Large-Scale Energy Infrastructure Optimization: Breakthroughs and Challenges of CO₂ Capture and Storage (CCS) Modeling

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Abstract Secure, sustainable, and cost-effective energy development will be one of the greatest global challenges in coming decades. This development will include an extensive range of energy resources including coal, conventional and unconventional oil and natural gas, wind, solar, biofuels, geothermal, and nuclear. CO_2 capture and storage (CCS) infrastructure is a key example; meaningful CCS in the US could involve capturing CO₂ from hundreds of CO₂ sources, including coal-fired and natural gas power plants, and transporting a volume of CO₂ greater than US oil consumption. Here, we highlight breakthroughs and future challenges for CCS infrastructure optimization and modeling. We start with the evolution of CCS infrastructure modeling from early attempts to represent the capture (sources), transport (network), and storage (sinks) of CO₂, through to the integration of more advanced spatial optimization (or location-allocation) approaches including mixed integer-linear programming. We then highlight key future challenges and opportunities, including the representation of significant uncertainties throughout the CCS supply chain and the ability to represent policy and business decisions into CCS infrastructure optimization. Finally, we examine the role that next-generation CCS infrastructure modeling can have in wider massive-scale energy network investments.

Keywords CO₂ capture and storage (CCS) • Spatial optimization • Uncertainty • Mixed integer-linear programs (MIP)

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© Springer-Verlag Berlin Heidelberg 2018 J.-C. Thill (ed.), *Spatial Analysis and Location Modeling in Urban and Regional Systems*, Advances in Geographic Information Science, https://doi.org/10.1007/978-3-642-37896-6_14

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Introduction

Secure, sustainable, and cost-effective energy development will be one of the greatest global challenges in coming decades. This development will include an extensive range of energy resources including coal, conventional and unconventional oil and natural gas, wind, solar, biofuels, geothermal, and nuclear. To meet global energy demands with these resources, energy infrastructure will have to be constructed on an unprecedented scale. In the US alone, this will include construction of perhaps hundreds of power plants, including wind and solar farms and several hundred thousand kilometers of pipelines and transmission lines. Integrating this diverse range of energy sources into an integrated, cost-effective system will take careful and comprehensive planning. Location-allocation modeling, or spatial optimization, should and will be a critical tool in this planning.

 CO_2 capture and storage (CCS) is a climate change mitigation technology that reduces CO_2 emissions by capturing CO_2 at large stationary sources (e.g., coalfired power plants), transporting the CO_2 in dedicated pipelines, and injecting and storing the CO_2 in geologic reservoirs (e.g., deep saline aquifers or depleted oil and gas reservoirs) (Middleton et al. 2012a; Stauffer et al. 2011). To have a meaningful impact, the US alone would have to install CO_2 capture infrastructure on hundreds of coal-fired and gas power plants as well as build a CO_2 pipeline network capable of transporting a volume of CO_2 greater than US oil consumption (Middleton et al. 2012b). Optimizing CCS infrastructure on this scale is large and complex problem, a problem well-suited to spatial optimization. For example, commercial-scale CCS involves capturing CO_2 from point sources, transporting the CO_2 over a network, and delivering the CO_2 to specific sinks. That is, this is a classic source-networksink optimization problem.

Here, we explore and discuss the evolution of CCS infrastructure modeling, from early developments introduced by CCS researchers through to the current state-of-the-art led by experts in infrastructure modeling and optimization. The early researchers used their CCS technology expertise to identify that there was an important source-network-sink problem to solve, but did not necessarily have the required tools to adequately solve CCS problems. Later, researchers with operations research and optimization backgrounds were brought into the equation, establishing classic optimization approaches to the problems. And more recently, CCS infrastructure modeling has begun to mature to the stage where advanced concepts-such as system uncertainty, fluctuating CO₂ flows, and real-world policy-have been integrated into models. Specifically, we identify how spatial optimization has solved many research gaps in CCS modeling, but also discuss how CCS presents a unique set of challenges particularly in scale and uncertainty and that these issues must be resolved going forward. We also highlight how many of the breakthroughs and challenges developed by CCS infrastructure modeling can be solved by a flexible modeling approach and how the solutions developed for CCS modeling can be applied to energy infrastructure in general.

