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Electronic Supporting Information

Power generation from chemically cleaned coals: do environmental benefits of firing cleaner coal outweigh environmental burden of cleaning?

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Content

S1 Details of chemical cleaning of coals

Recall, that the configuration of the system (such as types of equipment needed) for acid and alkali-acid leaching procedures was based on that proposed by Brooks et al. (2004), and was combined with process conditions (such as types and concentration of acids and/or alkali, reaction temperature and duration) retrieved from studies identified during the literature review.

Chemical cleaning consist of either two leaching steps (alkali and acid leaching), or one step (acid leaching). Both steps are done by mixing the coal with a liquid into a slurry that is heated to leach out ash and sulfur (Brooks et al. 2004). During alkali leaching, alkali dissolves silica and alumina from clay and also other silica and alumina bearing materials present in the coal, forming soluble sodium silicate and sodium aluminate (Mukherjee and Borthakur 2001) (see Eq. S1 and Eq. S2). Ash removal efficiency generally increases steadily as a function of NaOH concentrations, until around 20% NaOH where the rate of ash removal slows down. This is likely due to an initial transformation of the easily accessible minerals which already occurs at low NaOH concentrations. At higher NaOH concentrations the leaching starts to affect firmly bound minerals within the coal matrix, these are not easily removed so the extent of ash removal will not increase much from increasing NaOH concentration (Dash et al. 2013).

$$SiO_2 + 2NaOH \rightarrow Na_2SiO_3 + H_2O \tag{S1}$$

$$Al_2O_3 + 2NaOH \rightarrow 2NaAlO_2 + H_2O \tag{S2}$$

The reaction products in Eq S1 and Eq S2 are not very soluble in alkaline solutions, while the products are soluble under acidic conditions (Sharma and Gihar 1991). This is important for the acidic leaching as this removes the soluble derivatives during the acid leaching (Eq. S3 show an example of this reaction with sulfuric acid).

$$Na_2SiO_3 + H_2SO_4 \rightarrow Na_2SO_4 + H_2SiO_3 \tag{S3}$$

Increasing temperature is known to increase the speed of chemical reactions. An increase in temperature will therefore yield a faster reaction between leaching solutions and the coal minerals. This has previously been shown by experimental work, where increased temperature gave larger ash reductions (Waugh and Bowling 1984; Z.Y. Wang et al. 1986; Çulfaz et al. 1996).

S2 Geographical scope of important processes in coal life cycle

Details of the geographical scope for the base scenario (*i.e.* Europe) and for the geographical sensitivity scenarios (*i.e.* U.S.A. and China) are shown in Table S1.

Table S1 Geographical scope of the main process used for the base and geographical sensitivity scenarios

	European scenario (base scenario)		**U.S.A. scenario**		**China scenario**	
Process	Geographical scope	*Details*	Geographical scope	*Details*	Geographical scope	*Details*
Bituminous and Sub-bituminous extraction and supply	German	*Coal supply is based on information about import of coal to Germany from various global coal mining locations.*	U.S.A.	*Coal is mined and extracted in U.S.A. and transported from mining location to storage area by train* (Dones et al. 2007)	China	*Coal is mined and extracted in China and transported from mining location to storage area by train* (Dones et al. 2007)
Lignite extraction and supply	EU average	*Inventory only includes EU averages. Lignite for European use is primarily extracted in Germany (40%), Poland (15%) and Greece (15%)* (Dones et al. 2007)	EU average	*Inventory data on lignite mining in U.S.A. is not available. Because lignite mining is considered as an established technology, lignite mining in Europe and the impacts associated are assumed to be the same for U.S.A.*	EU average	*Inventory data on lignite mining in China. is not available. Because lignite mining is considered as an established technology, lignite mining in Europe and the impacts associated are assumed to be the same for China*
Electricity mix	EU average	*The electricity mix for Europe primarily consists of nuclear power (28%), hydropower (23%), coal power (17%), natural gas (17%), and lignite (8%)* (Dones et al. 2007)	U.S.A.	*The electricity mix for U.S.A. primarily consists of coal power (48%), nuclear power (20%), natural gas (18%) and hydropower (7%)* (Dones et al. 2007)	China	*The electricity mix for China consists of coal power (79%), hydropower (16%), oil (3%) and nuclear power (2%)* (Dones et al. 2007)
Heat mix	EU average	*Inventory is based on European production conditions of heat from natural gas.*	U.S.A.	*Heat production from natural gas in Europe is assumed similar to U.S.A. conditions. However, the electricity used for heat production is based on U.S.A. electricity grid mix*	China	*Heat production from natural gas in Europe is assumed similar to Chinese conditions. However, the electricity used for heat production is based on Chinese electricity grid mix*
NaOH production	EU average	*Inventory only includes EU averages.*	EU average	*Inventory data on NaOH production in U.S.A. was not available. Because NaOH production is considered an established and mature technology, the production and the impacts associated with production in Europe were assumed to be the same for U.S.A.*	EU average	*Inventory data on NaOH production in China was not available. Because NaOH production is considered an established and mature technology, the production and the impacts associated with production in Europe were assumed to be the same for China*
Acid production	EU average	*Inventory only includes EU averages.*	EU average	*Because acids are globally traded commodities and production of acids are considered a mature technology, the production and the impacts associated with production in Europe were assumed to be the same for U.S.A.*	EU average	*Because acids are globally traded commodities and production of acids are considered a mature technology, the production and the impacts associated with production in Europe were assumed to be the same for China*
Methanol production	EU/Global	*Electricity is based on EU grid mix. The feedstock and metals are based on global data as these are normally extracted from a global market.*	U.S.A./Global	*Electricity is based on U.S.A. electricity mix. The feedstock and metals are based on global data as these are normally extracted from a global market*	China/Global	*Electricity is based on Chinese electricity mix. The feedstock and metals are based on global data as these are normally extracted from a global market*
Pulverized coal power plant	German	*Pulverized coal power plant is based on German power plant as included in ecoinvent v2.2.* (Frischknecht et al. 2004) *and described by* (Dones et al. 2007). *The inventory is modified based on coal properties, such as energy output (higher heating value dependent) and emissions (e.g. CO_2 emission and emissions of particulate matter).*	U.S.A.	*The pulverized coal power plant is based on conditions for U.S.A. as included in ecoinvent v2.2.* (Frischknecht et al. 2004) *and described by* (Dones et al. 2007). *Pulverized coal plant is modified to account for coal specific inputs, such as CO_2 emission and emissions of particulate matter which depend on the composition of the coal.*	China	*The pulverized coal power plant is based on Chinese power plants as included in ecoinvent v2.2* (Frischknecht et al. 2004) *The process is modified to account for coal specific inputs, such as CO_2 emission and emissions of particulate matter which depend on the composition of the coal. Based on* (Dones et al. 2007) *the Chinese power plant has limited installation of flue gas cleaning, hence, NOx and SOx is not removed from the flue gas, emissions are therefore directly emitted to air.*

S3 Data points used for chemical cleaning process

Table S2 presents 239 data points on process conditions and ash removal from coal via chemical cleaning. The data is based on 10 studies where the efficiency of ash removal with chemical cleaning using alkali-acid or acid leaching has been assessed. The data points include information on process conditions (*e.g.* acid used, temperature and time of leaching) which were used to model the chemical cleaning process. Full LCAs were conducted for each data point to assess the variance in environmental impacts as a result of different chemical cleaning process conditions and coal types cleaned.

