*Desalination and Water Treatment*
www.deswater.com

51 (2013) 1487–1493
February

Taylor & Francis
Taylor & Francis Group


doi: 10.1080/19443994.2012.714727

# A $CO_2$-PENS model of methods and costs for treatment of water extracted during geologic carbon sequestration

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Received 1 March 2012; Accepted 18 July 2012

**ABSTRACT**

Extraction of water during subsurface carbon sequestration may be useful for the control of $CO_2$ placement, reducing pressure risks, and mitigating environmental risks. Desalination of this water may be possible if costs are kept low, in order to minimize the quantity that must be reinjected or otherwise disposed. Added value may be recovered in the form of treated water that can be reused by carbon capture, sequestration, and other industrial processes. Total dissolved solids will range from 10,000 mg/L up to over 100,000 mg/L, and temperatures may range up to 120°C, once the water is brought to the surface. We have developed a system-level, mesoscale analysis module for the $CO_2$-Predicting engineered natural system model to analyze the feasibility of treatment, the costs of treatment, the value of energy recovery, and the costs of concentrate disposal. Costs are derived from a database of reported literature values. The model allows the user to select the most economic options for treatment, to compare costs, and to understand the trade-off of risks and costs. Results of preliminary modeling indicate that while reverse osmosis is feasible within certain temperature and salinity ranges, nanofiltration and thermal methods may be more cost-effective or otherwise feasible.

*Keywords:* Carbon sequestration; Reverse osmosis; Nanofiltration; Multiple-effect distillation; Multistage flash distillation; Thermal distillation; Brine concentrate disposal

## 1. Introduction

Sequestration of captured $CO_2$ into geologic formations requires assessment of the risks associated with subsequent unanticipated movement of both $CO_2$ and water in subsurface rock formations. Extraction of water at or near the injection site can help control the movement of the $CO_2$ and control pressures to within desired ranges in order to minimize the risk of uncontrolled movement and escape of $CO_2$. Minimization of the volume of the extracted water that needs to be reinjected or otherwise disposed is desirable. The potential costs of treating this water can then be compared to the perceived value of pressure control for

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*Presented at the International Conference on Desalination for the Environment, Clean Water and Energy, European Desalination Society, 23–26 April 2012, Barcelona, Spain*

the system and the subsequent risks [1]. In order to better understand the trade-off of costs vs. processes and risks, we have developed a modular approach within LANL's $CO_2$-PENS model, which is an overarching systems model that can be used for carbon sequestration site risk assessment [2].

Water that is extracted will be saline (>10,000 mg/L total dissolved solids [TDS]), and may have characteristics of deep brine aquifer waters (greater hardness or silica contents) or of oil and gas produced waters (increased organic content). The low end of the salinity range is set by regulation [1]. The volumes of water extracted have been estimated to exceed rates of 436 $m^3$/d [2]. These waters will require pretreatment and desalination along with posttreatment to optimize use. The complexity of the treatment process is likely to be greater for brackish waters (~5,000 mg/L TDS) that are typically treated by municipalities in the USA for supplemental supplies, and more similar to marine waters (~35,000 mg/L TDS).

Mesoscale models are more generalized than site-specific engineering analyses and are more easily applied in the early development stages of a site. They can be used to prompt discussion of the water treatment needs, process needs, and the potential value added by creating treated water at a site. Generalized models have not been developed to analyze system costs and risks for the water extraction scenario. We utilized existing literature cost data for pretreatment, treatment, posttreatment, and Pelton Wheel energy recovery methods to develop a generalized model for cost analysis. The model is then used to predict ranges of cost to treat vs. $m^3$ of treated water or vs. tons of injected $CO_2$. Site designers and operators can optimize the model to fit their location, expected water quality, and desired quality of treated water. This paper presents results of cost modeling for expected pretreatment scenarios, treatment methods, disposal methods, and pressure cost recovery.