Early CCS Development

The IPCC's Special Report on CCS, published in 2005, illustrates the early emphasis on CO_2 capture technology and economics, with much less emphasis on CO_2 transport and storage (Metz et al. 2005), let alone any mention of integrated infrastructure modeling. This is of no surprise. For instance, the cost to capture CO_2 is still perhaps as much as an order of magnitude more expensive than either the transport or storage of CO₂, hence the early focus on CO₂ capture technology and economics. Arguably, this capture-focus remains today since capture costs still have the greatest flexibility for cost reduction. Similarly, without any large-scale CCS source-network-sink infrastructure in place (largely still true today), system CCS infrastructure modeling and optimization received scant attention. Although geological storage had been proposed in some detail over more than a decade before the IPCC report (Koide et al. 1992), later including storage below the ocean seafloor (Koide et al. 1997), very little advancement in economic characterization of geological storage had been made by the time the IPCC report was compiled and published. At the time, geological storage in deep saline aquifers was widely regarded as a sequestration option with the largest physical potential, a belief borne out by subsequent refinements of storage characterization, most notably the continuing efforts of the US Department of Energy to map out storage potential in North America (USDOE 2010).

The IPCC report devotes some attention to transport costs and very little to storage costs. Without widespread adoption of CCS technology at the time, and indeed with only perhaps a single large commercial CCS project using a pipeline of any length—Weyburn (Petroleum Technology Research Centre 2011)—little attention was paid to CO₂ transportation. Conversely, even without CCS in place, millions of tonnes of natural (i.e., non-anthropogenic) CO₂ have been transported large distances for several decades, taking CO₂ from natural geologic formations (such as salt domes) and injecting the CO₂ into depleted oil fields for enhanced oil recovery (EOR). Currently, EOR annually stores between 50 and 70 million tonnes (50–70 MtCO₂/year) in the US. However, transportation and integrated infrastructure modeling were not a high priority. In short, the IPCC report heavily concentrated on CO₂ capture technology, devoted some attention to geologic storage engineering and costs, but with almost no emphasis on CO₂ transportation and integrated CCS modeling.

The IPCC report relied on just three reports for CO₂ injection and storage costs: Bock (2002), Allinson et al. (2003a), and Hendriks and Bock (1993), a covering a broad geographic range (Australia, the United States, and Europe, respectively). In the US, Bock's report for the Electric Power Research Institute (with the US DOE) found ranges between $0.40/tCO_2$ and $4.50/tCO_2$. In Australia, Allinson et al.'s article in the APPEA Journal found a similar 0.20 to 5.10 per tonne (Allinson et al. 2003b). Hendriks et al. (2004), in a report for Ecofys with the Netherland's TNO, found a range between 1.90 and 6.20 for Europe. Offshore costs were slightly higher and had a wider range, and oil and gas fields were roughly the same (Metz et al. 2005). Perhaps because the ranges were relatively narrow or because their magnitude was so small compared to the estimated cost of capture, most large models seemed to focus on variations in capture parameters as controlling the degree of penetration of CCS. It is in fact rare to find any kind of documentation of transport or storage costs in the stabilization scenario modeling that accompanies many IPCC reports (Bernstein et al. 2007) or in, for example, the US Energy Information Administration's National Energy Modeling system at the time (EIA 2007). Highly sophisticated techno-economic models for power plants focused their attention on capture (Rubin et al. 2005, 2007) since the characteristics of power plant/capture systems were easier to model with little computational effort.

