RSC Advances

Supplementary Information

Prospective Life-cycle Modeling of a Carbon Capture and Storage System Using Metal-Organic Frameworks for CO_2 Capture

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http://dx.doi.org/10.1039/c3ra40265g

Tables

Figures

Table S1. Low, middle (base-case), and high estimates of key model parameters.

Parameter	Unit	Low	Middle	High
Coal supply				
Coal from newly constructed mines	percent	20%	**50%**	80%
Coal transport distance	km	400	**1000**	1600
MEA capture				
MEA consumption	kg per tCO_2 captured	1.50	**2.50**	4.00
MEA cost [a]	\$ per t	1275	**1700**	2125
MEA production GHG emissions	tCO_2e per t	2.6	**3.4**	4.3
MOF capture				
MOF working capacity [b]	percent	14%	**18%**	24%
MOF regeneration energy	MJe/tCO_2	200	**400**	600
Capture/regeneration cycle time	minutes	30	**60**	90
Life span of MOF	number of capture cycles	12000	**8000**	4000
Relative capture auxiliary load, MOF/MEA [c]	percent	100%	**100%**	150%
Capture bed utilization factor	percent	100%	**100%**	90%
Organic ligand cost	\$ per t	1000	**1400**	1800
Organic ligand production energy	GJ per t	50	**68**	96
Organic ligand production GHG	tCO_2e per t	0.2	**1.3**	3.2
Metal cost [d]	\$ per t	260	**300**	1000
Metal production energy	GJ per t	0.9	**8.3**	20.9
Metal production GHG	tCO_2e per t	0.1	**1.0**	3.0
Recycling rate for metal in post-use MOF	percent	99%	**95%**	80%
Solvent cost	\$ per t	400	**800**	1300
Solvent production energy	GJ per t	45	**75**	100
Solvent production GHG	tCO_2e per t	1.2	**2.4**	4
Mass ratio, solvent/MOF	ratio	0	**70**	200
Solvent recycling rate	percent	98%	**90%**	75%
MOF synthesis cost	\$ per t	400	**940**	3240
MOF synthesis energy	GJ per t	0.27	**15**	61
MOF synthesis GHG	tCO_2e per t	0.02	**0.88**	3.6
MOF synthesis reaction yield	percent	100%	**85%**	70%
CO_2 transport and storage				
Length of feeder line from plant to trunk line	km	50	**100**	150
Length of trunk line to sequestration site	km	100	**200**	300
Compression pressure	bar	160	**150**	140
Wall thickness of pipeline	mm	15	**18**	21
CO_2 leakage	t CO_2 per year per km pipeline	0.14	**1.4**	14
Downstream re-compression needed	yes or no	no	**yes**	yes
Baseline transport cost	\$ per tCO_2 transported	4.5	**6.0**	7.6
Baseline injection cost	\$ per tCO_2 injected	4.0	**5.3**	6.6
Depth of injection well	m	800	**1200**	2000
Costs of MOF system relative to MEA system				
Capital cost of flue gas cleaning, MOF/MEA	percent	100%	**100%**	150%
Capital cost of capture system, MOF/MEA	percent	100%	**150%**	200%
O&M cost of flue gas cleaning, MOF/MEA	percent	100%	**100%**	150%
O&M cost of capture system, MOF/MEA	percent	100%	**100%**	150%
Learning rates				
Learning rate, capital cost, generation	[e]	0.09	**0.06**	0.03
Learning rate, O&M cost, generation	[e]	0.3	**0.15**	0.07
Learning rate, capital cost, flue gas cleaning	[e]	0.18	**0.12**	0.06
Learning rate, O&M cost, flue gas cleaning	[e]	0.3	**0.22**	0.1
Learning rate, capital cost, CO_2 capture (MEA)	[e]	0.17	**0.11**	0.06
Learning rate, O&M cost, CO_2 capture (MEA)	[e]	0.3	**0.22**	0.1
Learning rate, capital cost, CO_2 capture (MOF)	[e]	0.17	**0.11**	0.06
Learning rate, O&M cost, CO_2 capture (MOF)	[e]	0.3	**0.22**	0.1
Learning rate, capital cost, CO_2 compression	[e]	0.1	**0**	0
Learning rate, O&M cost, CO_2 compression	[e]	0.1	**0**	0
Learning rate, CO_2 transport	[e]	0.09	**0.06**	0.03
Learning rate, CO_2 injection	[e]	0.09	**0.06**	0.03
Learning rate, minimum installed capacity	GW	5	**10**	10
Learning rate, maximum installed capacity	GW	150	**100**	50

Learning rate, maximum cumulative transport	Gt-km	390	**260**	130
Learning rate, maximum cumulative injection	$MtCO_2$	4500	**3000**	1500

[a] High/low values are plus/minus 25% of base-case value

[b] Mass of recoverable CO_2 per cycle, as a percentage of the mass of the MOF material

[c] Auxiliary energy load (for pumps, fans, etc.) of MOF capture system relative to MEA capture system

[d] Middle cost value is for magnesium nitrate hexahydrate (98%) as feedstock; High cost value is for refined magnesium metal, adjusted to account for lower elemental metal content in base-case metal salt

[e] Learning rates are expressed as fractional reduction in unit cost for each doubling of total production or capacity

Table S2. Base-case performance and cost assumptions for three generations of power plants with no CO_2 capture and with MEA- and MOF-based capture systems.