## 2. Model development

Fig. 1 shows the expected TDS range in mg/L vs. expected temperature ranges for extracted water at $CO_2$ sequestration sites [3]. These sites range from saline water reservoirs, oil and gas reservoirs, coal seams, organic rich basins, and fractured basalts [4]. The dark blue shaded areas indicate ranges typically acceptable for reverse osmosis (RO), while the red dashed lines bracket typical temperature ranges expected for waters extracted and treated without additional cooling. The dark red line indicates the

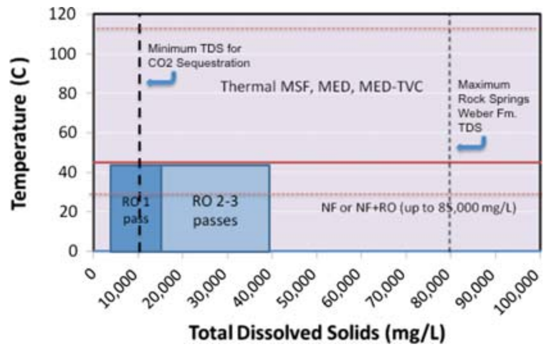


Fig. 1. Ranges of salinity and temperature expected for water extracted from $CO_2$ sequestration formations.

maximum temperature anticipated for RO to be feasible (45˚C). Salinity ranges over 100,000 mg/L may occur at some sites; however, there is little data available on the costs for desalinating these waters.

Water quality information for these waters is available through the databases, such as National Carbon Sequestration Database and Geographic Information System [5], and through the literature. Frequently, the type of chemical data needed for detailed treatment evaluation is not available, limiting the analysis to a generalized model. Research indicates that the injection of $CO_2$ may increase solution concentrations of major cations, such as Fe(II), Ca, Mg, and K, with time and spatial variability within the injected formation [6,7]. Extracted waters thus may need increased pretreatment over typical marine or brackish waters. Dissolved gases ($CH_4$ and volatile organics) also may need to be removed prior to treatment, although breakthrough of $CO_2$ is likely to be suppressed by site management practices, because $CO_2$ migration is an undesirable outcome of permanent sequestration.

Pretreatment scenarios within the model are outlined as shown in Fig. 2. Fig. 3 shows treatment choices. Four different treatment scenarios were considered. The model makes a choice of treatment type based on the temperature and salinity of the water to be treated (from Fig. 1), and desired output quality (mg/L TDS). The RO and nanofiltration (NF) methods can be looped for up to three passes with costs accumulating during each pass.

Choices of RO are also limited by the desired output quality (<1,000 mg/L TDS), while NF output quality is not limited. Thermal output quality is assumed to always be <500 mg/L TDS. Posttreatment costs are included for each method at a fixed rate per $m^3$.

## 3. Model construction

The system model was developed using the GoldSim© platform [8]. GoldSim© provides utilities that

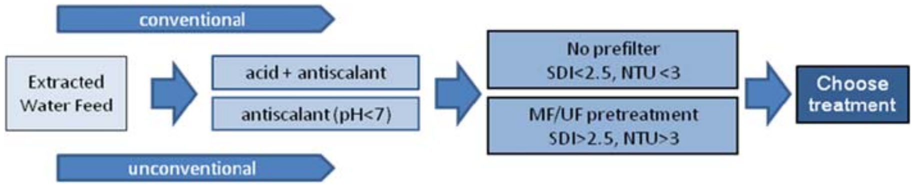


Fig. 2. Conventional and unconventional pretreatment choices available in the model.

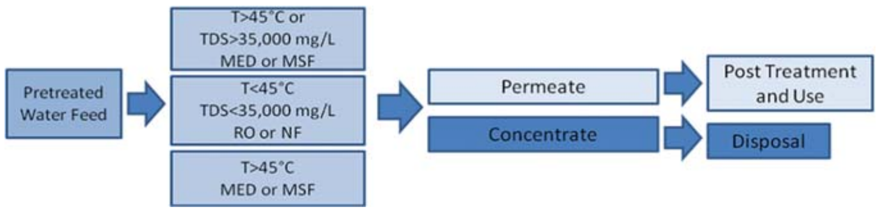


Fig. 3. Treatment choices available and criteria for model selection of a particular treatment.

can be used to develop analysis models designed to perform multirealization, probabilistic simulations. A Fortran code was used to capture the logic of treatment process selection shown in Figs. 2 and 3 and was linked within GoldSim©. The model has various data elements to input user-specified parameters including stochastic distributions. The model captures all decision points and either range or constant data input values, and samples within those value ranges to produce a cost distribution output for feasible treatment process scenarios.