The preferred method for incorporating transport and storage cost estimation into large scale modeling is well-illustrated by Bock's analysis of transport and storage cost for deep saline aquifers in the United States (Bock 2002). By 2000, the Bureau of Economic Geology at the University of Texas at Austin had compiled and digitized maps for 20 aquifers with information on over a dozen geological parameters, all of which might impact the storage capacity of the aquifer, the cost of injecting CO₂, or both (BEG 2000). Bock used this information to estimate the injection rate of CO₂ through a single well, which is an important value because it determines the number of wells that a sequestration site would require and the cost of drilling those wells is a major component of the overall cost of storage (Bock 2002). Although this analysis was almost certainly flawed—for example, it appeared to overestimate the injection rate by a considerable amount (Eccles et al. 2009)—it is certainly a good initial framework for estimating storage costs. The framework presented related total costs and injection rate, which continues to be a good way of representing the cost of CO₂ abatement in cost per tonne. Beyond this, however, the variation in geology and its effect on cost and capacity vanished when this component of the cost model was coupled to the transport component.

Similarly, the cost of transport was simplified drastically. Literature on transport costs at the time revealed that there might be a dramatic variation in the cost of transport depending on the scale at which CO_2 was transported (Kuby et al. 2011b) and the distance the pipeline had to cover (Chandel et al. 2010). Indeed, data on natural gas pipelines showed fairly clearly that although there was a great deal of variation in cost for short pipelines, cost of long pipelines was largely dependent on these two factors (Parker 2004). The transport component of models, then, could simply focus on arriving at two summary statistics for the pipeline network: the average length of pipeline and the average size of a source (or cluster of sources).

Bock's report is an excellent example of this method, in which the author estimates the cost of transport by determining an average distance and power plant size and determining the cost of transport from them (Bock 2002). This philosophy also appears in the IPCC report, where transport costs tend to be summarized by these two variables. Several figures demonstrate how far the understanding of source-sink matching has come just by the scale of their axes—plotting transport costs as a function of distance, the distance variable stretches up into the many thousands of kilometers, which now seems quite unlikely (Metz et al. 2005).

This approach very clearly discards the important fact that although one might summarize any pipeline network by the average size and length of pipelines, the development of that network will rarely include any pipelines that are actually at the average size and length. That is, most sources would face a cost to link to a sink that is different than the average, which might in turn affect their decision to link to that sink or to even capture in the first place. Critical in determining whether it is appropriate to distill the cost of transport (and storage) to average values is understanding the distribution of costs associated with transport. If the cost is not normally distributed or has a high variance, very little certainty is gained by reporting or using average figures in integrated modeling. The averaging approach was clearly meant to simplify first-order calculations in a complex problem, but could not survive very long without investigation as to the nature of variation in actual transport or storage costs.

Later investigations revealed variations in transport cost ranging over tens of dollars per tonne of CO_2 , which is clearly large enough to impact decisions from pipeline routing and storage location all the way to the decision to capture itself, generally dominated by the cost of capture. Using an average length completely discards critical decision information and renders the results of these analyses suspect at best. Early transport cost figures did not include the variation in transport costs that would enable valuable conclusions to be drawn from CCS models.

This variation was clearly understood by the authors of the early studies, but they especially lacked a good framework for estimating how this variation would interact with the geographic and geologic variation in storage costs. This led to a combination of approaches in which each component was analyzed separately and a summarizing statistic or two was used to couple the components together. Thus, instead of interacting, the components could simply be added together to get the total cost of a CCS system.

Until recently, this was how major CCS modeling by the EPA (Dooley et al. 2008) and the EIA (2007) was conducted—the best understanding of a combined average cost of transport and storage was added to better-understood economics of capture and used to estimate the deployment or potential of CCS. This was not limited to government agencies or research organizations; various private estimates also took this approach (e.g., BCG 2008; McKinsey Climate Change Initiative 2008), since it had major advantages in terms of complexity, computational requirements, and data availability.

It was fairly clear, however, that this was not a permanent solution, even to the authors of the IPCC special report, who note that "[t]he full range of costs is acknowledged to be larger than shown" (Metz et al. 2005). While large-scale efforts to improve characterization of storage capacity focused on physical capacity (Ciferno et al. 2010), research into the impact of geological factors on storage cost by Eccles et al. found storage costs that ranged over several orders of magnitude just from the basic cost of injection, ranging from the sub- $1/tCO_2$ found by Bock (2002) all the way up to thousands of dollars per tonne (Eccles et al. 2009).