Table S2. List of data points used and key information used for modelling the chemical cleaning process

Leaching process	Ash Initial [%]	Tempera-ture, alkali leaching [C]	Time, alkali leaching [hr]	NaOH conc. [%]	Temper a-ture, acid leaching [C]	Time, acid leaching [hr]	Acid used	Acid conc. [%]	Coal type	Measured ash content [%]	Reference
Alkali-acid	15.5	157	2.5	5	100	0.2	HCl	10	Bituminous coal	13.5	(Z.Y. Wang et al. 1986)
Alkali-acid	15.5	127	2.5	21	100	0.2	HCl	10	Bituminous coal	8.1	
Alkali-acid	15.5	157	2.5	21	100	0.2	HCl	10	Bituminous coal	6.0	
Alkali-acid	15.5	187	2.5	21	100	0.2	HCl	10	Bituminous coal	3.0	
Alkali-acid	15.5	127	2.5	52	100	0.2	HCl	10	Bituminous coal	6.0	
Alkali-acid	15.5	157	0.3	52	100	0.2	HCl	10	Bituminous coal	14.8	
Alkali-acid	15.5	157	1.0	52	100	0.2	HCl	10	Bituminous coal	10.5	
Alkali-acid	15.5	157	1.8	52	100	0.2	HCl	10	Bituminous coal	6.0	
Alkali-acid	15.5	157	2.5	52	100	0.2	HCl	10	Bituminous coal	4.1	
Alkali-acid	15.5	187	2.5	52	100	0.2	HCl	10	Bituminous coal	2.7	
Alkali-acid	15.5	187	24.0	52	100	0.2	HCl	10	Bituminous coal	1.7	
Alkali-acid	15.5	157	2.5	98	100	0.2	HCl	10	Bituminous coal	3.1	
Alkali-acid	7.0	157	1.0	5	100	0.2	HCl	10	Bituminous coal	4.4	
Alkali-acid	7.0	127	1.0	21	100	0.2	HCl	10	Bituminous coal	3.7	
Alkali-acid	7.0	157	1.0	21	100	0.2	HCl	10	Bituminous coal	2.6	
Alkali-acid	7.0	127	1.0	52	100	0.2	HCl	10	Bituminous coal	3.5	
Alkali-acid	7.0	157	1.0	52	100	0.2	HCl	10	Bituminous coal	1.4	
Alkali-acid	7.0	187	1.0	52	100	0.2	HCl	10	Bituminous coal	0.9	
Alkali-acid	7.0	157	1.0	98	100	0.2	HCl	10	Bituminous coal	1.2	
Alkali-acid	15.0	85	2.5	10	85	0.5	HCl	10	Bituminous coal	7.8	(Dash et al. 2013)
Alkali-acid	15.0	85	2.5	20	85	0.5	HCl	10	Bituminous coal	7.6	
Alkali-acid	15.0	85	2.5	30	85	0.5	HCl	10	Bituminous coal	7.5	
Alkali-acid	15.0	85	2.5	40	85	0.5	HCl	10	Bituminous coal	7.5	
Alkali-acid	17.9	85	2.5	10	85	0.5	HCl	10	Bituminous coal	11.0	
Alkali-acid	17.9	85	2.5	20	85	0.5	HCl	10	Bituminous coal	7.9	
Alkali-acid	17.9	85	2.5	30	85	0.5	HCl	10	Bituminous coal	7.5	
Alkali-acid	17.9	85	2.5	40	85	0.5	HCl	10	Bituminous coal	7.3	
Alkali-acid	26.4	85	2.5	10	85	0.5	HCl	10	Bituminous coal	18.0	
Alkali-acid	26.4	85	2.5	20	85	0.5	HCl	10	Bituminous coal	15.1	
Alkali-acid	26.4	85	2.5	30	85	0.5	HCl	10	Bituminous coal	12.0	
Alkali-	26.4	85	2.5	40	85	0.5	HCl	10	Bituminous coal	11.0	

Leaching process	Ash Initial [%]	Tempera-ture, alkali leaching [C]	Time, alkali leaching [hr]	NaOH conc. [%]	Temper a-ture, acid leaching [C]	Time, acid leaching [hr]	Acid used	Acid conc. [%]	Coal type	Measured ash content [%]	Reference
acid											
Alkali-acid	8.4	95	2.0	2	95	8.0	HCl	10	Bituminous coal	5.2	(Mukherjee and Borthakur 2001)
Alkali-acid	8.4	95	2.0	4	95	8.0	HCl	10	Bituminous coal	5.2	
Alkali-acid	8.4	95	2.0	8	95	8.0	HCl	10	Bituminous coal	4.8	
Alkali-acid	8.4	95	2.0	16	95	8.0	HCl	10	Bituminous coal	4.4	
Alkali-acid	10.4	95	2.0	2	95	8.0	HCl	10	Bituminous coal	6.5	
Alkali-acid	10.4	95	2.0	4	95	8.0	HCl	10	Bituminous coal	6.5	
Alkali-acid	10.4	95	2.0	8	95	8.0	HCl	10	Bituminous coal	6.3	
Alkali-acid	10.4	95	2.0	16	95	8.0	HCl	10	Bituminous coal	6.2	
Alkali-acid	11.1	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.4	(Yang and Das 1985)
Alkali-acid	6.9	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.3	
Alkali-acid	4.8	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.2	
Alkali-acid	8.7	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.5	
Alkali-acid	3.2	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.2	
Alkali-acid	16.8	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	5.2	
Alkali-acid	12.2	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.5	
Alkali-acid	6.8	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.3	
Alkali-acid	9.4	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	0.6	
Alkali-acid	5.9	210	2.0	10	80	1.0	H_2SO_4	10	Bituminous coal	1.0	
Alkali-acid	20.1	210	2.0	10	80	1.0	H_2SO_4	10	Subbituminous coal	7.0	
Alkali-acid	28.1	95	1.0	10	95	1.0	HCl	10	Lignite	17.4	(Karaca and Önal 2003)
Alkali-acid	28.9	95	1.0	20	95	1.0	HCl	10	Lignite	14.2	
Alkali-acid	26.0	95	1.0	30	95	1.0	HCl	10	Lignite	10.2	
Alkali-acid	28.1	95	1.0	10	95	1.0	H_2SO_4	10	Lignite	16.4	
Alkali-acid	28.9	95	1.0	20	95	1.0	H_2SO_4	10	Lignite	14.2	
Alkali-acid	26.0	95	1.0	30	95	1.0	H_2SO_4	10	Lignite	10.6	
Alkali-acid	18.8	95	1.0	10	95	1.0	HCl	10	Lignite	3.9	
Alkali-acid	17.0	95	1.0	20	95	1.0	HCl	10	Lignite	3.8	
Alkali-acid	15.0	95	1.0	30	95	1.0	HCl	10	Lignite	3.3	
Alkali-acid	18.8	95	1.0	10	95	1.0	H_2SO_4	10	Lignite	6.2	
Alkali-acid	7.0	127	0.5	3	100	0.2	HCl	10	Bituminous coal	4.8	(Çulfaz et al. 1996)
Alkali-acid	7.0	157	0.5	3	100	0.2	HCl	10	Bituminous coal	4.5	
Alkali-acid	7.0	187	0.5	3	100	0.2	HCl	10	Bituminous coal	4.1	
Alkali-acid	7.0	127	1.0	3	100	0.2	HCl	10	Bituminous coal	4.4	
Alkali-acid	7.0	157	1.0	3	100	0.2	HCl	10	Bituminous coal	4.0	
Alkali-acid	7.0	187	1.0	3	100	0.2	HCl	10	Bituminous coal	3.6	
Alkali-acid	7.0	127	2.5	3	100	0.2	HCl	10	Bituminous coal	4.1	
Alkali-acid	7.0	157	2.5	3	100	0.2	HCl	10	Bituminous coal	3.7	