	Sub-critical			Super-critical			Ultra-super-critical		
	No capture	MEA capture	MOF capture	No capture	MEA capture	MOF capture	No capture	MEA capture	MOF capture
Heat rate (MJ/MWh)	10498	14349	13353	9359	12344	11574	8314	10551	10007
--Turbines	10498	10498	10498	9359	9359	9359	8314	8314	8314
--Capture media regeneration	0	2093	1219	0	1623	938	0	1216	725
--CO_2 compression	0	1465	1363	0	1136	1065	0	851	807
--Auxiliary capture loads	0	293	273	0	227	213	0	170	161
Generating efficiency (%, HHV)	34.3	25.1	26.9	38.5	29.3	31.2	43.3	34.1	35.8
Coal feed (t/MWh)	0.41	0.57	0.53	0.37	0.49	0.46	0.33	0.42	0.39
CO_2 emitted (t/MWh)	0.93	0.13	0.12	0.83	0.11	0.10	0.74	0.09	0.09
CO_2 captured (t/MWh)	0.00	1.15	1.07	0.00	0.98	0.92	0.00	0.84	0.80
Levelized capital costs (¢/kWh)									
Boiler/turbine/generator	0.00[a]	0.00[a]	0.00[a]	2.63	3.26	3.05	2.69	3.18	3.02
Flue gas cleaning	0.00	0.63	0.58	0.49	0.60	0.56	0.50	0.59	0.56
CO_2 capture	0.00	0.94	1.31	0.00	0.90	1.27	0.00	0.88	1.25
CO_2 compression	0.00	0.21	0.19	0.00	0.20	0.19	0.00	0.20	0.19
Levelized O&M costs(¢/kWh)									
Boiler/turbine/generator	0.50	0.61	0.56	0.50	0.61	0.57	0.50	0.61	0.57
Flue gas cleaning	0.36	0.44	0.41	0.36	0.44	0.41	0.36	0.44	0.41
CO_2 capture w/o media	0.00	0.34	0.32	0.00	0.34	0.32	0.00	0.34	0.32
CO_2 capture media	0.00	0.44	0.63	0.00	0.44	0.63	0.00	0.44	0.63
CO_2 compression	0.00	0.04	0.04	0.00	0.04	0.04	0.00	0.04	0.04
Fuel costs (¢/kWh)									
Fuel cost in 2010	1.90	2.60	2.42	1.70	2.23	2.09	1.51	1.91	1.82
Fuel cost in 2050 (reference)	1.92	2.63	2.44	1.71	2.25	2.11	1.52	1.93	1.83
Fuel cost in 2050 (high)	4.17	5.71	5.31	3.72	4.90	4.59	3.30	4.20	3.98

[a] Capital costs of existing plants are assumed to be fully amortized.

Table S3. Energy use, CO_2 emissions, and energy cost per ton of material, for gate-to-gate processing of 36 proxy materials. Feedstock energy and supply chain energy is not included.

Material	Primary energy [a] (GJ per ton)	CO_2 emissions [b] (ton CO_2 per ton)	Energy cost [c] ($ per ton)
Ethylene	20.8	1.25	157
Polyethylene	7.0	0.38	34
Ethylene Dichloride	9.6	0.57	68
Polyvinyl Chloride	4.1	0.24	27
Ethylene Oxide	6.4	0.36	39
Ethylene Glycol	7.3	0.42	46
Polyester	33.6	2.00	242
Propylene	4.3	0.25	29
Polypropylene	2.1	0.12	12
Propylene Oxide	8.2	0.48	54
Acrylonitrile	3.0	0.18	20
Acrylic Fibers	60.7	3.60	433
BTX	3.3	0.20	25
Benzene	2.9	0.17	22
Ethylbenzene	3.5	0.21	27
Styrene	39.2	2.39	315
Polystyrene	5.9	0.36	44
Cumene	1.7	0.10	13
Phenol/Acetone	20.1	1.21	152
Terephthalic Acid	7.1	0.40	42
Cyclohexane	4.8	0.28	35
Adipic Acid	49.1	2.91	351
Caprolactam	35.1	2.10	259
Nylon 6,6	55.6	3.24	366
Nylon 6	34.0	2.01	236
Chlorine/Sodium Hydroxide	42.2	2.33	216
Sodium Carbonate	8.5	0.51	65
Ammonia	32.6	1.87	214
Urea	2.5	0.15	17
Nitric Acid	0.6	0.04	5
Ammonium Nitrate	1.4	0.08	8
Ammonium Sulphate	12.8	0.74	85
Sulfuric Acid	0.3	0.02	1
Phosphoric Acid	5.8	0.34	38
Ammonium Phosphate	1.1	0.07	7
Superphosphate	3.2	0.18	18
Mean	15.0	0.88	103
Minimum	0.27	0.02	1.4
Maximum	60.7	3.60	433

[a] End-use fuels and primary energy associated with end-use electricity used within the production facility (Reference 33). Energy export from exothermic processes, feedstock energy value, and raw material supply chain energy use is not included.

[b] CO_2 emissions from energy use. Fuel emissions based on IPCC default emission factors for stationary fuel combustion in manufacturing industries (Reference 34). Electricity emissions based on average US electricity grid emission intensity in 2008.

[c] Cost of end-use fuels and electricity in 2010 dollars, based on projected average cost from 2010 to 2050 of fuels (Reference 13) and electricity (calculated within the model).