Such research paralleled decades-old conventional wisdom in the oil and gas industry as well as any other extractive industry: resources are rarely utilized at their average cost, and the economic ease of extraction plays a major role in the resource utilization (Craft et al. 1991). Leaders in the CCS field called for more advanced characterization of storage sites, including the use of techno-economic models to evaluate realistic or economic storage potential (Bachu et al. 2007).

At the same time, modelers began to acknowledge (or advocate) that storage and transport costs could not be taken separately and just added together (Dooley et al. 2008). This was especially clear in the special case of geological storage with enhanced oil recovery. Although deep saline aquifers could (incorrectly) be imagined to be large, homogeneous bodies with similarly homogeneous characteristics, it was entirely obviously that oil fields are quite different from one another, and that not only would the costs of injecting CO_2 in oil fields vary based on the geology, the offsetting revenue from recovered oil would also vary (Nemeth et al. 2011).

Geographic Optimization and CCS

The problem, as presented starkly by EOR assessments, was an excellent opportunity for simple optimization: given various options for storage, each with a capacity and cost, and various agents who might utilize this storage, what configuration of source-sink matching would minimize total costs for the storage and transport system (Middleton et al. 2011)? This early optimization was pioneered by Dooley et al. (2004), who developed an optimization framework that could solve relatively simple versions of the source-sink matching problem. The approach represented a considerable advance over the uncoupled summary statistic one and represented an important move toward geographic optimization.

However, this approach still suffered from a number of drawbacks, possibly stemming from the research questions it may have been meant to solve. The authors devoted time and attention on enhanced oil recovery and geological characterization of the oil fields, but treated saline aquifers as economically homogeneous bodies (Dahowski and Dooley 2004). Although the documentation of the model is sparse, it appears that the cost of storage in saline aquifers for evaluations that are relatively massive in scale (i.e. all of North America and later China) is exactly the same over thousands of square kilometers of these aquifer's surface footprint (Dahowski et al. 2009; Dooley et al. 2004). The saline aquifers, moreover, completely dominate the source-sink matching, in which hundreds of sources in their analysis optimize simply the distance to the closest saline formation and nothing else, which renders the results largely unusable for policy planning.

At the same time, other modelers focused more heavily on understanding or integrating realistic costs of storage and, where possible, doing integrated sourcesink matching with transport optimization (McCoy and Rubin 2008; Middleton and Bielicki 2009; Middleton et al. 2012d). After Dooley et al.'s evaluation of North America, but before Dahowski et al.'s evaluation of China, the EPA (2008) published a detailed estimate of roughly 80 cost categories for geological storage, many of which would depend on geological characteristics or project requirements that stem from the characteristics such as the number of wells required. This allowed researchers to develop advanced semi-analytical models for geological storage, such the one underlying *SimCCS* (Middleton and Bielicki 2009). As more geological data became available, numerical simulations or models based on them, such as CO_2 -*PENS* (Stauffer et al. 2009; Viswanathan et al. 2008), also became more prolific, allowing a much better characterization of geological potential.

At the same time, pipeline optimization and the methods associated with location optimization began to appear in CCS literature. An MIT project developed a cost weighting surface (Herzog et al. 2007), a necessary prerequisite for the cost distance/backlink calculations that form the basis of pipeline routing algorithms. *SimCCS* uses a similar but more detailed surface (Middleton and Bielicki 2009, 2013; Middleton et al. 2012d). Since then, a proliferation of transport models that utilize geographic optimization methods have emerged including Han and Lee (2011), Mendelevitch et al. (2010), Morbee et al. (2012), Kemp and Kasim (2010), and van den Broek et al. (van den Broek et al. 2010).

At this point, the development of transport and storage modeling is now mature enough to have completely integrated capture, transport, and storage components that consider all elements of the CCS system in combination (Keating et al. 2010). The results from integrated models have provided interesting perspectives on the potential of carbon capture and storage.