Leaching process	Ash Initial [%]	Tempera-ture, alkali leaching [C]	Time, alkali leaching [hr]	NaOH conc. [%]	Tempera-ture, acid leaching [C]	Time, acid leaching [hr]	Acid used	Acid conc. [%]	Coal type	Measured ash content [%]	Reference
Alkali-acid	7.0	187	2.5	3	100	0.2	HCl	10	Bituminous coal	3.3	
Alkali-acid	7.0	127	0.5	5	100	0.2	HCl	10	Bituminous coal	4.3	
Alkali-acid	7.0	157	0.5	5	100	0.2	HCl	10	Bituminous coal	4.0	
Alkali-acid	7.0	187	0.5	5	100	0.2	HCl	10	Bituminous coal	3.6	
Alkali-acid	7.0	127	1.0	5	100	0.2	HCl	10	Bituminous coal	3.5	
Alkali-acid	7.0	157	1.0	5	100	0.2	HCl	10	Bituminous coal	3.1	
Alkali-acid	7.0	187	1.0	5	100	0.2	HCl	10	Bituminous coal	2.9	
Alkali-acid	7.0	127	2.5	5	100	0.2	HCl	10	Bituminous coal	3.2	
Alkali-acid	7.0	157	2.5	5	100	0.2	HCl	10	Bituminous coal	2.8	
Alkali-acid	7.0	187	2.5	5	100	0.2	HCl	10	Bituminous coal	2.5	
Alkali-acid	7.0	127	0.5	21	100	0.2	HCl	10	Bituminous coal	3.9	
Alkali-acid	7.0	157	0.5	21	100	0.2	HCl	10	Bituminous coal	3.5	
Alkali-acid	7.0	187	0.5	21	100	0.2	HCl	10	Bituminous coal	3.2	
Alkali-acid	7.0	127	1.0	21	100	0.2	HCl	10	Bituminous coal	2.4	
Alkali-acid	7.0	157	1.0	21	100	0.2	HCl	10	Bituminous coal	2.1	
Alkali-acid	7.0	187	1.0	21	100	0.2	HCl	10	Bituminous coal	1.7	
Alkali-acid	7.0	127	2.5	21	100	0.2	HCl	10	Bituminous coal	1.9	
Alkali-acid	7.0	157	2.5	21	100	0.2	HCl	10	Bituminous coal	1.6	
Alkali-acid	7.0	187	2.5	21	100	0.2	HCl	10	Bituminous coal	1.2	
Alkali-acid	7.0	127	0.5	98	100	0.2	HCl	10	Bituminous coal	3.1	
Alkali-acid	7.0	157	0.5	98	100	0.2	HCl	10	Bituminous coal	2.7	
Alkali-acid	7.0	187	0.5	98	100	0.2	HCl	10	Bituminous coal	2.1	
Alkali-acid	7.0	127	1.0	98	100	0.2	HCl	10	Bituminous coal	1.3	
Alkali-acid	7.0	157	1.0	98	100	0.2	HCl	10	Bituminous coal	1.1	
Alkali-acid	7.0	187	1.0	98	100	0.2	HCl	10	Bituminous coal	0.9	
Alkali-acid	7.0	127	2.5	98	100	0.2	HCl	10	Bituminous coal	1.0	
Alkali-acid	7.0	157	2.5	98	100	0.2	HCl	10	Bituminous coal	0.7	
Alkali-acid	7.0	187	2.5	98	100	0.2	HCl	10	Bituminous coal	0.3	
Alkali-acid	35.6	127	0.5	3	100	0.2	HCl	10	Lignite	30.2	
Alkali-acid	35.6	157	0.5	3	100	0.2	HCl	10	Lignite	30.3	
Alkali-acid	35.6	187	0.5	3	100	0.2	HCl	10	Lignite	28.9	
Alkali-acid	35.6	127	1.0	3	100	0.2	HCl	10	Lignite	30.1	
Alkali-acid	35.6	157	1.0	3	100	0.2	HCl	10	Lignite	28.1	
Alkali-acid	35.6	187	1.0	3	100	0.2	HCl	10	Lignite	27.2	
Alkali-acid	35.6	127	2.5	3	100	0.2	HCl	10	Lignite	29.8	
Alkali-acid	35.6	157	2.5	3	100	0.2	HCl	10	Lignite	22.9	
Alkali-acid	35.6	187	2.5	3	100	0.2	HCl	10	Lignite	22.1	
Alkali-	35.6	127	0.5	5	100	0.2	HCl	10	Lignite	29.9	

Leaching process	Ash Initial [%]	Tempera-ture, alkali leaching [C]	Time, alkali leaching [hr]	NaOH conc. [%]	Tempera-ture, acid leaching [C]	Time, acid leaching [hr]	Acid used	Acid conc. [%]	Coal type	Measured ash content [%]	Reference
acid											
Alkali-acid	35.6	157	0.5	5	100	0.2	HCl	10	Lignite	28.8	
Alkali-acid	35.6	187	0.5	5	100	0.2	HCl	10	Lignite	23.7	
Alkali-acid	35.6	127	1.0	5	100	0.2	HCl	10	Lignite	29.5	
Alkali-acid	35.6	157	1.0	5	100	0.2	HCl	10	Lignite	28.1	
Alkali-acid	35.6	187	1.0	5	100	0.2	HCl	10	Lignite	21.3	
Alkali-acid	35.6	127	2.5	5	100	0.2	HCl	10	Lignite	20.1	
Alkali-acid	35.6	157	2.5	5	100	0.2	HCl	10	Lignite	14.3	
Alkali-acid	35.6	187	2.5	5	100	0.2	HCl	10	Lignite	14.1	
Alkali-acid	35.6	127	0.5	21	100	0.2	HCl	10	Lignite	26.4	
Alkali-acid	35.6	157	0.5	21	100	0.2	HCl	10	Lignite	21.9	
Alkali-acid	35.6	187	0.5	21	100	0.2	HCl	10	Lignite	14.8	
Alkali-acid	35.6	127	1.0	21	100	0.2	HCl	10	Lignite	21.8	
Alkali-acid	35.6	157	1.0	21	100	0.2	HCl	10	Lignite	15.8	
Alkali-acid	35.6	187	1.0	21	100	0.2	HCl	10	Lignite	7.5	
Alkali-acid	35.6	127	2.5	21	100	0.2	HCl	10	Lignite	14.1	
Alkali-acid	35.6	157	2.5	21	100	0.2	HCl	10	Lignite	6.5	
Alkali-acid	35.6	187	2.5	21	100	0.2	HCl	10	Lignite	5.8	
Alkali-acid	35.6	127	0.5	98	100	0.2	HCl	10	Lignite	24.6	
Alkali-acid	35.6	157	0.5	98	100	0.2	HCl	10	Lignite	12.0	
Alkali-acid	35.6	187	0.5	98	100	0.2	HCl	10	Lignite	9.1	
Alkali-acid	35.6	127	1.0	98	100	0.2	HCl	10	Lignite	13.3	
Alkali-acid	35.6	157	1.0	98	100	0.2	HCl	10	Lignite	10.4	
Alkali-acid	35.6	187	1.0	98	100	0.2	HCl	10	Lignite	6.2	
Alkali-acid	35.6	127	2.5	98	100	0.2	HCl	10	Lignite	9.3	
Alkali-acid	35.6	157	2.5	98	100	0.2	HCl	10	Lignite	5.1	
Alkali-acid	35.6	187	2.5	98	100	0.2	HCl	10	Lignite	3.4	
Acid	7.9	0	0.0	0	65	3.0	HF	1.3	Bituminous coal	5.6	(Steel and Patrick 2001)
Acid	7.9	0	0.0	0	65	3.0	HF	3	Bituminous coal	4.1	
Acid	7.9	0	0.0	0	65	3.0	HF	3	Bituminous coal	3.4	
Acid	7.9	0	0.0	0	65	3.0	HF	4	Bituminous coal	2.5	
Acid	7.9	0	0.0	0	65	3.0	HF	5	Bituminous coal	3.5	
Acid	7.9	0	0.0	0	65	3.0	HF	6	Bituminous coal	2.4	
Acid	7.9	0	0.0	0	65	3.0	HF	8	Bituminous coal	2.6	
Acid	7.9	0	0.0	0	65	3.0	HF	9	Bituminous coal	2.5	
Acid	7.9	0	0.0	0	65	3.0	HF	10	Bituminous coal	2.6	
Acid	7.9	0	0.0	0	65	3.0	HF	12	Bituminous coal	2.8	
Acid	7.9	0	0.0	0	65	3.0	HF	13	Bituminous coal	2.8	
Acid	7.9	0	0.0	0	65	3.0	HF	15	Bituminous coal	2.3	
Acid	7.9	0	0.0	0	65	3.0	HF	19	Bituminous coal	2.6	
Acid	7.9	0	0.0	0	65.0	3.0	HF	25.5	Bituminous coal	2.7	
Acid	30.3	0	0.0	0	95	1.0	HCl	10	Lignite	24.6	(Karaca and Önal 2003)
Acid	30.3	0	0.0	0	95	1.0	H_2SO_4	10	Lignite	22.1	
Acid	15.4	0	0.0	0	95	1.0	HCl	10	Lignite	5.3	
Acid	15.4	0	0.0	0	95	1.0	H_2SO_4	10	Lignite	6.2	
Acid	21.4	0	0.0	0	30	2.0	H_2O_2	30	Lignite	12.7	