Table S4. Primary energy use and GHG emissions associated with cradle-to-gate production of 10 organic materials.

Material	Primary energy use (GJ per ton)[a]				GHG emissions (tCO_2e/t)[b]
	Process energy	Feedstock energy	Raw material supply chain	Total embodied energy	
BTX	3.3	74.3	0.9	78.5	0.24
Cyclohexane	4.8	49.3	3.9	57.9	0.39
Benzene	2.9	54.1	1.0	58.1	0.25
Ethylbenzene	3.5	44.2	6.9	54.6	0.69
Styrene	39.2	46.6	10.4	96.2	3.18
Cumene	1.7	44.3	3.7	49.7	0.24
Phenol/Acetone	20.1	35.1	5.1	60.3	1.59
Terephthalic acid	7.1	43.7	2.1	52.9	0.56
Adipic acid	49.1	33.5	3.4	85.9	3.17
Caprolactam	35.1	48.8	4.9	88.8	2.47
Mean	16.7	47.4	4.2	68.3	1.28
Minimum	1.7	33.5	0.9	49.7	0.24
Maximum	49.1	74.3	10.4	96.2	3.18

[a] Primary energy use based on Reference 33

[b] GHG emissions are based on average US electricity grid emission factor and IPCC default emission factors for stationary fuel combustion in manufacturing industries (Reference 34). Emissions from raw material supply chain assume diesel fuel is used for mining, drilling, transportation, etc. No emissions are assigned to feedstock energy.

Table S5. Estimated global mine production and global reserves of various metals in 2010 (Reference 45). In cases where end-use is a metal compound, we converted mass to elemental metal.

Metal	Global mine production (million tons per year)	Global reserves (million tons)	Major mine producing countries
Aluminum	41.4	7409	China, Russia, USA
Chromium	7.6	120	South Africa, Kazakhstan, India
Cobalt	0.088	7	Congo, Zambia, China
Copper	16.2	630	Chile, Peru, USA
Iron	1130[a]	87000	China, Brazil, Australia
Manganese	13.0	630	China, Australia, South Africa
Magnesium	6.3[a]	775[b]	China, Russia, Israel
Nickel	1.6	76	Russia, Indonesia, Philippines
Titanium	3.9	414	China, Japan, Russia
Vanadium	0.056	14	China, South Africa, Russia
Zinc	12.0	250	China, Peru, Australia
Zirconium	0.88	41	Australia, South Africa, USA

[a] 2008 data

[b] Data from: S.E. Kesler, *Mineral Resources, Economics, and the Environment*, Macmillan College Publishing, New York, 1994.