Multiple realizations (either 100 or 500) were run for several sequestration/extraction scenarios. Cost scenarios were based on ranges of data found in the literature for brackish (up to 15,000 mg/L TDS) through highly saline (up to 80,000 mg/L TDS) water qualities, four electricity cost values (0.04, 0.07, 0.10, and 0.20 US $/kWh), and variable temperature ranges from 15 to 120℃ (to account for superheating of high-salinity waters). We also evaluated three fixed treated volume scenarios: 50, 75, and 90% of input feed volume for RO (Table 1). The costs of pumping to move water from the extraction point to the treatment system are not included in the module, because these are included elsewhere in the $CO_2$-PENS model.

Pelton Wheel pressure recovery was included as a model option for RO and NF processes [9]. Cost reductions using pressure recovery are amplified by the number of cycles selected by the model (up to three, depending on desired output quality).

Percentages of energy recovery from RO systems were calculated using the following equation:

$$\text{RO rate} = \{(\$/\text{kWh}_{\text{RO}} - \$/\text{kWh}_{\text{PR}}) * \text{kWh/m}^3\} + \{\$/\text{m}^3_{\text{NE}}\} \quad (1)$$

where RO = reverse osmosis; PR = pressure recovery; and NE = nonenergy costs.

Energy recovery scenarios include the following factors: OPEX on capital (UF or conventional); 1st pass seawater RO OPEX; and permeate conditioning OPEX. A low range of energy recovery costs, utilizing only a Pelton Wheel option, was used for modeling, because RO treatment cost ranges found in the literature did not match well (recovery value must be < RO cost). In other words, claimed recovery values were often greater than actual calculated or reported costs for RO options. Further cost recovery is claimed possible but is likely system-specific and may not be reducible to percentages of total energy costs.

The model includes six options for concentrate disposal [9]: Class I, Class II, and Class V well disposal, evaporation ponds, ocean disposal, and zero liquid discharge. The model queries for location information from the user to select the most feasible option.

## 4. Model scenarios

We performed calculations using data ranges derived from the literature for three representative geologic formations which are potential future geologic sequestration targets, including the Weber Formation and Madison Formations within the Rock Springs Uplift (Wyoming) [10] and the Frio Formation (Texas) [11,12]. For comparison, we also plot known values of treatment costs for two sites: the Al-Shoaiba multistage flash (MSF) desalination plant in Saudi Arabia [13] and the Key Bailey Hutchinson Brackish Water RO desalination plant in El Paso, Texas (KBH-El Paso) [14]. During each realization, costs were calculated for the treatment and pretreat-

Table 1
Independent variables chosen for modeling scenarios

| Criterion | Minimum value | Maximum value | Fixed ranges or values | Units | Note |
|---|---|---|---|---|---|
| Feed water volume | NA | NA | 37,854 | $m^3$ | Equals 10 MGD |
| Supply quality (TDS) | 10,000 | 80,000 | NA | ppm | |
| Permeate volume as desired percentage of feed volume | NA | NA | 50, 75, 90 | Percent (%) | NF only 75–90% |
| Permeate quality (desired quality) | 500 | 1,500 | NA | ppm TDS | |
| Temperature of feed water | 15 | 120 | NA | deg C | |
| Cost of energy | NA | NA | 0.04, 0.07, 0.10, 0.20 | $/kWh | |
| Feed pH | 4 | 10 | NA | pH units | |
| Feed turbidity | 1 | 10 | NA | NTU | |

*The value of 10,000 mg/L TDS is the lowest value of salinity allowed for formations used as $CO_2$ reservoirs, and, thus, for water extracted.

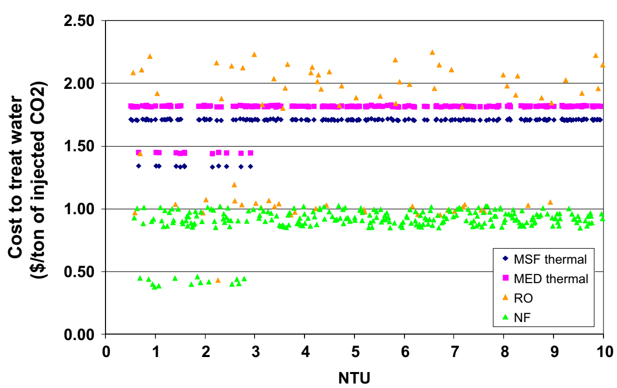


Fig. 4. Range of costs to treat (in $/ton $CO_2$ injected) for four methods in terms of NTU conditions.

ment processes selected based upon the input fixed and stochastic data.