Leaching process	Ash Initial [%]	Tempera-ture, alkali leaching [C]	Time, alkali leaching [hr]	NaOH conc. [%]	Temper a-ture, acid leaching [C]	Time, acid leaching [hr]	Acid used	Acid conc. [%]	Coal type	Measured ash content [%]	Reference
Acid	16.7	0	0.0	0	30	2.0	H_2O_2	30	Lignite	11.5	
Acid	8.8	0	0.0	0	25	4.0	H_2O_2	3	Bituminous coal	7.3	(Mukherjee et al. 2001)
Acid	8.8	0	0.0	0	25	4.0	H_2O_2	5	Bituminous coal	7.2	
Acid	8.8	0	0.0	0	25	4.0	H_2O_2	10	Bituminous coal	7.1	
Acid	8.8	0	0.0	0	25	4.0	H_2O_2	15	Bituminous coal	7.0	
Acid	11.0	0	0.0	0	25	4.0	H_2O_2	3	Bituminous coal	9.8	
Acid	11.0	0	0.0	0	25	4.0	H_2O_2	5	Bituminous coal	9.6	
Acid	11.0	0	0.0	0	25	4.0	H_2O_2	10	Bituminous coal	9.5	
Acid	11.0	0	0.0	0	25	4.0	H_2O_2	15	Bituminous coal	9.4	
Acid	8.4	0	0.0	0	95	8.0	HCl	10	Bituminous coal	6.3	(Mukherjee and Borthakur 2001)
Acid	8.8	0	0.0	0	95	0.5	HCl	10	Bituminous coal	6.6	(Mukherjee and Borthakur 2004)
Acid	8.8	0	0.0	0	95	4.0	HCl	10	Subbituminous coal	6.5	
Acid	8.8	0	0.0	0	95	8.0	HCl	10	Subbituminous coal	6.3	
Acid	8.8	0	0.0	0	30	8.0	HCl	10	Subbituminous coal	6.8	
Acid	8.8	0	0.0	0	95	0.5	HCl	20	Subbituminous coal	6.5	
Acid	8.8	0	0.0	0	95	4.0	HCl	20	Subbituminous coal	6.4	
Acid	8.8	0	0.0	0	95	8.0	HCl	20	Subbituminous coal	6.2	
Acid	8.8	0	0.0	0	30	8.0	HCl	20	Subbituminous coal	6.8	
Acid	8.8	0	0.0	0	95	0.5	HCl	30	Subbituminous coal	6.4	
Acid	8.8	0	0.0	0	95	4.0	HCl	30	Subbituminous coal	6.3	
Acid	8.8	0	0.0	0	95	8.0	HCl	30	Subbituminous coal	6.1	
Acid	8.8	0	0.0	0	30	8.0	HCl	30	Subbituminous coal	6.7	
Acid	8.8	0	0.0	0	95	0.5	HNO_3	10	Subbituminous coal	6.3	
Acid	8.8	0	0.0	0	95	4.0	HNO_3	10	Subbituminous coal	6.0	
Acid	8.8	0	0.0	0	95	8.0	HNO_3	10	Subbituminous coal	5.8	
Acid	8.8	0	0.0	0	30	8.0	HNO_3	10	Subbituminous coal	6.8	
Acid	8.8	0	0.0	0	95	0.5	HNO_3	20	Subbituminous coal	5.8	
Acid	8.8	0	0.0	0	95	4.0	HNO_3	20	Subbituminous coal	5.6	
Acid	8.8	0	0.0	0	95	8.0	HNO_3	20	Subbituminous coal	5.6	
Acid	8.8	0	0.0	0	30	8.0	HNO_3	20	Subbituminous coal	6.3	
Acid	8.8	0	0.0	0	95	0.5	HNO_3	30	Subbituminous coal	5.6	
Acid	8.8	0	0.0	0	95	4.0	HNO_3	30	Subbituminous coal	5.4	
Acid	8.8	0	0.0	0	95	8.0	HNO_3	30	Subbituminous coal	5.3	
Acid	8.8	0	0.0	0	30	8.0	HNO_3	30	Subbituminous coal	5.9	
Acid	8.8	0	0.0	0	95	0.5	H_2SO_4	10	Subbituminous coal	6.2	
Acid	8.8	0	0.0	0	95	4.0	H_2SO_4	10	Subbituminous coal	5.9	
Acid	8.8	0	0.0	0	95	8.0	H_2SO_4	10	Subbituminous coal	5.8	
Acid	8.8	0	0.0	0	30	8.0	H_2SO_4	10	Subbituminous coal	6.6	
Acid	8.8	0	0.0	0	95	0.5	H_2SO_4	20	Subbituminous coal	6.1	
Acid	8.8	0	0.0	0	95	4.0	H_2SO_4	20	Subbituminous coal	5.9	
Acid	8.8	0	0.0	0	95	8.0	H_2SO_4	20	Subbituminous coal	5.6	
Acid	8.8	0	0.0	0	30	8.0	H_2SO_4	20	Subbituminous coal	6.4	

Leaching process	Ash Initial [%]	Tempera-ture, alkali leaching [C]	Time, alkali leaching [hr]	NaOH conc. [%]	Tempera-ture, acid leaching [C]	Time, acid leaching [hr]	Acid used	Acid conc. [%]	Coal type	Measured ash content [%]	Reference
Acid	8.8	0	0.0	0	95	0.5	H_2SO_4	30	Subbituminous coal	5.4	
Acid	8.8	0	0.0	0	95	4.0	H_2SO_4	30	Subbituminous coal	5.3	
Acid	8.8	0	0.0	0	95	8.0	H_2SO_4	30	Subbituminous coal	5.1	
Acid	8.8	0	0.0	0	30	8.0	H_2SO_4	30	Subbituminous coal	6.1	
Acid	11.0	0	0.0	0	95	0.5	HCl	10	Bituminous coal	9.4	
Acid	11.0	0	0.0	0	95	4.0	HCl	10	Bituminous coal	9.0	
Acid	11.0	0	0.0	0	95	8.0	HCl	10	Bituminous coal	8.8	
Acid	11.0	0	0.0	0	30	8.0	HCl	10	Bituminous coal	9.4	
Acid	11.0	0	0.0	0	95	0.5	HCl	20	Bituminous coal	9.3	
Acid	11.0	0	0.0	0	95	4.0	HCl	20	Bituminous coal	8.8	
Acid	11.0	0	0.0	0	95	8.0	HCl	20	Bituminous coal	8.5	
Acid	11.0	0	0.0	0	30	8.0	HCl	20	Bituminous coal	9.3	
Acid	11.0	0	0.0	0	95	0.5	HCl	30	Bituminous coal	8.9	
Acid	11.0	0	0.0	0	95	4.0	HCl	30	Bituminous coal	8.5	
Acid	11.0	0	0.0	0	95	8.0	HCl	30	Bituminous coal	8.3	
Acid	11.0	0	0.0	0	30	8.0	HCl	30	Bituminous coal	9.1	
Acid	11.0	0	0.0	0	95	0.5	HNO_3	10	Bituminous coal	8.9	
Acid	11.0	0	0.0	0	95	4.0	HNO_3	10	Bituminous coal	8.5	
Acid	11.0	0	0.0	0	95	8.0	HNO_3	10	Bituminous coal	8.4	
Acid	11.0	0	0.0	0	30	8.0	HNO_3	10	Bituminous coal	9.4	
Acid	11.0	0	0.0	0	95	0.5	HNO_3	20	Bituminous coal	8.7	
Acid	11.0	0	0.0	0	95	4.0	HNO_3	20	Bituminous coal	7.6	
Acid	11.0	0	0.0	0	95	8.0	HNO_3	20	Bituminous coal	7.6	
Acid	11.0	0	0.0	0	30	8.0	HNO_3	20	Bituminous coal	9.2	
Acid	11.0	0	0.0	0	95	0.5	HNO_3	30	Bituminous coal	7.8	
Acid	11.0	0	0.0	0	95	4.0	HNO_3	30	Bituminous coal	7.5	
Acid	11.0	0	0.0	0	95	8.0	HNO_3	30	Bituminous coal	7.4	
Acid	11.0	0	0.0	0	30	8.0	HNO_3	30	Bituminous coal	8.4	
Acid	11.0	0	0.0	0	95	0.5	H_2SO_4	10	Bituminous coal	8.7	
Acid	11.0	0	0.0	0	95	4.0	H_2SO_4	10	Bituminous coal	8.7	
Acid	11.0	0	0.0	0	95	8.0	H_2SO_4	10	Bituminous coal	8.6	
Acid	11.0	0	0.0	0	30	8.0	H_2SO_4	10	Bituminous coal	9.5	
Acid	11.0	0	0.0	0	95	0.5	H_2SO_4	20	Bituminous coal	8.6	
Acid	11.0	0	0.0	0	95	4.0	H_2SO_4	20	Bituminous coal	8.4	
Acid	11.0	0	0.0	0	95	8.0	H_2SO_4	20	Bituminous coal	8.1	
Acid	11.0	0	0.0	0	30	8.0	H_2SO_4	20	Bituminous coal	9.2	
Acid	11.0	0	0.0	0	95	0.5	H_2SO_4	30	Bituminous coal	8.6	
Acid	11.0	0	0.0	0	95	4.0	H_2SO_4	30	Bituminous coal	8.0	
Acid	11.0	0	0.0	0	95	8.0	H_2SO_4	30	Bituminous coal	7.5	
Acid	11.0	0	0.0	0	30	8.0	H_2SO_4	30	Bituminous coal	9.2	
Acid	34.3	0	0.0	0	30	0.3	HCl	5	Bituminous coal	20.7	(Gulen et al. 2005)
Acid	34.3	0	0.0	0	30	0.3	HCl	10	Bituminous coal	20.8	
Acid	34.3	0	0.0	0	30	0.3	HNO_3	5	Bituminous coal	23.6	
Acid	34.3	0	0.0	0	30	0.3	HNO_3	10	Bituminous coal	21.7	