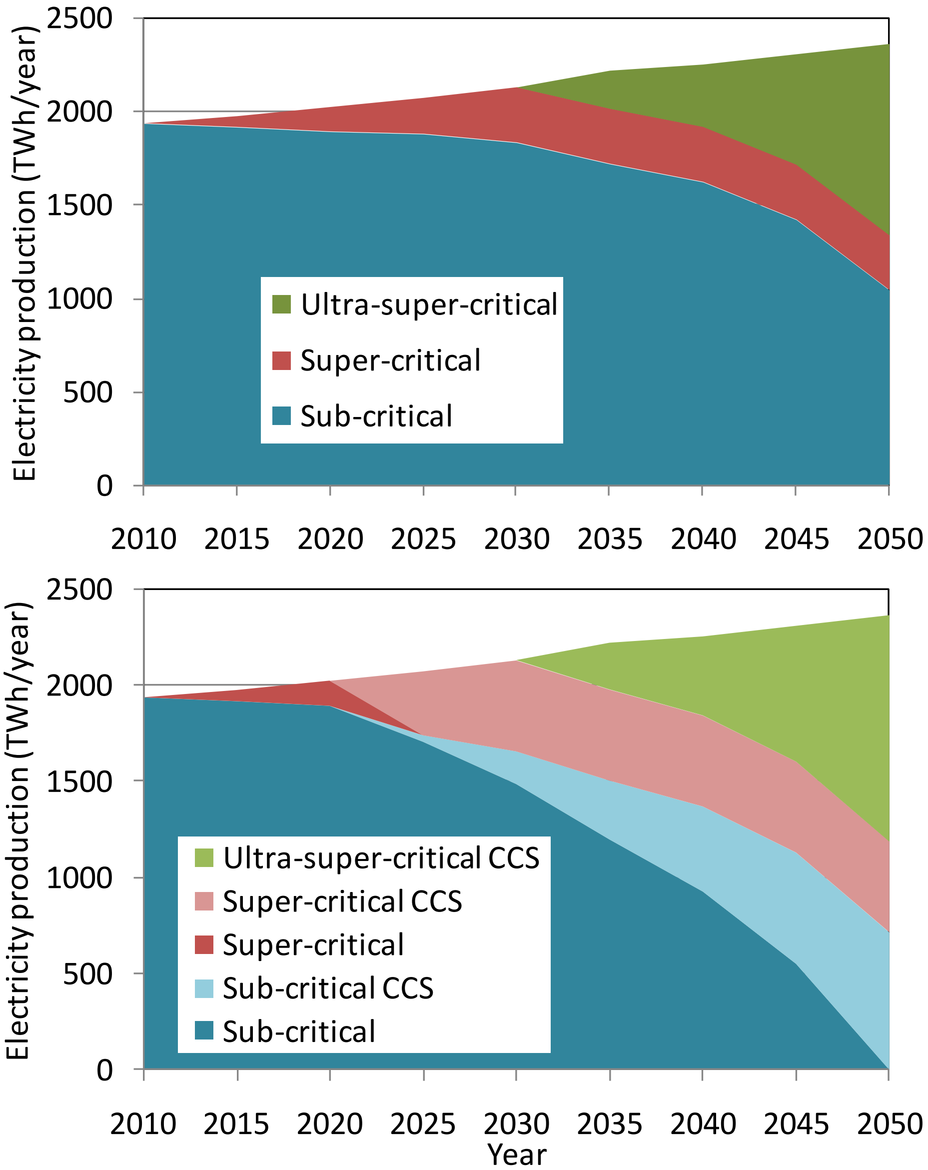

Figure S1. Illustrative scenarios of US coal-fired electricity production from 2010 to 2050 with three successive generations of efficiency technologies, without CCS (top) and with CCS deployed in retrofitted and new power plants (bottom).

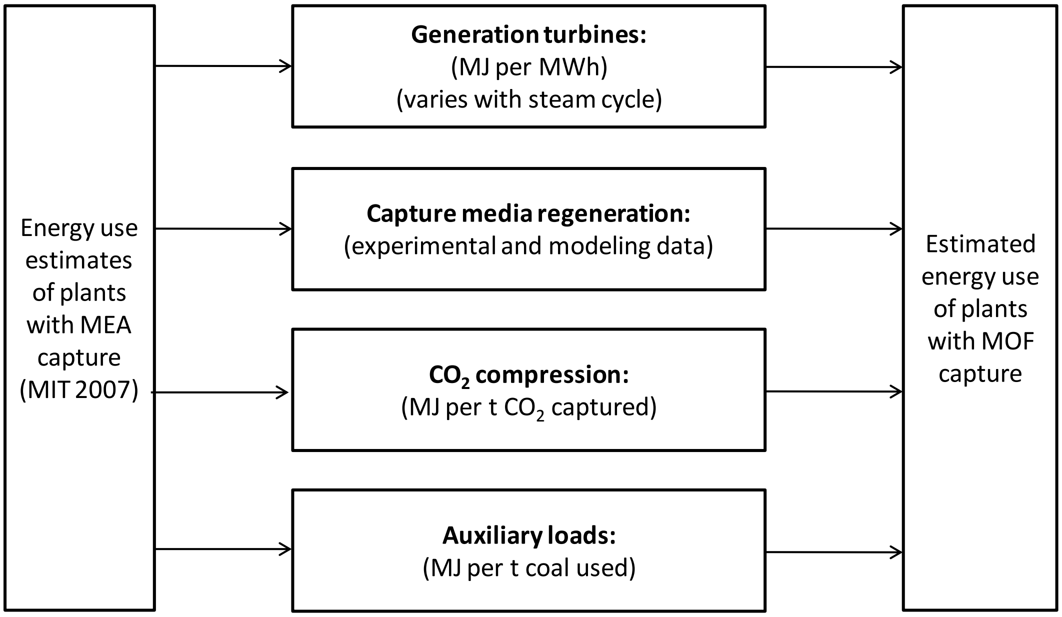

Figure S2. Framework for energy use modeling of power plants with MOF capture.

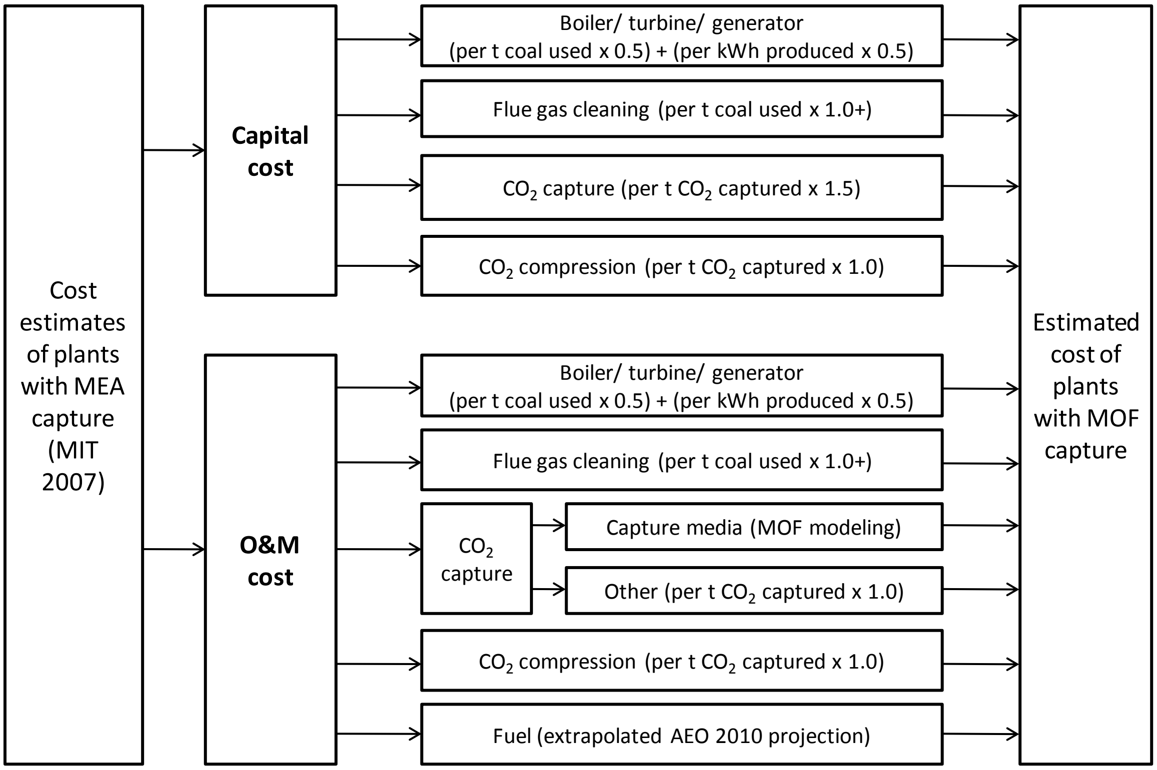

Figure S3. Framework for cost modeling of power plants with MOF capture.