## 5. Results and discussion

We viewed results in terms of two metrics: output treated water volume and injected mass of $CO_2$. Both metrics are important for the evaluation of site management costs and risk trade-offs. For these scenarios, we held the density of the injected $CO_2$ constant and assumed a constant treated water volume of 37,854 $m^3$ (10 million gallons per day). As such, our results do not reflect cost dependency on injection conditions that might change the $CO_2$ density and thus, change the volume of water that might be extracted. Results were plotted for condition (TDS and T) ranges that reflect the Weber, Madison, and Frio formations.

The model incorporates statistical variation in ranges of turbidity for RO and NF methods, but not for MSF and MED methods, where the system is less sensitive. Fig. 4 illustrates this effect. This plot incorporates the modeled conditions of variable TDS, fixed $T = 35$°C, a desired treated volume = 50% of feed volume, energy costs = $0.10/kWh, no pressure recovery, no disposal costs included, and over 500 realizations. The stochastic data ranges and the effect of model statistical sampling on the data ranges create cost data that is scattered around a central mean. The effect on final costs from each step of the treatment process selected by the model is reflected in these cost ranges. Because the model does not incorporate changes in costs as a result of TDS composition (e.g. ratios of Na: Ca) for thermal treatment or for NF, these costs are relatively flat when plotted vs. TDS. Others [15] have discussed the impacts of geochemistry on RO process costs; however, there is little data in the literature that can be used to incorporate real cost variation for thermal processes with changes in geochemistry.

Fig. 5 shows the effect of increasing costs for RO as TDS increases [16]. Thermal method costs reported in the literature do not vary with salinity, as most thermal processes are designed for seawater within ranges of about 20,000–40,000 mg/L TDS. This illustrates a need for further research into application of thermal processes to very highly saline waters in the range from 45,000–100,000 mg/L. Low points for each of the processes typically reflect lower costs due to lower turbidity and lower pretreatment costs. Costs range from less than $0.50 to $2.20/ton $CO_2$ injected. In comparison, costs to capture $CO_2$ from power generation facilities are estimated to vary from 15 to 75

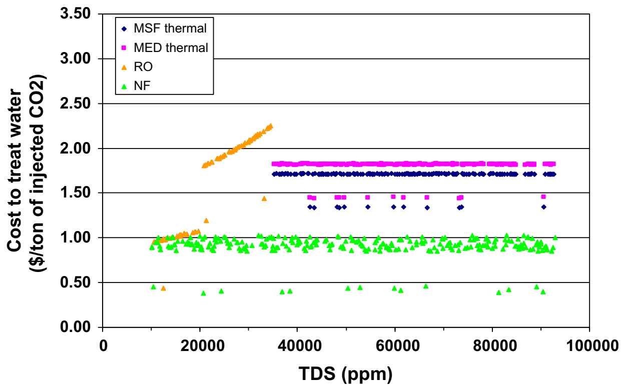


Fig. 5. Cost comparison of all treatment methods in terms of tons injected $CO_2$.

\$/ton $CO_2$, while costs for geologic sequestration may vary from 0.5 to 8 \$/ton $CO_2$ [17].

As salinity increases, RO becomes less efficient, in terms of the percentage of feed water treated per day (Fig. 6), as a result of increasing RO rounds (capped at three for practical purposes, as is typical in the industry). Thermal methods do not lose efficiency because the output water volume is a function of system design, not salinity. The model output can be configured to show costs in terms of output volume of treated water (Fig. 6). Model output costs for treatment are constrained by the input literature ranges; costs of about \$1/$m^3$ are now typical for many treatment processes [18]. In this case, the model runs included variable TDS (<35,000 mg/L TDS) and temperatures (<65°C), final treated volumes of either 50 or 90% of feed volume, an oil and gas produced water type, energy costs = \$0.10/kWh, no pressure recovery, and no disposal treatment costs.