Leaching process	Ash Initial [%]	Tempera-ture, alkali leaching [C]	Time, alkali leaching [hr]	NaOH conc. [%]	Temper a-ture, acid leaching [C]	Time, acid leaching [hr]	Acid used	Acid conc. [%]	Coal type	Measured ash content [%]	Reference
Acid	34.3	0	0.0	0	30	0.3	H_2SO_4	5	Bituminous coal	27.7	
Acid	34.3	0	0.0	0	30	0.3	H_2SO_4	10	Bituminous coal	27.8	

S4 European power plant efficiencies

The average power plant efficiency of pulverized coal power plants (sub-critical and super-critical) in European countries as presented by Graus et al. (2008) is shown in Table S3. Table S3 also includes the average power plant efficiency for Europe and the 95 % confidence interval to illustrate the variability in the overall power plant efficiency. This information was used for defining the average power plant efficiency for Europe as used in the basis LCA scenario. As stated in the main paper, the average and variability ranges for Europe were also applied for power plants in China and U.S.A. This choice does not influence the main goal of this study *i.e.* the comparison between coal cleaning technologies, but will to some extent influence the environmental performance of coal burning in general. The variability in the power plant efficiency was used in the uncertainty and variability analysis.

Table S3. Power plant efficiency in 2005 and average age of operational pulverized coal power plants by the end of 2005 (weighted by capacity), shown for European countries and as a total European average.

Coal-fired plants	Average age	Power plant efficiency
Austria	21	41%
Belgium	34	38%
Bulgaria	30	29%
Czech Republic	31	31%
Denmark	23	43%
Finland	26	38%
France	30	39%
Germany	25	40%
Greece	23	35%
Hungary	37	32%
Ireland	19	40%
Italy	31	37%
Netherlands	21	43%
Poland	29	37%
Portugal	16	39%
Romania	27	35%
Slovakia	36	26%
Slovenia	34	36%
Spain	25	39%
Sweden	31	31%
United Kingdom	33	39%
Arithmetic mean	27.7	36.6%
Standard deviation	5.8	0.045
2.5 percentile	18	28%
97.5 percentile	37	43%

S5 Calculation of heat demand for demineralization

The demineralization process requires heating of the coal slurry for both the leaching steps and for the hydrothermal washing. Data on the heat energy required is not available, and as a best estimate the heat requirements were estimated using the heat equation for calculating the energy required for heating the slurry. The heat equation used is shown in Eq. S4 (Young and Freedman 2008):

$$Q = mc\Delta T \qquad \text{(S4)}$$

where Q [cal] is the heat energy required for heating the slurry, ΔT is difference in temperature between the heated material and the outside temperature, m [g] is the mass of the slurry, and c [cal g^{-1} $°C^{-1}$] is the specific heat capacity of the slurry, which is assumed to be the same as water. The slurry is assumed kept and heated in a 5 mm stainless steel cylinder insulated with 10 mm glass wool. The heat loss equation is based on conductive heat transfer through a material. Eq. S5 shows the heat transfer through two materials used for insolation.

$$q = \Delta T / ((s_1 / k_1 A) + (s_2 / k_2 A)) \qquad \text{(S5)}$$

where q is heat transfer (W), A is heat transfer area (m^2), k_1 is thermal conductivity of material 1 ($W\ m^{-1}\ K^{-1}$), k_2 is thermal conductivity of material 2 ($W\ m^{-1}\ K^{-1}$) where, s_1 is thickness of material 1 (m) and s_2 is thickness of material 2 (m)

For coal leaching we assume that the process is performed in a stainless steel reactor insulated with glass wool. The steel is assumed to be 0.05 m and $k_{Stainless\ steel} = 16\ W\ m^{-1}\ K^{-1}$. The glass wool insulation is assumed to be 0.1 m and $k_{Glass\ wool\ insulation} = 0.4\ W\ m^{-1}\ K^{-1}$. Based on this the heat loss for a 100 °C liquid with a 0.00010 m^3 volume per hour is 0.0020 MJ hr^{-1}. The energy required for heating the liquid from 12 °C to 100 °C is 37 MJ. The energy from heat loss per hour accounts for ca. 0.005% of the energy required for the initial heating. Because of this small contribution heat loss is considered negligible in the total energy balance.

S6 Modeling of sulfur removal

A general problem with combustion of coal is the formation of NO_x and SO_x whom both contribute to air pollution, and are emitted as a result of the content in the coal used (Franco and Diaz 2009). Mukherjee and Borthakur (2001) showed that treatment with alkali or acid yields a reduction in sulfur content, while combined leaching such as alkali-acid leaching yields a larger reduction compared to treatment with alkali or acid alone. Sulfur is removed by reactions with NaOH as shown in Eq. S6 where pyrite is transformed into a sodium salt, which can be removed during the leaching.

$$30NaOH + 8FeS_2 \rightarrow 4Fe_2O_3 + 14Na_2S + Na_2S_2O_3 + 15H_2O \tag{S6}$$

S6.1 Modelling approach

The regression model for sulfur reduction is based on curve fitting to measured data (Mukherjee et al. 2001; Mukherjee and Borthakur 2001; Mukherjee and Borthakur 2003) (see Table S4). The data sets included variables which were recognized as important *i.e.* NaOH concentration and acid concentration (in terms of molarity) and time of NaOH leaching. The data was analysed to reveal the overall trend in sulfur reduction as a function of change. For the time of acid leaching a trend similar to NaOH leaching is assumed. A sulfur reduction factor (SRF) is derived for multiplication with the initial sulfur content (see Eq. S7 and Eq. S8).

$$SRF_{Coal} = SRF_{NaOH} \times SRF_{Acid} \times SRF_{Time,NaOH} \times SRF_{Time,Acid} \tag{S7}$$

$$\text{Sulfur content}_{\text{Treated coal}} = S_{Start} \times SRF_{Coal} \tag{S8}$$

Where SRF_{NaOH} is the reduction factor from alkali leaching, SRF_{Acid} is the reduction factor from acid leaching, $SRF_{Time,NaOH}$ is the reduction factor as a function of alkali leaching time and the $SRF_{Time,Acid}$ is the reduction factor as a function of acid leaching time. The reduction factors are multiplied to give the SRF_{Coal} in Eq. S7. The SRF_{Coal} is multiplied with the initial sulfur content (S_{Start}) to produce the resulting sulfur content after chemical cleaning (see Eq. S8).

For deriving the SRF_{Coal}, studies isolating and varying parameters during the experimental work was needed to identify the actual change sulfur content from a change to a specific parameter independent of other parameters. The references used for identifying the effect of varying isolated parameters are shown in Table S4. The data for each parameter was fitted to 17 different regression curves of the types: linear, exponential, power and sigmoidal. The regression curve with the highest R^2 was used. The curve type chosen and the original regression parameters are given in Table S4.

Table S4 Overview of input parameters used for deriving the sulfur reduction model, this includes best fitting function, regression parameters and R^2.