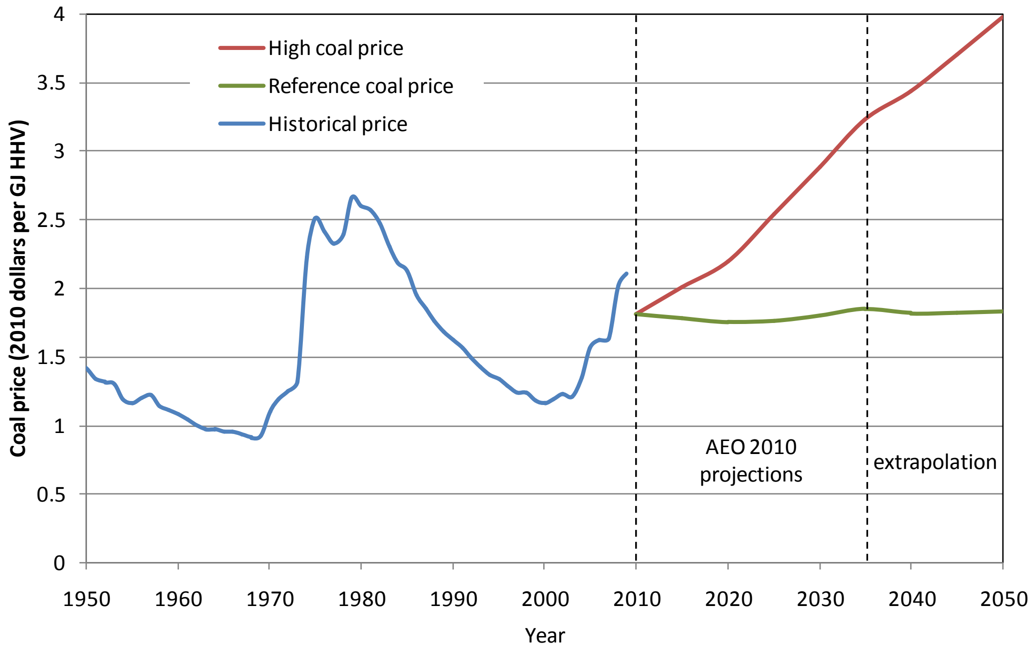

Figure S4. Historical and projected coal prices ($\$ GJ^{-1}$). Coal is Illinois bituminous with HHV ≈ 25.35 $GJ\ t^{-1}$.