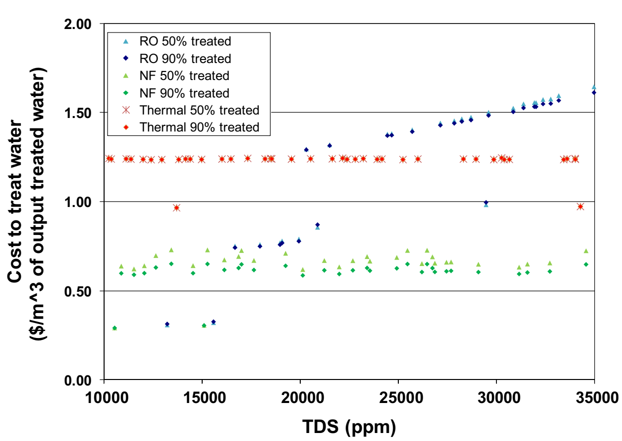


Fig. 6. Cost comparison of three methods and two recovery goals in terms of output treated water volume.

Single-pass RO is the least expensive scenario chosen by the model, at salinities less than 20,000 mg/L TDS. Above this, multiple passes of RO are enacted as the model is constrained to produce a fixed output volume (50% of influent volume). Above 35,000 mg/L TDS, thermal desalination is chosen. For comparison to model results, data from Al Shoaiba and KBH-El Paso are shown in Fig. 7. Significantly, even at a low influent temperature, many of the RO scenarios are more expensive at the higher energy cost ranges than thermal, contrary to common impressions of thermal as being considerably more expensive than membrane methods. NF (e.g. Fig. 4) is a very cost-effective treatment if final salinities needed exceed typical freshwater ranges of 500–1,000 mg/L TDS. Thermal treatment becomes an automatic selection if the influent water is above 45°C, as most RO membranes cannot tolerate higher temperatures, and high temperatures also increase the salinity of the final water quality. Similar results (not shown) were found for higher recovery rates. When viewed as a percentage of feed volume, RO gradually becomes less cost efficient than thermal processes up to an imposed cut-off salinity (in Fig. 7, 35,000 mg/L TDS). This indicates that feasibility should be evaluated not only as a function of simple cost to treat, but also as a part of the whole system cost model.

Fig. 8 shows the effect of inclusion of different disposal options based on a Rock Springs scenario. This scenario was chosen because of the wide potential TDS range, wide temperature range, and location (an inland arid region) which allows for a large number of different options to be chosen. The model accounts for a temperature range of 15–120°C, a TDS range of 15,000–35,000 mg/L, energy costs of \$0.10/kWh, and a desired output treated volume percentage of 50%. The Class II well disposal option dominates the cost scenario, because of the wide range of potential disposal

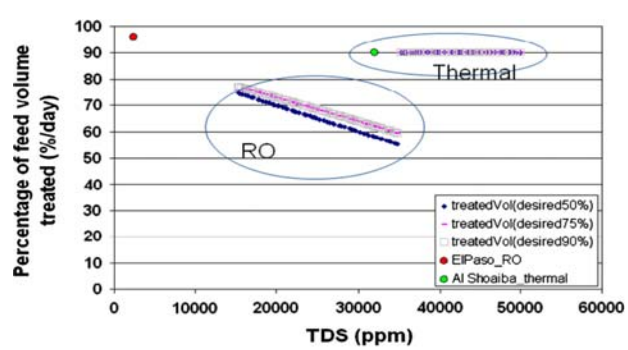


Fig. 7. Percentage of volume treated per day, as a function of variable feed TDS: $T = 25$°C, no NF option. Does not include energy recovery or concentrate disposal costs.

