0.28 – 4.7), and the baseline NER is 1.3 (range of 0.48– 4.5). NEER tend to be lower than NER values for all cases except for the multiple well, Umax and maximum-yield cases, which have large gas yields relative to the energy required. Figure 9 compares the range of UCTT NERs to other sources of liquid transportation fuels and to electricity generated from coal. NERs for some transportation fuels vary widely, and limited NERs are reported for oil shale.²⁷⁻²⁹ Recognizing that oil shale has a limited commercial production history, particularly in situ, a good deal of uncertainty is associated with oil shale NERs, with NERs ranging from less than 1²⁷ to 2.5 (if gas is exported)²⁸ or 2.6²⁹ for refined fuel. The baseline NER for UCTT is less than half that for oil sands and in the range of that for oil shale (0.48 and 2.6).^{27,29} The in situ shale and coal processes face similar challenges with energy losses, i.e., waste energy to the formation. However, the multiple-well case (NER of 4.5 at 2.5 years) compares favorably with oil sands (NER of 2.8).⁴² A number of factors would limit UCTT's feasibility including coals with high moisture content ($>5\%$) and/or low volatile yield ($<30\%$).

Selecting the formation heating time would likely need to be a balance between the economics and NER. To overcome the fixed cost of well drilling and infrastructure, a minimum yield will be necessary. However, longer formation heating times lead to larger volumes of coal that are heated to low temperatures, resulting in wasted energy and lower NERs.

3.2 CO₂ Emissions

Of the life-cycle stages, heating the formation clearly drives the CO₂ emissions (Figure 10). The results presented in this figure assume that all of the natural gas is combusted to generate the electricity needed to heat the formation and that gasoline is the only remaining product. Transport and refining CO₂ emissions are similar to those for other sources of liquid fuels. On an energy content basis, well-to-pump (WTP) life-cycle CO₂ emissions are 178 g CO₂e/MJ baseline (50 – 558 g CO₂e/MJ range).

The WTP GHG emissions for the liquid fuel produced from the UCTT process with the low-moisture coal (50 – 558 g CO₂e/MJ range) are dominated by the process of heating the coal formation, which contributes 169 g CO₂e/MJ of the 178 g CO₂e/MJ WTP GHG emissions (baseline at 2.5 years of heating time). Literature values for GHG emissions from in situ recovery of coal resources are limited. However, in situ recovery of oil shale and sands can serve as useful benchmarks, as does coal-to-liquid conversion such as the Fischer Tropsch process.

Figure 11 compares the range of WTP GHG emissions for gasoline produced by UCTT with GHG emissions from other transportation fuels. The emissions are several times greater than the US average WTP GHG emissions of 18.1 g CO₂e/MJ.⁹ As with the NER values, the multiple-well, U_{max} and the maximum-yield cases provide the most attractive (lowest GHG) emissions, and U_{min}, high moisture and minimum-yield cases lead to the highest GHG emissions. This evaluation's WTP GHG emissions overlap with the upper end of the range of GHG emissions reported for the Shell in situ conversion process (ICP) of 38-63 g CO₂e/MJ transportation fuel¹⁰ and generally fall into the range of values reported by Kelly et al.²⁷ of 60 - 120 g CO₂e/MJ for in situ production of crude from oil shale. UCTT's GHG emissions also generally fall within the

wider range of values reported for ex situ oil shale operations (40-180 g CO₂ e/MJ gasoline).^{30,31} These values are nearly double those reported for production of reformulated gasoline produced from in situ recovery of Canadian oil sands (29 - 35 g CO₂ e/MJ) reported by McKellar et al.³² The comparatively low GHG emissions from Canadian oil sands reflect the relative ease in recovering bitumen from sands and the shallow depth of the sands. WTP GHG for transformations of coal to liquid fuels via the Fischer Tropsch process (73 - 140 g CO₂ e/MJ, diesel product³³) are also in the range of those reported for the conceptual UCTT process described in this paper (50-558 g CO₂ e/MJ, gasoline product).