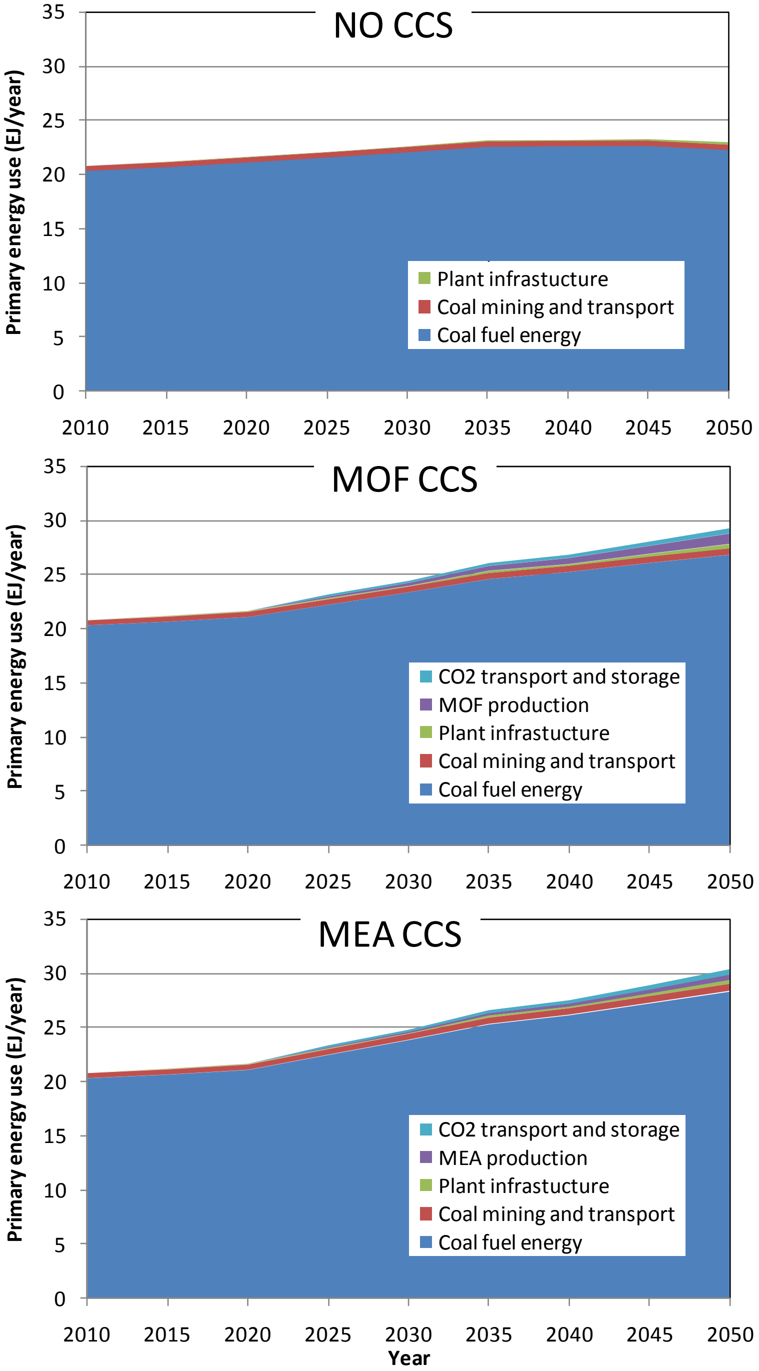

Figure S5. Estimated system-wide primary energy use (EJ y^{-1}) from 2010 to 2050 for cases with no CO_2 capture and with MOF- and MEA-based capture systems.

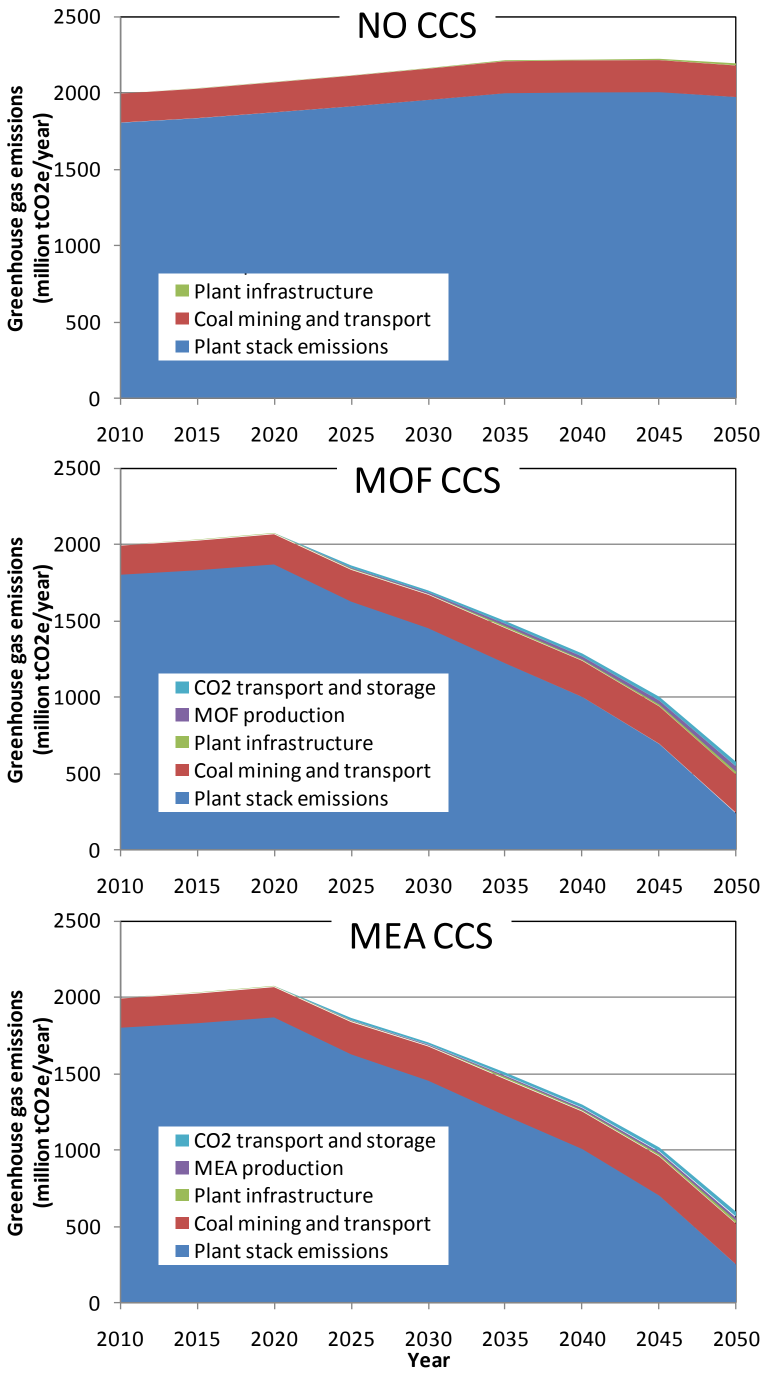

Figure S6. Estimated system-wide GHG emissions (million $tCO_2e\ y^{-1}$) from 2010 to 2050 for cases with no CO_2 capture and with MOF- and MEA-based capture systems.