Sulfur reduction							
Variable	Model type	Regression curve	Regression parameters	Data points	Variable	R^2	Data reference
Acid concentration	Weibull model	$SRF_{Acid} = A_1 - A_2 \times \exp\left(-A_3 \times x^{A_4}\right)$	A_1=0.92 A_2=0.24 A_3=0.94 A_4=-0.78	18	Acid concentration in solution [M]	0.95	(Mukherjee et al. 2001)
NaOH concentration	Logistic model	$SRF_{NaOH} = \frac{A_1}{1 + A_2 \times \exp\left(-A_3 \times x\right)}$	A_1=0.81 A_2=-0.19 A_3=0.83	8	NaOH concentration in solution [%]	0.93	(Mukherjee and Borthakur 2001)
$Time_{NaOH}$	Logarithm model	$SRF_{Time,NaOH} = A_1 + A_2 \times \ln(x)$	A_1=0.86 A_2=-0.02	50	Time of leaching [hr]	0.93	(Mukherjee and Borthakur 2001)
$Time_{Acid}$	Logarithm model	$SRF_{Time,Acid} = A_1 + A_2 \times \ln(x)$	A_1=3.92 A_2=-0.05	Same as $Time_{NaOH}$	Time of leaching [hr]	Same as $Time_{NaOH}$	Same as $Time_{NaOH}$

After the determination of each parameter specific SRF, the overall sulfur removal is compared with measured data. The combined SRF_{Coal} is compared to 86 data point from three peer-reviewed studies. Based on these comparisons, all regression parameters in Table S4 were adjusted to produce the best with the available data points. The quality of the fit was based on the R^2 value, in this way all regression parameters are adjusted to yield the highest R^2. The model was compared to an external data set consisting of 41 data point from 4 peer-reviewed studies. The model fit using an external data set produced a predictive squared correlation coefficient for external validation (Q^2) equal to 0.8. A 1:1 plot showing the predictability of the sulfur reduction model for the internal and the external data set against measured data is shown in Figure S1. It shows from Figure S1 that the modelled sulfur content from chemical cleaning is slightly overestimating the sulfur content compared to the measured sulfur content. We consider these predictions as sufficiently accurate to employ the model for prediction of sulphur removal for the data points collected in our study.

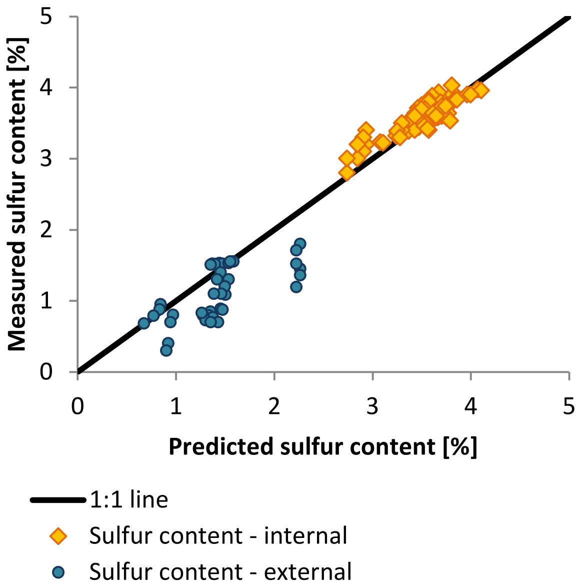

Figure S1. Performance of our model for prediction of sulphur removal from leaching conditions (eq S8). A perfect agreement between model and experimental results would result in alignment of the data points on the first diagonal (black line)

S7 Environmental impact scores for coal life cycle for ReCiPe

Environmental impacts scores for all 18 impact categories available in ReCiPe are shown in Figure S2. For terrestrial toxicity, Figure S2 shows that chemically cleaned coals do not perform better as compared to physically cleaned and raw coals. This worse performance of chemically cleaned coal is mainly due to emission of phosphorous to soil (from the methanol production process). However, rather than a toxicant (as classified in ReCiPe), phosphorus is a macro nutrient, contributing to eutrophication. When phosphorus is excluded from the comparison, terrestrial ecotoxicity impact scores from firing chemically cleaned coals show an impact profile similar to freshwater ecotoxicity.

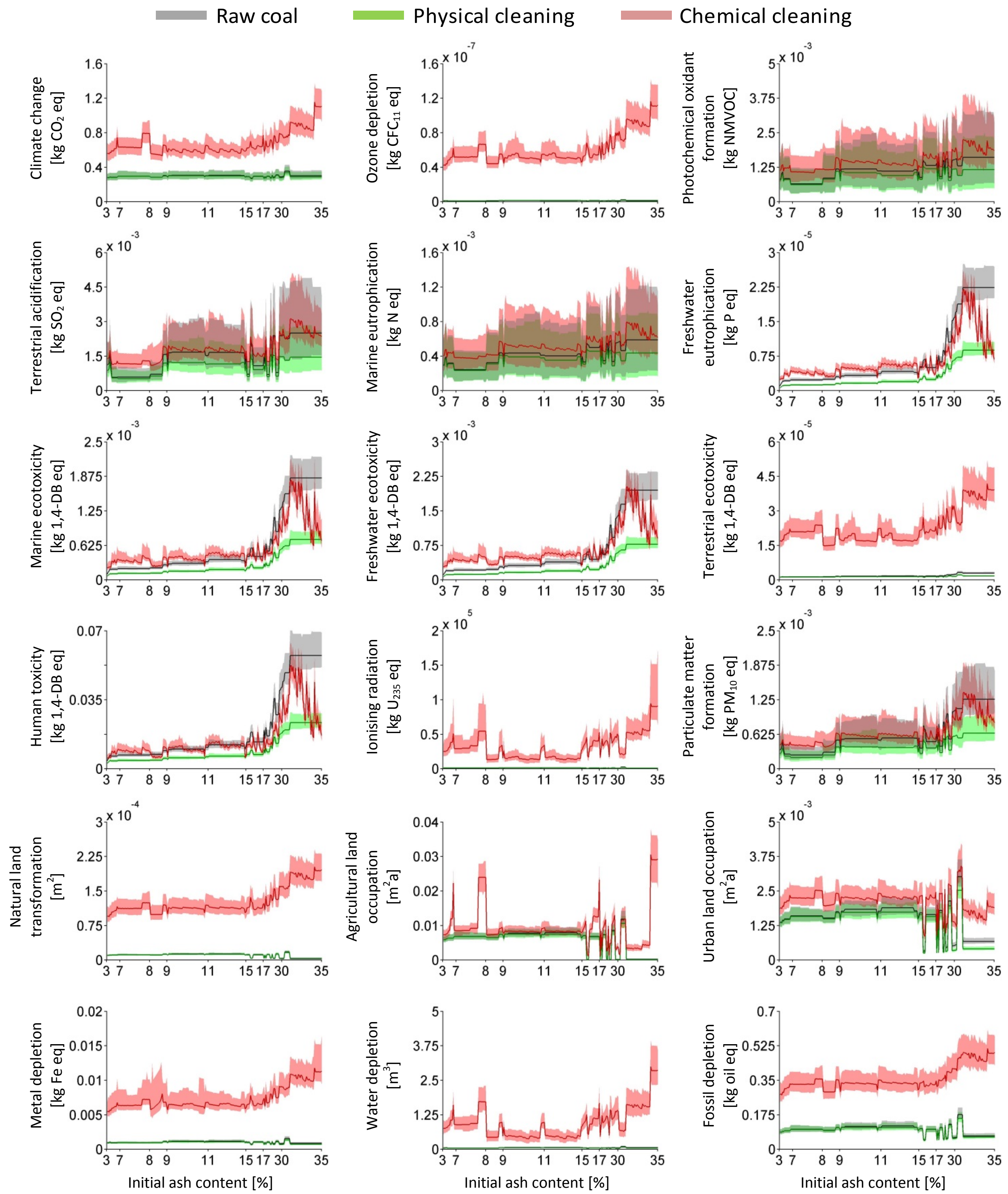

Figure S2. Impact scores and the associated 95% confidence intervals for the impact categories available in ReCiPe 2008 per functional unit ("output of 1 MJ of electricity produced from a pulverized coal power plant"). The results are sorted in ascending order after ash content in the raw coal.