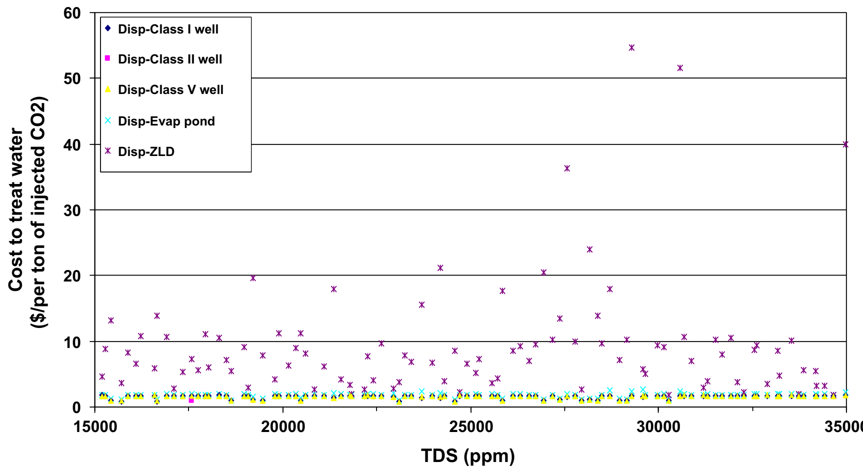


Fig. 8. Effect of different disposal options on total costs.

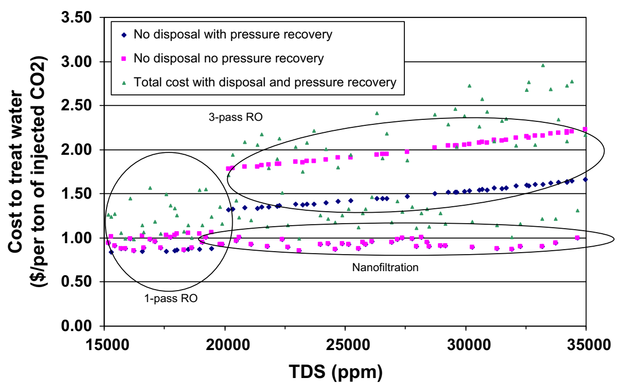


Fig. 9. Cost to treat water including both pressure recovery and disposal. Rock Springs evaporation pond example, fixed input T, fixed $/kWh, and RO recovery rate.

costs involved. Evaporation ponds are the next highest in cost and can be limited by volume constraints. Class I disposal well costs were the lowest and were derived from the largest number of reported data values.

Fig. 9 shows an example of the effect of energy recovery on total costs, with and without concentrate disposal included. This scenario is for the Rock Springs Fm. salinity ranges, at a fixed temperature of 35˚C, a 50% RO recovery rate, and a $0.10/kWh energy cost. Both 1-pass (<20,000 mg/L TDS) and 3-pass (>20,000 mg/L TDS) RO scenarios are shown along with NF (lowest cost range) results. Evaporation pond disposal adds a significant cost and variability to the results, although some of these costs are restrained by the addition of pressure recovery. Maximum costs rose from $2.50 to $3.00/ton $CO_2$ injected for the highest feasible salinities.

## 6. Conclusions

Treatment costs for waters extracted from sequestration can be reasonably estimated using a mesoscale generalized model. Evaluated scenarios yielded a cost range of $0.40–$2.30/ton $CO_2$ injected, without inclusion of pressure energy recovery (Pelton Wheel) and concentrate disposal, or about 2–3% of combined capture and sequestration costs. Addition of various concentrate disposal options increased costs considerably, up to more than 50% of sequestration costs in the worst-case scenarios. The most likely disposal cost scenario, Class I well disposal, however, was much more cost-effective. Addition of pressure recovery balances the significant costs incurred from disposal for RO processes. Pretreatment and treatment cost data need further research to expand the range of applicability for high salinity systems between 40,000 to 100,000 mg/L. Most significantly, the relative cost-effectiveness of thermal processes over membrane processes for many conditions expected at extraction sites indicates that these methods may be more applicable than expected, provided that pretreatment costs are not excessive.

## References

[1] R.L. Newmark, J. Samuel Friedmann, Susan A. Carroll, Water challenges for geologic carbon capture and sequestration, Environ. Manage. 45(4) (2010) 651–661.
[2] P.H. Stauffer et al., A system model for geologic sequestration of carbon dioxide, Environ. Sci. Technol. 43(3) (2009) 565–570.
[3] E.J. Sullivan, S. Chu, P.H. Stauffer, R. Middleton, R.J. Pawar, A method and cost model for treatment of water extracted during geologic carbon sequestration, Int. J. Greenhouse Gas Control (2012) 15.
[4] NETL. Carbon Sequestration Geologic Storage Focus Area. Available 27 February, 2012, from: http://www.netl.doe.gov/technologies/carbon_seq/corerd/storage.html.