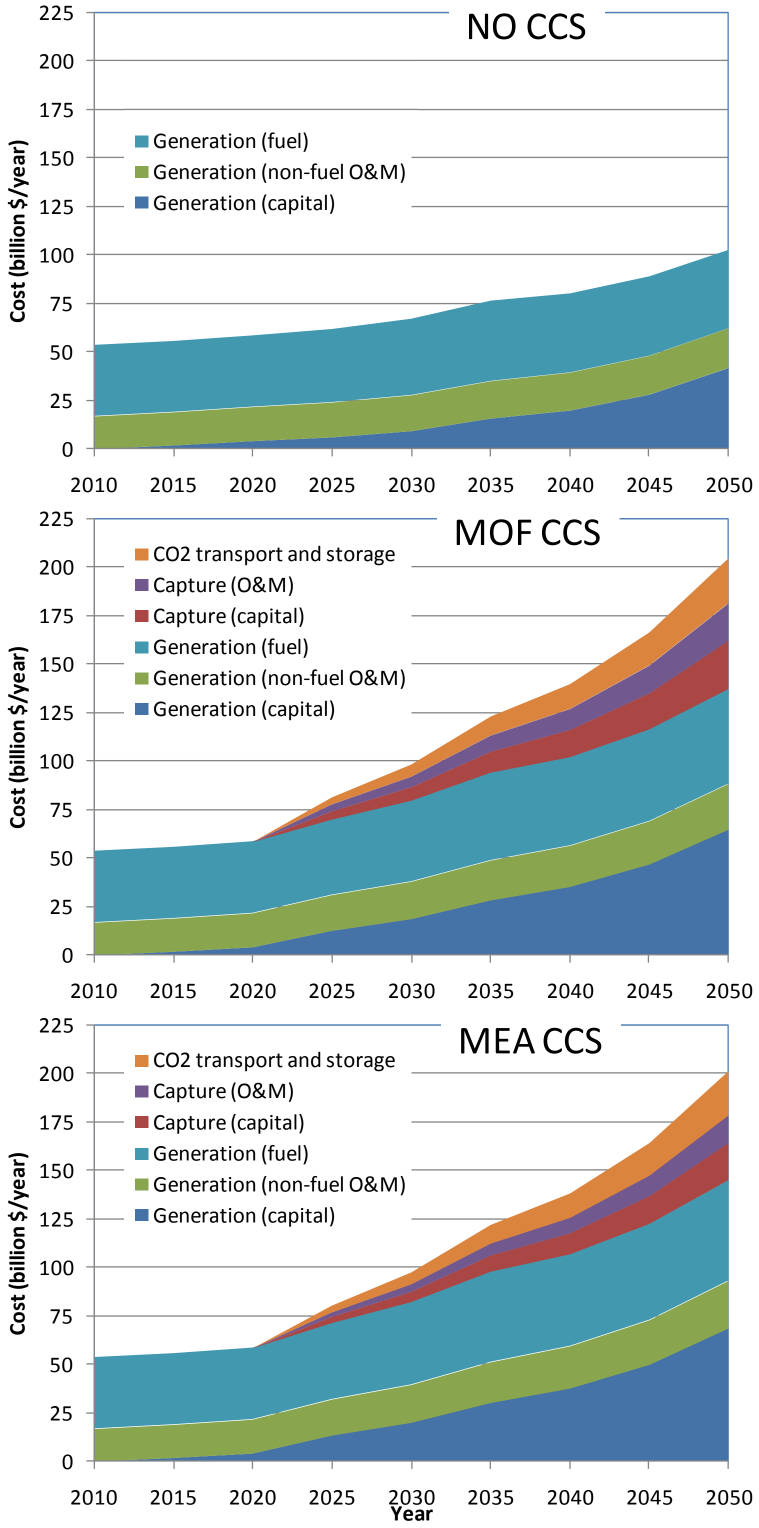

Figure S7. Estimated total system cost (G$ y^{-1}) from 2010 to 2050 for cases with no CO_2 capture and with MOF- and MEA-based capture systems.