This type of fuel resource, in situ coal, falls into the category of lower quality crudes that, if developed, would result in increased GHG emissions compared to conventional crude sources. Dooley et al.³⁴ suggest that the development of unconventional fuels in the United States would significantly increase GHG emissions. Brandt and Farrell³⁰ suggest that transitioning to low-quality crude sources, such as tar sands or coal-derived liquids, could raise upstream GHG emissions by several gigatonnes annually.

3.3 Sensitivity and Uncertainty

Of the factors considered in the sensitivity and uncertainty analysis, the yield model, the heater temperature, the number of heaters, and the moisture content of the coal had the greatest effect on both the GHG emissions and the NER. Because of the large volumes of coal heated to relatively low temperatures, using the maximum yield model (U_{max} includes maximum yield model and the most favorable ranges of other parameters) resulted in more favorable NERs and GHGs than any of the other single-well cases (Table 2). Existing yield models focus on rapid heating rates, typical of pulverized coal combustion. Better models are needed to predict product yields at the low ultimate temperatures and the very low heating rates typical of a UCTT process

($< 1^{\circ}\text{C/hr}$). This evaluation examined three yield models, all based on sigmoidal fits of the experimental data. These models produce yields that follow trends reported in the literature for coal devolatilization over temperatures ranging from approximately $200 - 600^{\circ}\text{C}$ at higher heating rates $>0.5^{\circ}\text{C/s}$.³⁵

Two subcomponents of the yield model are the ultimate yield and the product composition. The ultimate yield for the baseline coal is typical of a high-volatile bituminous coal (38 – 45%).³⁵ However, coal volatile content varies widely from 2 – 10% for anthracites, to 20 – 30% for low and medium-volatile bituminous coals and 40 – 50% for subbituminous and lignites.³⁵ The product composition and the liquid to gas ratio are also related to the yield model. The liquid products have a greater heating value than the gas products. The LHV of the liquid products is 43,000 kJ/kg, and the LHV for the gas product mixture is 16,500 kJ/kg (range of 12,200 to 19,300). The gas products contain approximately 30% by weight CO_2 and 7% H_2O , which contributes to the lower energy value of the gas products. Consequently, increasing the ratio of liquid to gas products improves the NER of the process.

Lower rank coals tend to exhibit high gas yields and low liquid yields, while high-volatile bituminous coals tend to exhibit high liquid and moderate gas yields.³⁵ The coal selected for this analysis is a high-volatile bituminous coal with a low moisture content. With these attributes, it is a more likely candidate for the UCTT process than a lower rank, higher moisture coal or a low-volatile high rank coal.

Heater configuration, heater temperature and coal moisture content also have a significant effect on the viability of the UCTT process. Multiple heating wells offer the most favorable NERs and GHG emissions, and this array of closely spaced heaters would be more operationally realistic than a single-well configuration. This dense well spacing improves product recovery per

unit energy input, making UCTT a potentially promising processes. The low-heater-temperature case NER is approximately one half of the baseline case. A heater temperature of 400°C would cause the UCTT process to become unfeasible. Although the baseline case has a heater temperature of 600°C, which corresponds to the experimental conditions, commercially available electrical heaters may have difficulty maintaining a temperature of 600°C over the distances required in a full-scale UCTT process.

The moisture content of the baseline coal is low, and increasing the moisture content from 3.2% (baseline) to 10 and 20% increases the GHG emissions by a factor of 30 and 38%, respectively. Different ranks of coal exhibit a wide variety of moisture contents, ranging from less than 5% for anthracites and bituminous/subbituminous coals to greater than 30% for lignites.^{35,36} Bituminous and subbituminous coals account for more than 90% of US coal production.³⁷ Selecting a low-moisture resource would be a key criterion of a UCTT process.

Although thermal diffusivity affects the time required to heat the coal seam and this property has a good deal of uncertainty, in the range considered in this evaluation its effect on the NER and GHG emissions is limited. Consequently it is not included in the results. However, diffusivity may be an important consideration for the economics of a UCTT process.