S8 Statistical comparison of impact scores

Table S5 shows a comparison between chemical and physical coal cleaning for all included impact categories. The table shows the percentage cases where chemical cleaning performs better than physical cleaning and vice versa. The two last columns show the percentage cases where chemical cleaning performs significantly better than physical cleaning and vice versa. The difference is considered significant if 95% confidence intervals do not overlap. The confidence intervals were estimated using Monte Carly simulation as described in the main paper.

Table S5 Number of cases where either chemically demineralized or physically demineralized coal perform better or perform significantly better (with 95 % confidence). Impact categories where chemically cleaned coals perform better are marked with bold italics.

	Cases performing better [%]		Cases performing significantly better [%]	
Impact category	Chemical demineralization	Physical demineralization	Chemical demineralization	Physical demineralization
Agricultural land occupation	0	100	0	33
Climate change	0	100	0	100
Fossil depletion	0	100	0	100
Freshwater ecotoxicity	0	100	0	97
Freshwater eutrophication	3	97	0	93
Human toxicity	4	96	0	81
Ionising radiation	0	100	0	100
Marine ecotoxicity	2	98	0	94
Marine eutrophication	0	100	0	0
Metal depletion	0	100	0	100
Natural land transformation	0	100	0	100
Ozone depletion	0	100	0	100
Particulate matter formation	0	100	0	23
Photochemical oxidant formation	0	100	0	0
Terrestrial acidification	0	100	0	15
Terrestrial ecotoxicity	0	100	0	100
Urban land occupation	0	100	0	59
Water depletion	0	100	0	100

S9 Details of sensitivity analysis

The sensitivity analysis included 27 parameters that were included in the LCA model for the coal life cycle. The parameters included the coal composition (*e.g.* ash, carbon and sulfur content), the chemical cleaning process conditions (*e.g.* leaching duration, leaching process temperature, acid recovery efficiency) and power plant conditions (*e.g.* life time of power plant, power plant efficiency and NOx and SOx removal efficiency). Only parameters which produced an average sensitivity coefficient, $|S_{coef}| \geq 0.3$ or a maximum $|S_{coef}| \geq 0.5$ were considered to be important for the model results. In addition, parameters which are well known and given as part of literature data in Table S2 (*i.e.* ash content, acid concentration and NaOH concentration) are not included in Table S6. The important parameters used for uncertainty and variability analysis which are not part of Table S2 are shown in Table S6.

Table S6 Sensitivity analysis of model parameters for the impact categories included in ReCiPe. Only parameters shown to be sensitive based on the S_{coef} and not part of Table S2 are included in this table. The coefficients in bold have an average $|S_{coef}| \geq 0.3$ or a maximum $|S_{coef}| \geq 0.5$. The sensitivity coefficients are shown as the average coefficient (the minimum coefficient; the maximum coefficient). The parameters in *italic* are included in the uncertainty/variability analysis.

	Demineralization process						**Power plant**		
Impact category	*Acid recovery eff.*	*Centrifuge electricity use*	*Filter press electricity use*	Methanol in hydrothermal washing liquid	*Sodium hydroxide recovery eff.*	Coal to liquid ratio	*Net overall efficiency*	*Eff. SOx removal*	*Eff. NOx removal*
Agricultural land occupation	-0.011 (-0.044;-0.002)	0.083 (0;0.12)	0.05 (0.019;0.062)	0.023 (0.008;0.028)	0.023 (-0.009;0.24)	**0.3 (0.015;1.54)**	**-0.8 (-0.8;-0.8)**	0 (0;0.001)	0.002 (0;0.004)
Climate change	-0.008 (-0.032;-0.001)	0.13 (0;0.18)	0.076 (0.065;0.095)	0.21 (0.17;0.26)	-0.006 (-0.022;0.068)	**0.25 (0.04;0.96)**	-0.8 (-0.8;-0.8)	0.001 (0;0.005)	0.003 (0;0.006)
Fossil depletion	-0.005 (-0.02;-0.001)	0.081 (0;0.1)	0.048 (0.045;0.053)	**0.45 (0.41;0.51)**	-0.013 (-0.04;0)	0.16 (0.082;0.34)	**-0.8 (-0.8;-0.8)**	0 (0;0.002)	0.003 (0;0.005)
Freshwater ecotoxicity	-0.042 (-0.15;-0.007)	0.068 (0;0.13)	0.04 (0.019;0.064)	**0.44 (0.2;0.65)**	-0.106 (-0.33;0)	0.12 (0.038;0.23)	**-0.8 (-0.8;-0.79)**	0.004 (0;0.013)	0.004 (0;0.006)
Freshwater eutrophication	-0.016 (-0.057;-0.003)	0.088 (0;0.17)	0.051 (0.024;0.079)	**0.37 (0.17;0.56)**	-0.032 (-0.097;0)	0.16 (0.082;0.26)	**-0.8 (-0.8;-0.8)**	0.001 (0;0.004)	0.003 (0;0.005)
Human toxicity	-0.129 (-0.45;-0.023)	0.16 (0;0.32)	0.094 (0.039;0.15)	0.11 (0.044;0.18)	-0.059 (-0.17;0)	0.2 (0.073;0.32)	**-0.8 (-0.8;-0.8)**	0.008 (0;0.028)	0.002 (0;0.004)
Ionising radiation	**-0.189 (-1.05;-0.049)**	**0.34 (0;0.48)**	0.25 (0.12;0.48)	0.16 (0.072;0.31)	**-0.517 (-1.81;0)**	**0.47 (0.28;0.85)**	**-0.8 (-0.8;-0.8)**	0.001 (0;0.006)	0.003 (0;0.008)
Marine ecotoxicity	-0.103 (-0.35;-0.017)	0.097 (0;0.2)	0.056 (0.023;0.098)	0.24 (0.095;0.4)	-0.122 (-0.36;0)	0.19 (0.083;0.32)	**-0.8 (-0.8;-0.79)**	0.005 (0;0.017)	0.006 (0;0.011)
Marine eutrophication	-0.013 (-0.032;0.017)	0.11 (0;0.23)	0.057 (0.023;0.13)	0.22 (0.091;0.4)	-0.035 (-0.087;0)	0.15 (-0.005;0.34)	**-0.798 (-0.8;-0.77)**	0.005 (0;0.033)	**-1.707 (-3.07;0.033)**
Metal depletion	-0.069 (-0.26;-0.01)	0.098 (0;0.14)	0.058 (0.052;0.073)	**0.54 (0.47;0.64)**	**-0.13 (-0.59;0)**	**0.25 (0.12;0.52)**	**-0.799 (-0.8;-0.79)**	0.003 (0;0.018)	0.017 (0;0.034)
Natural land transformation	-0.009 (-0.033;0.003)	0.051 (0;0.071)	0.03 (0.027;0.037)	**0.66 (0.58;0.74)**	-0.017 (-0.05;0)	0.19 (0.1;0.47)	**-0.8 (-0.8;-0.79)**	0.001 (0;0.008)	0.007 (0;0.015)
Ozone depletion	-0.12 (-0.43;-0.019)	0.074 (0;0.1)	0.044 (0.032;0.051)	**0.63 (0.44;0.73)**	-0.002 (-0.015;0.068)	**0.34 (0.21;0.91)**	**-0.8 (-0.8;-0.8)**	0.001 (0;0.006)	0.007 (0;0.013)
Particulate matter formation	-0.024 (-0.057;-0.003)	0.1 (0;0.24)	0.055 (0.027;0.12)	0.18 (0.087;0.36)	-0.06 (-0.15;0)	0.17 (0.041;0.4)	**-0.799 (-0.8;-0.78)**	**-0.322 (-1.05;0.022)**	**-0.894 (-1.76;0.022)**
Photochemical oxidant formation	-0.012 (-0.028;0.016)	0.1 (0;0.22)	0.055 (0.024;0.12)	0.25 (0.11;0.44)	-0.029 (-0.074;0)	0.14 (-0.008;0.43)	**-0.799 (-0.8;-0.78)**	-0.051 (-0.17;0.029)	**-1.586 (-2.87;0.029)**
Terrestrial acidification	-0.025 (-0.05;-0.003)	0.13 (0;0.24)	0.067 (0.032;0.12)	0.22 (0.11;0.38)	-0.072 (-0.19;0)	0.16 (0.005;0.39)	**-0.799 (-0.8;-0.79)**	**-0.594 (-1.74;0.017)**	**-0.881 (-1.87;0.017)**
Terrestrial ecotoxicity	**-0.176 (-0.59;-0.028)**	0.082 (0;0.11)	0.048 (0.04;0.055)	**0.66 (0.53;0.77)**	-0.036 (-0.13;0)	**0.2 (0.092;0.52)**	**-0.8 (-0.8;-0.8)**	0.001 (0;0.006)	0.006 (0;0.012)
Urban land occupation	**-0.078 (-0.5;-0.017)**	**0.37 (0;0.51)**	**0.26 (0.095;0.57)**	0.18 (0.061;0.38)	-0.146 (-0.37;0)	**0.5 (0.051;1.52)**	**-0.8 (-0.8;-0.8)**	0.004 (0;0.02)	0.003 (0;0.011)
Water depletion	-0.014 (-0.054;0)	0.096 (0;0.13)	0.057 (0.05;0.064)	0.12 (0.1;0.14)	-0.029 (-0.11;0)	0.12 (0.028;0.38)	**-0.8 (-0.8;-0.79)**	0.001 (0;0.008)	0.003 (0;0.008)