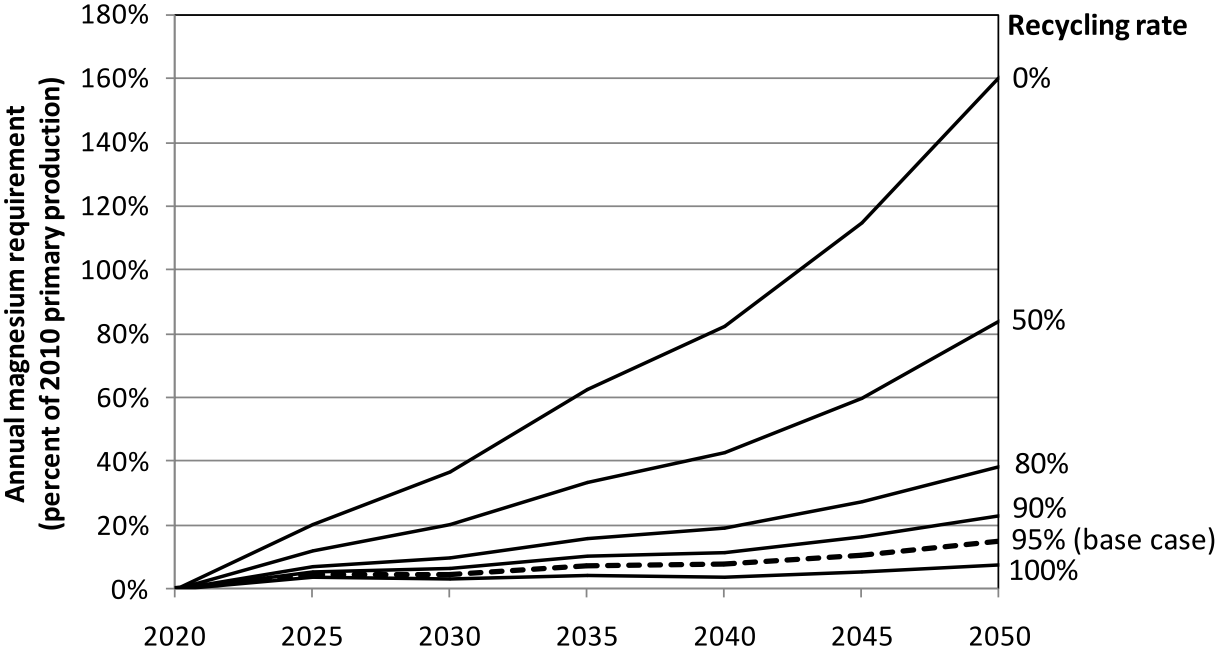

Figure S8. Estimated annual primary metal requirement for MOF production, expressed as a percentage of 2010 primary magnesium production, as a function of recycling rate of metal in post-use MOF material.

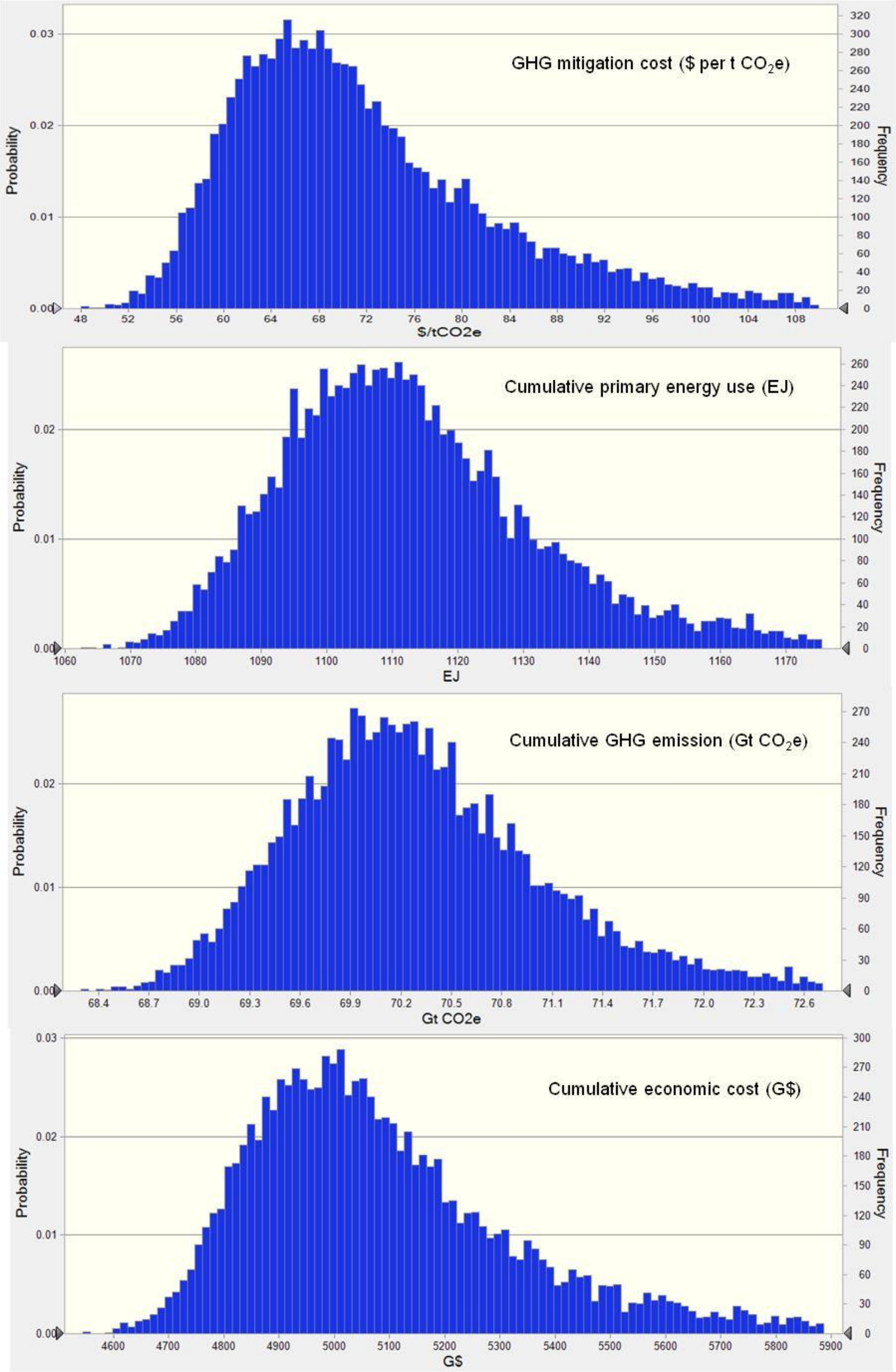

Figure S9. Outcomes of Monte Carlo simulation of full-scale deployment of MOF-based carbon capture and storage in the US coal-fired power fleet through 2050: GHG mitigation cost ($ per tCO_2e), total cumulative primary energy use (EJ), total cumulative GHG emissions (Gt CO_2e), and total cumulative cost for coal-fired electricity production (G$).