3.4 Other Uncertainties

The sensitivity and uncertainty analysis began to address potential uncertainties in the UCTT process including formation and coal/product properties, experimental error, and product yield. However additional uncertainties will affect the feasibility of UCTT. These include the behavior of water in the formation, mineral matter, which affects pyrolysis behavior, the environmental fate of the liquid- and gas-phase products, design and maintenance of well casing, and operational challenges associated with recovering the liquid products from the formation. It is

not known whether water in the formation would flow into the heating zone as the product is recovered. Any additional water would continue to absorb energy and make the energy balance less favorable. If CBM was extracted from the formation, the coal seam would have been dewatered, thus limiting water flow into the formation. In addition to water, other light hydrocarbons may flow into the heating zone and be recovered, which would improve UCTT's feasibility. This study did not consider the environmental fate of any unrecovered products. However as shown in Figure 6, the pyrolysis zone extends approximately 3 meters from the heater after 2.5 years of heating. Unrecovered product would likely adsorb to the heated coal seam as it cools.

The yield models explored in this evaluation do not cover the full range of possible models, such as Biagini and Tognotti³⁸ or Kobayashi et al.³⁹ Furthermore, the yield models considered in this analysis did not account for any recovery losses associated with gathering the products from the well and transporting these to the surface.

4 CONCLUSIONS

The experimental results suggest that UCTT may be promising because it can produce a high-quality liquid product as well as a gas that could help heat the formation. UCTT tends to leave the carbon in the ground and produce a lower carbon fuel than the parent coal. Heater temperature and configuration, product yield at low temperatures and the moisture content of the coal are the key factors in determining the feasibility of UCTT. Accurate low-temperature, low heating rate yield information is critical to further evaluation of UCTT. In spite of this limitation, this evaluation suggests that high volatile, low moisture coal would be a good target for UCTT. The most favorable UCTT results (NER and GHG emissions) occur for multiple heater wells with a heater temperature of 600°C (or greater) combined with a low moisture (5%

or less), high volatile content (30% or more) coal. The NER and GHG emissions for the process are less favorable than those for oil sands and are in the general range of that for oil shale. However due to the limited commercial adoption of in situ oil shale production and the low natural gas and liquid fuel prices, UCTT is unlikely to become commercially viable in the near term.

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Figure 1. Example of a UCTT process. The process is not drawn to scale.

Figure 2. System boundaries for the analysis of UCTT. The shaded box indicates that heating the formation is critical to the analysis.

Table 1. Sufco coal properties. These are presented on a dry ash free basis. This is based on the average of 6 samples. The average moisture content is 3.21% and the average ash content is 5.04%.

Fixed carbon (%)	Heating value (MJ/kg)	Carbon (%)	Hydrogen (%)	Nitrogen (%)	Oxygen (%)	Sulfur (%)
54.75	32.7	78.46	5.61	1.72	13.56	0.65

Figure 3. Sigmoidal fit of the experimental results. The baseline model uses the scoping data, while the Umin and Umax models fit the range of all experimental results and use the minimum and maximum experimental yields, respectively.

652 **Table 2.** Emission factors, coal properties, and selected parameters used in the sensitivity and uncertainty analyses.