First, large-scale characterizations of geological storage potential indicate that there is plenty of storage capacity (USDOE 2010). The total technical potential may reach tens of billions of tonnes of storage space in North America alone, which is more than enough to sequester decades or centuries of emissions. This abundance, however, is not necessarily evenly distributed geographically. Just as with oil and gas extraction, it is not possible to utilize a storage resource anywhere. Although sedimentary formations are common across the United States, Eccles et al. (2011) find that the vast majority of cheap, abundant storage potential is concentrated in the Michigan and Ohio Basins, in Cretaceous sediments along the East Coast, and in Texas, especially along the Gulf Coast. Fortunately, these areas are easily accessible for many large CO_2 sources, but in terms of physical surface area, they make up a relatively small portion of sedimentary basins in the United States in general (Eccles et al. 2011).

These findings indicate that at least at first, carbon storage might be utilized for *below* the "average" cost of storage because these large, cheap reservoirs could be easily exploited. From the wrong perspective, the variation in carbon storage potential might lead to the conclusion that because many geological formations are unsuitable for cheap, large-scale storage, the technology does not have much potential for abating climate change. However, an integrated examination of geographic variation in geology indicates that cheap, large-scale storage sites might be deployed first, and thus the initial cost of utilization might be less than a summary statistic might indicate.

Second, transport of CO_2 over long distances can be relatively cheap, with appropriate coordination and scale, enabling the use of large, low-cost reservoirs that may not be proximate to sources. This may be apparent even when simply

examining techno-economic models (McCoy and Rubin 2008) or summaries of transport costs for pipelines (Chandel et al. 2010)—transporting CO₂ at scale (greater than perhaps 10 MT of CO₂ per pipeline route per year) decreases the cost per tonne of transport by a significant amount. Chandel et al. indicate that cost for transport (including labor and materials, both for pipelines and pumping stations) can drop from \$0.018 per tonne per km for low volume transport (roughly 1 MT per year) to under \$0.010 per tonne per km for 10 MT per year; even larger pipelines might see cost drop as low as \$0.006 per tonne per km (Chandel et al. 2010). These numbers put the levelized cost of transport for 250 km of pipeline and 10–20 MT of CO₂ per year at a relatively low \$2/t. This does not include the cost of rights of way, but is obviously smaller in scale than the variation in the cost of geological storage and the total cost of capture.

In earlier versions of geographic optimization, we see the argument that transport and storage will be low-cost because most sources are close to some kind of sink (Dooley et al. 2004; Wildenborg et al. 2004). Geological variations and their impact on cost appear to contradict this, because not every storage site is going to a feasible sink economically. However, we can see that geographic optimization indicates that large-scale transport is relatively low cost and national-scale geological data indicates that there are at least a few huge, low-cost storage options; whether sources and sinks are close to each other may be largely irrelevant.

Large-scale optimization brings these elements together and can more or less easily determine what the nature of an integrated, planned network of pipelines would be and how much it would cost. Integrated optimization is fairly standard for transport and storage modeling. As compared to a decade ago, there are many different models competing for attention in academic literature, where geographers have made a substantial impact on improving and refining our understanding of the physical potential for CO_2 storage and the nature of the infrastructure that would support that storage system.

Issues with Optimization

Advances brought by traditional geographic optimization have not been able to overcome some interesting challenges posed by geological storage and the CCS system in general.

The first most obvious of these is geological uncertainty. CO_2 storage pilot projects have until recently been demonstration-scale, with a few large commercialscale endeavors (Michael et al. 2010). Of these, Sleipner Vest is probably the most well-known of non-EOR projects. From a geological perspective, the Utsira sand, into which the Sleipner project injects about a million tonnes of CO_2 per year, is an ideal environment. It is high-permeability, unconsolidated sand, and even though it is almost 200 m thick, the horizontal well-bore is perforated along only 100 m and can still sustain injection rates of nearly 3000 tonnes per day (Eccles et al. 2009). The Snovhit project was expected to have similar performance to Sleipner Vest, but rapid increases in reservoir pressure early in its operation indicated that the Snovhit geology was not exactly as expected. Consequently, engineers at Statoil had to intervene to increase injectivity (Eiken et al. 2011). From a technical perspective this is a success story since, although the site did not operate as expected, Statoil was able to adapt to the situation. However, from a planning or operations perspective, the project is considered a minor disaster. In a large-scale storage system, Snovhit would not have been a one-off project, it would have been one of an interconnected series of CO₂ storage sites selected for their physical and economic characteristics as better than other sites that would have been more costly to utilize. The unexpected characteristics of Snovhit would have increased its cost and made it less reliable as a CO₂ sink than other sites, but the source-sink matching algorithm would obviously not have been able to take that into account.