[5] NETL. National Carbon Sequestration Database and Geographic Information System (NATCARB). Available 28 February, 2012, from: http://www.netl.doe.gov/technologies/carbon_seq/natcarb/index.html.
[6] A.H. Karamalidis, J. Alexandra; Griffith, Craig; Hedges, Sheila; Lu, Jiemin, Laboratory investigaion of $CO_2$-Rock-Brine interactions using natural sandsone and brine samples from the SECARB Tuscaloosa injection zone, in 2010 Geological Society of America Annual Meeting, Geological Society of America (GSA), Denver, Co, 2010.
[7] D.L. Newell, J.P. Kaszuba, H.S. Viswanathan, R.J. Pawar, T. Carpenter, Significance of carbonate buffers in natural waters reacting with supercritical CO2: Implications for monitoring, measuring and verification (MMV) of geologic carbon sequestration, Geophys. Res. Lett. 35(23) (2008) L23403.
[8] GoldSim Probabilistic Simulation Environment User's Guide, Version 10.5. Volumes 1 and 2. GoldSim Technology Group LLC, Issaquah, Washington, 2010.
[9] E.J. Sullivan, S. Chu, R.J. Pawar, Effects of concentrate disposal and energy recovery on costs for treatment of water produced during geologic sequestration, in Tenth Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, 2011.
[10] R.C. Surdam, Z. Jiao, The Rock Springs Uplift-An Outstanding Geological $CO_2$ Sequestration Site in Southwestern Wyoming, Wyoming State Geological Survey (2) (2007) 1–31.
[11] S.D. Hovorka, M.H. Holtz, S. Sakurai, P.R. Knox, D. Collins, P. Papadeas, D. Stehli, Report to the Texas commission on environmental quality to accompany a class V application for an experimental technology pilot injection well: GCCC Digital Publication Series #03-04: Frio Pilot in $CO_2$ sequestration in brine-bearing sandstones, in GCCC Digital Publication Series 2003, The University of Texas at Austin, Bureau of Economic Geology, Austin, TX, 175.
[12] S.D. Hovorka, C.M. Doughty, P.R. Knox, C.T. Green, K. Pruess, S.M. Benson, Evaluation of brine-bearing sands of the Frio Formation, Upper Texas Gulf Coast for geological sequestration, in Proceedings, First National Conference on Carbon Sequestration, May 14-17, 2001, Gulf Coast Carbon Center, GCCC Digital Publication Series #01-01, Washington, DC, 13.
[13] O.A. Hamed, Mubarak S. Al-Dossary, Jameel H. Baksh, Ibrahim Al-Khayat, Hassan Al-Harthi, Prospects of increasing water production by elevating operational temperature in Al-Shoaiba Phase-1 desalination plant, Saline Water Desalination Research Institute; Saline Water Conversion Corporation, Al-Jubail, 2005.
[14] P.J. Gorder, Development of Brackish grroundwater as a sustainable supply to support growth and military base expansion in El Paso-the Kay Bailey Hutchison desalination facilities project-El Paso water utilities, in: 9th Annual National Salinity Summit, 2009, Las Vegas, NV, 2009.
[15] W.L. Bourcier, T.J. Wolery, T. Wolfe, C. Haussmann, T.A. Buscheck, R.D. Aines, A preliminary cost and engineering estimate for desalinating produced formation water associated with cabon dioxide capture and storage, Int. J. Greenhouse Gas Control 5(5) (2011) 1319–1328.
[16] E.J. Sullivan, S. Chu, P.H. Stauffer, R.J. Pawar, A system model of methods, processes, and costs for treatment of water produced during CO2 sequestration, 9th Annual Carbon Capture and Sequestration Conference, Pittsburgh, PA, May 10–13, 2010.
[17] S. Benson, P. Cook, B. Metz, O. Davidson, H. de Coninck, M. Loos, L. Meyer, IPCC Special Report on Carbon Dioxide Capture and Storage, Cambridge, England, Cambridge University Press, 2005, p. 195.
[18] A. Al-Qaraghuli, Renewable Energy Applications in Water Desalination, New Mexico Water Resources Research Institute 56th Annual Water Conference, New Mexico New Water New Energy, December 11–13, 2011. Alamogordo, NM.