Process	Baseline	Umax	Umin	Max Yield	Min Yield	Max NER	Min NER	10% water	20% water	Low heat	Enhanced k	Multiple well
Coal moisture	3.2 %	3.2%	3.2%	3.2%	3.2%	3.2%	3.2%	10%	20%	3.2%	3.2%	3.2 %
Background temperature (°C)	20	20	20	20	20	20	20	20	20		20	20
Drilling diesel fuel consumption (l/m)	12.4 ¹⁶	12.4 ¹⁶	12.4 ¹⁶	12.4 ¹⁶	12.4 ¹⁶	12.4 ¹⁶	12.4 ¹⁶	12.4 ¹⁶	12.4 ¹⁶		12.4 ¹⁶	12.4 ¹⁶
Heating the formation												
Heater temperature (°C)	800	800	800	800	800	800	800	800	800	600	800	800
Cp coal (J/g°C)	1.41	1.14	1.47	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41
Maximum yield (%)	45.25	46.2	44.6	46.2	44.6	50	40	45.25	45.25	45.25	45.25	45.25
Liquid product (%)	50	58.2	29.5	58.2	29.5	60	40	50	50	50	50	50
Yield model	b	c	d	c	d	b	b	b	b	b	b	b
Refining (MJ/kg crude) ⁸	3.2	3.2	3.2	3.2	3.2	2.88	3.52	3.2	3.2	3.2	3.2	3.2
Transport (J/MJ) ²⁴	6720	6720	6720	6720	6720	6720	6720	6720	6720	6720	6720	6720
Efficiency of NGCC electricity generation	50%	50%	50%	50%	50%	50%	50%	50%	50%	50%	50%	50%

653 a) At 600°C. b) $Yield = \frac{0.4525}{1 + e^{0.02096(472 - Temp)}}$ (baseline yield model). c) $Yield = \frac{0.462}{1 + e^{0.02096(357 - Temp)}}$. d) $Yield = \frac{0.446}{1 + e^{0.02096(567 - Temp)}}$.

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Figure 4. Moles of carbon (C), hydrogen (H), nitrogen (N), oxygen (O), and sulfur (S) in the original coal (as received) and in the char, liquid, and gas. The coal was heated to an internal temperature of 540°C at ambient pressure and held for 3 hours.

Figure 5. Energy produced, energy required, energy required with simultaneous production and NER as a function of time for the process of heating the formation.

Figure 6. Temperature profile at various radial distances from the heater (distance 0.25 m increments) a 2.5-year heating period for the baseline case.

Figure 7. The temperature profile for the multiple well configuration after 2.5 years of heating.

Figure 8. Comparison of NERs for the process of heating the coal formation. MinNER is not shown because it overlaps with the lower NER cases.

Table 3. Summary of WTP NER and NEER values at 2.5 and 5 years of UCTT production.

	Base	Umax	Umin	Max yield	Min yield	Max NER	Min NER	10% Water	20% Water	Low heat	Mult well
<i>2.5 years</i>											
NER	1.26	3.13	0.48	2.81	0.51	1.58	1.04	1.01	0.75	0.577	4.48
NEER	1.11	3.86	0.28	3.20	0.40	1.51	0.82	0.86	0.61	0.458	4.74
<i>5 years</i>											
NER	1.06	2.85	0.14	2.96	0.39	1.13	0.87	0.84	0.62	0.421	4.14
NEER	1.01	3.33	0.08	3.66	0.30	1.27	0.74	0.77	0.54	0.327	4.68

Figure 9. NER/EROI for gasoline produced from the UCTT process, oil shale^{13,27}, corn ethanol^{40,41}, Canadian oil sands⁴², conventional crude⁴³, and electricity generated from coal⁴¹. The highest oil shale NER²⁹ in this figure was adjusted from a shale-oil crude basis to a refined fuel basis assuming a refining energy requirement of 507.5 MJ/ton shale processed and a ratio of HHV of refined product to upgraded shale oil of 0.9 from Brandt⁴⁴.

Figure 10. GHG emissions (CO₂ e) from baseline, maximum uncertainty (favorable), maximum yield, NER max, 10% water, 20% water, and lower heater temperature cases at a 2.5-year heating period. The Umin case is not shown on this scale. It is 558 g CO₂ e/MJ.

Figure 11. Range of CO₂ e emissions per MJ of transportation fuel for UCTT, oil shale (low, for Shell's in situ conversion process¹⁰ and, high, for ex situ shale³⁰), diesel produced from coal via the Fischer Tropsch process³³, corn ethanol^{45,40}, Canadian oil sands³², and gasoline from crude oil³².