Geological uncertainty is especially pernicious because Snovhit was supposedly well characterized (Eiken et al. 2011). Uncertain geologic characteristics can be challenging to incorporate into linear optimization, but Monte Carlo frameworks and other techniques could be used to create hybrid optimization models that would incorporate uncertain characteristics; uncertainty in storage and cost estimates are somewhat linked (Middleton et al. 2012c).

First, optimization models will have to be constrained to require the inclusion of reserve capacity. Snovhit isn't the only storage project with uncertain operating parameters. Even the very small (48 t/day) Nagaoka project experienced wide variations in injection performance, and systems that manage 100-megaton-scale emissions must be able to handle such intermittent performance (Research Institute of Innovative Technology for the, 2007). The cost of possible intermittency must be traded off against the cost of emissions, putting CCS in the same reliability boat as renewables like wind and solar.

Second, models must be able to appropriately digest uncertain operating parameters and provide useful results the incorporate the known uncertainty in geology. This is distinct from the problem of including reserve capacity in that reserve capacity is generally meant to accommodate short-term issues with performance. In electrical production and transmission, this might be the failure of a generator but not necessarily the complete removal of that generator from the grid. With geological storage, there can be considerable uncertainty as to the performance of the sequestration site on a long-term basis, as with Snovhit. Although various sensing techniques can mitigate this uncertainty, it is entirely possible that in addition to seeing daily fluctuations in the capacity of an injection well, a storage site operator might encounter systemic flaws in geology which permanently reduce the operating capacity of the site (Middleton et al. 2012c).

This might not even be the result of geological uncertainty. Underground injection has long-lived effects on the pressure environment, which reduces the injectivity of wells and requires compensation through either increased injection pressure or active reservoir management or simply toleration of the reduced performance (Eccles et al. 2012). In some cases, active reservoir management may be too expensive (because of fluid disposal costs) or increasing pressure may not be

feasible (because the pressure may be near the fracture limit), which would mean that tolerance for decreased performance might be the only option. If wells are not correctly spaced, this decreased performance could be dramatic (Eccles et al. 2012). Perhaps most importantly, the decreased performance is more or less directly related to the permeability of the formation, the parameter at issue in the Snovhit problems.

The optimization framework must therefore not only account for short-term reserve capacity, but also the cost of building out the system to account for possible long-term disruptions. The degree and nature of the long-term disruptions is in many ways quite uncertain, more or less in direct relation to the degree to which geological conditions are well-characterized.

In addition to accounting for geological uncertainty, spatial optimization must take into consideration complex decision variables in which different components of the CCS system might interact in unexpected ways. This somewhat ambiguous statement is best illustrated in the consideration of peaking plants and the dispatch of power (Middleton and Eccles 2013). Traditionally, CCS is modeled as a monolithic technology with constant operation that matches the capacity factor of the source to which it is attached. For baseload coal plants, this is not necessarily incorrect, but for plants with high ramp rates that operate as peaking plants or load-following plants, there is an interesting problem: what size should the capture facility be? It could be sized anywhere from zero to the maximum CO_2 output of the plant – depending on the plant's dispatch characteristics, though, it could be underutilized to a considerable degree. If the plant is a peaking natural gas plant, it might sit unused for most of the day, which obviously affects the economics of its operation.

The key element of the problem is the cost of CO_2 disposal vs. the cost of emissions (Middleton and Eccles 2013); with a high enough carbon price (or, critically, a low enough disposal cost) the plant would oversize its capture equipment. The carbon price is a matter of policy and is essentially out of the hands of the modeler (Kuby et al. 2011a), but the disposal cost can be a decision parameter. Whether the plant sends its emissions to a local EOR producer vs. sending them to a big, centralized CCS facility a few states over is critical to the initial decision of installing capture equipment, a feedback loop that is challenging to incorporate into the structure of geographic optimization models.

Broadly speaking, this decision comes down to incorporating the option to underutilize infrastructure. There are other reasons to underutilize infrastructure (or the equivalent, to oversize its initial construction), which includes resources coming online at different times and the storage capacity or reserve capacity of underutilized infrastructure. But these decision options need to be integrated very carefully with the simple but powerful source-sink matching optimization that currently exists. Even something as unobtrusive as fault tolerance (what happens when a pipeline goes down?) needs consideration in planning, optimization, and cost estimation.

Finally, slow movement on climate change policy has thrown into sharp relief the unusual question of the nature of the objective function. Lacking a financial incentive to avoid emissions, proponents of CCS have turned to carbon utilization as a motivation for CCS deployment. Carbon dioxide is currently used most widely in EOR, where each tonne of injected CO_2 might extract 3 (using industry standards) or more (using reservoir modeling) barrels of oil. At the current price of oil, it is not difficult to see that the financial incentives for capture are much different than we might expect under a carbon price, which has led to renewed interest in enhanced oil recovery using CCS as the source for the CO_2 .

In this environment, it is not necessarily appropriate to minimize costs: the actors in the system would rather want to maximize revenue, especially the oil producers. It was never particularly clear what entities would be operating the pipeline transport or CO_2 storage portions of the CCS system, but in the current environment, it seems it is almost certainly not going to be the same entity that operates the CO_2 source, so the different motivations must be integrated into optimization modeling. Additionally, echoing earlier issues of uncertainty, this environment might dramatically change over the planning lifetime of a CCS project. It is certainly not out of the question that even the somewhat recalcitrant United States might have a carbon price in the next two decades; what impact would this have halfway through the planning and/or deployment of a large-scale carbon storage system? How will the policy treat stranded capital or ongoing investments? Perhaps more importantly, will the policy itself be based on the lessons learned or results from optimization modeling and deployment of CCS systems?

Beyond these questions of uncertainty and motivation, it is clear that deployment of CCS on the scale that would impact CO_2 emissions dramatically is an application of geographic optimization that has never been seen before. The CO_2 emissions from the US electric power sector alone would produce the same volume of (compressed) CO_2 as the entire would consumes in oil. We have certainly used geographic optimization for pipeline planning and transport optimization, but never at such a large scale. The idea of designing a system that would move a billion tonnes of CO_2 from the ground up is mind-boggling, and there are almost certainly challenges of working at that scale that have not even been considered, much less integrated into modeling.

Flexible Modeling Approach

To deal with these issues, a flexible modeling approach that draws from the best traditions of spatial optimization is necessary. As the name implies, flexible modeling could involve many different techniques to modify basic network-sink optimization. Some of these variations might be innovative applications of linear programming, and some might involve extending linear optimization to mixed-integer programming, using creative constraints or decision variables, or even shifting to hybrid approaches, especially involving unconventional optimization modeling.

Mixed-integer programming is the easiest technique to incorporate, as is clear from the fact that it is already used in several optimization models (Middleton and Bielicki 2009; Morbee et al. 2012). One reason to use mixed-integer programming is the prevalence of fixed pipeline sizes in industry and modeling; pipelines have to be scaled to accommodate the optimum CO_2 flux but have to use one of the fixed pipeline sizes, so MIP has to be used (Middleton 2013). MIP techniques are common in transport optimization, and thus it may not be particularly revolutionary to say that they should be used here. At the same time, however, MIP solutions take more computation to find, so MIP models have to be constructed or deployed carefully in complex or very large-scale optimization problems.

MIP's limitations are especially important when the issues of geological uncertainty and peaking plant's decision options (i.e. how much capture capacity to install) are considered. At first glance, this may not be apparent. Reserve requirements that can mitigate daily fluctuations in transport or sequestration capacity may simply require constraints in a MIP model that would overbuild capacity given probabilities, expected values, and so on. Even longer-term issues might also be solved with clever MIP applications such as, for example, multiple time periods for capacity to come online to deal with reduced performance with possible acceleration or the equivalent of spinning reserves in electricity transmission applied to CCS systems (Middleton et al. 2012e). This dramatically increases the complexity of the MIP problems to be solved, but that is not necessarily prohibitive.

However, modelers may want to consider a more flexible solution, which is to employ a variety of techniques at different scales specifically designed to incorporate uncertainty and probability. At local scales for individual projects, this might not be much different than the techniques we see today. But at larger scales with more uncertainty, modelers may wish to take advantage of Monte Carlo techniques. To deal with large-scale geological uncertainty, Monte Carlo models might solve many variations on the same problem to arrive at a variety of outcomes and distributions of their costs; this has previously been done with CCS and MIPs (Middleton et al. 2012c). In transportation routing, this is of course very challenging to interpret, because it is in some ways only the beginning of the decision process that leads to a build-out on the ground. Nonetheless, it can be paired with the moredetailed local routing to give industry stakeholders and policymakers a multi-scale tool that could correctly incorporate uncertainty and risk at some levels but provide useful, detailed routing and cost information at other levels.

Beyond iterating network-sink problems in a Monte Carlo framework, evolutionary or agent-based algorithms deployed at the right scale could also narrow decision options and also provide a "fuzzier" picture of optimal decisions. These types of algorithms, in some ways like Monte Carlo models, can give multiple decision options that are close to the optimum, which might be especially useful in accounting for geological uncertainty or determining how to plan simulations are a more detailed scale. They have another advantage, which is that they tend to incorporate behavior by the agents involved (like power plant, pipeline, and storage site operators) that is easier to tweak or to limit so as to match the conditions or behavior that are observed in the real world. These agent models might be especially effective if the agents solve simple transport optimization problems as part of the model structure.

A variety of models using different techniques at different scales might thus incorporate varying degrees of complexity in transport optimization yet in their entirety provide more value than a rigid approach to multi-scale modeling using linear or mixed integer programming alone. The flexible suite of models allows evaluation of CCS resources, decisions, and policy and many levels and with many degrees of confidence, from the detailed and somewhat traditional pipeline routing at a local or project level used to actually plan a CCS installation to the plethora of techniques that can be applied at national or international scales to assess the mitigation potential of the resource.

Regardless of the structure of these models in the future, it is fairly clear that spatial optimization has dramatically improved the assessment of CCS at all scales already. The flexible approaches of the future will continue to refine our understanding of CCS potential in the energy system. Perhaps most importantly, the unique challenges presented in CCS modeling may provide valuable insight into hybrid or flexible modeling techniques in other arenas, generalizing the issues and solutions to spatial optimization as a field.

The scalable, flexible approach is almost certainly applicable to energy infrastructure modeling as a whole. Spatial optimization is critical in understanding the deployment of future energy projects, from transmission for wind projects (e.g., Phillips and Middleton 2012) to the CCS pipeline infrastructure issues described above. Other resources are likely to have the same or more uncertainty as we find in CCS. Intermittency in renewable generation is another critical issue that will impact its deployment and the deployment of infrastructure that supports it, another clear application of spatial optimization with uncertain parameters that might require a flexible approach. Integrating plugin hybrid electric vehicles as an energy storage system in the smart grid of the future likewise requires different approaches to deal with uncertainty at different scales.

The techniques that will be developed to deal with the issues in CCS optimization will almost certainly have value in these and other arenas, making them not simply useful to the CCS research community, but to the larger energy infrastructure research community and to the field of spatial optimization. Flexible modeling approaches can help solve critical challenges in energy production in the future, in a world constrained by climate change and resource allocation as well as increasing demand. Spatial distribution of resources will be a feature of the energy infrastructure of the future for decades to come, and location allocation will thus be an invaluable tool in understanding and planning for the energy needs of civilization in years to come (Figs. 1 and 2).



Fig. 1 Schematic of the CO₂ capture and injection/storage process; CO₂ transport is not depicted



Fig. 2 Variability of CO_2 injection and storage costs for major deep saline aquifers in the United States (Eccles et al. (2011))

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