S 10 Unit processes

The full model inventory as created in GaBi is shown in Table S7. The table is divided into main processes (*e.g.* the chemical cleaning process). The source (*i.e.* ecoinvent v2.2 is “ecoinvent” and specifically developed processes are named “own”), geographic coverage and reference year is indicated for all processes.

Table S7. Unit processes used to model life cycle inventories for European baseline scenario

Process	Process name	Source	Geographical scope	Year	Comment
Supply of coal to Germany					
Supply of hard coal to Germany	DE: hard coal supply mix <u-so>				
Coal mined and transported from Latin America	RLA: hard coal, at regional storage <agg>	ecoinvent	Latin America and the Caribbean	1989	
Coal mined and transported from Australia	AU: hard coal, at regional storage <agg>	ecoinvent	Australia	1989	
Coal mined and transported from Asia	CPA: hard coal, at regional storage <agg>	ecoinvent	Centrally Planned Asia and China	1989	
Coal mined and transported from Kazakhstan	ZA: hard coal, at regional storage <agg>	ecoinvent	Kazakhstan	1989	
Coal mined and transported from North America	RNA: hard coal, at regional storage <agg>	ecoinvent	North America	1989	
Coal mined and transported from Russia	RU: hard coal, at regional storage <agg>	ecoinvent	Russian Federation	1989	
Coal mined and transported from Central and Eastern Europe	EEU: hard coal, at regional storage <agg>	ecoinvent	Central and Eastern Europe	1989	
Coal mined and transported from Western Europe	WEU: hard coal, at regional storage <agg>	ecoinvent	Western Europe	1989	
Transport of coal within Europe with ship	RER: transport, barge <agg>	ecoinvent	Europe	2000	
Transport of coal within Europe with train	RER: transport, freight, rail <agg>	ecoinvent	Europe	2000	
Transport of coal from Australia with ship	OCE: transport, transoceanic freight ship <agg>	ecoinvent	Oceanic	2000	
Electricity for storage and preparation of coal	UCTE: electricity, medium voltage, production UCTE, at grid <u-so>	ecoinvent	Union for the Co-ordination of Transmission of Electricity	2004	
European electricity grid	RER: electricity, production mix RER <agg>	ecoinvent	Europe	2004	Electricity from European grid for production of medium voltage electricity
Supply of lignite to Europe					
Supply of lignite to Europe	RER: lignite, at mine <agg>	ecoinvent	Europe	1994	
Physical coal cleaning process					
The removal of ash and sulphur via physical cleaning	Coal to energy 1 (Selector) <agg>	Own			This process accounts for the ash and sulphur removed from the raw coal. This includes the electricity usage required for the physical cleaning process.
Chemical coal demineralization process					
NaOH leaching	NaOH leaching <u-so>	Own			This process is specifically developed for this study. The inputs for this process are: electricity, heat, water and Sodium hydroxide. The unit processes for the inputs are described in the designated sections in this table.
Centrifuge of coal slurry	Centrifuge <u-so>	Own			This process is specifically developed for this study. The input for this process is: electricity. The unit process for European electricity described in the designated section in this table.
Acid leaching	Acid leaching <u-so>	Own			This process is specifically developed for this study. The inputs for this process are: electricity, heat, water and acid. The unit processes for the inputs are described in the designated sections in this table.
Filter pressing of coal slurry	Filter press <u-so>	Own			This process is specifically developed for this study. The input for this process is: electricity. The unit process for European electricity described in the designated section in this table.

Process	Process name	Source	Geographical scope	Year	Comment
Hydrothermal wash	Hydrothermal wash <u-so>	Own			This process is specifically developed for this study. The inputs for this process are: heat, water and methanol. The unit processes for the inputs are described in the designated sections in this table.
Filter pressing of washed coal slurry	Filter press (hydrothermal wash) <u-so>	Own			This process is specifically developed for this study. The input for this process is: electricity. The unit process for European electricity described in the designated section in this table.
Drying of cleaned coal	Dryer <u-so>	Own			This process is specifically developed for this study. The input for this process is: heat. The unit process for European heat described in the designated section in this table.
Transport from chemical cleaning process to power plant	RER: transport, lorry >16t, fleet average <agg>	ecoinvent	Europe	2005	
Recovery of sodium hydroxide with lime	Sodium hydroxide recovery <u-so>	Own			This process is specifically developed for this study. The input for this process is: electricity. The unit process for European electricity described in the designated section in this table.
Recovery of acids with gypsum	Acid recovery <u-so>	Own			This process is specifically developed for this study. The input for this process is: electricity. The unit process for European electricity described in the designated section in this table.
Inputs and recovery/disposal of feedstock for chemical demineralization process					
Production of sodium hydroxide	RER: sodium hydroxide, 50% in H2O, production mix, at plant ecoinvent <agg>	ecoinvent	Europe	2000	
Recovery of sodium hydroxide	RER: sodium hydroxide, 50% in H2O, production mix, at plant ecoinvent <agg>	ecoinvent	Europe	2000	Process is inverted to model recovery and avoidance of virgin sodium hydroxide
	Production of acids				
Production of sulphuric acid	RER: sulphuric acid, liquid, at plant <agg>	ecoinvent	Europe	2001	
Production of hydrochloric acid	RER: hydrochloric acid, 30% in H2O, at plant ecoinvent <agg>	ecoinvent	Europe	2000	
Production of nitric acid	RER: nitric acid, 50% in H2O, at plant <agg>	ecoinvent	Europe	2001	
Production of hydrogen fluoride	GLO: hydrogen fluoride, at plant <agg>	ecoinvent	World	2006	
Production of hydrogen peroxide	RER: hydrogen peroxide, 50% in H2O, at plant <agg>	ecoinvent	Europe	1995	
	Recovery of acids				
Recovery of sulphuric acid	RER: sulphuric acid, liquid, at plant <agg>	ecoinvent	Europe	2001	Process is inverted to model recovery and avoidance of virgin acid
Recovery of hydrochloric acid	RER: hydrochloric acid, 30% in H2O, at plant ecoinvent <agg>	ecoinvent	Europe	2000	Process is inverted to model recovery and avoidance of virgin acid
Recovery of nitric acid	RER: nitric acid, 50% in H2O, at plant <agg>	ecoinvent	Europe	2001	Process is inverted to model recovery and avoidance of virgin acid
Recovery of hydrogen fluoride	GLO: hydrogen fluoride, at plant <agg>	ecoinvent	World	2006	Process is inverted to model recovery and avoidance of virgin acid
Recovery of hydrogen peroxide	RER: hydrogen peroxide, 50% in H2O, at plant <agg>	ecoinvent	Europe	1995	Process is inverted to model recovery and avoidance of virgin acid
Production of process water	RER: tap water, at user	ecoinvent	Europe	2000	
Production of gypsum	CH: gypsum, mineral, at mine <agg>	ecoinvent	Switzerland	2003	
Production of lime	CH: lime, hydrated, packed, at plant <agg>	ecoinvent	Switzerland	2002	
Production of methanol	GLO: methanol, at plant <u-so>	ecoinvent	World	2001	
Production of natural gas	RER: natural gas, high pressure, at consumer <agg>	ecoinvent	Europe	2000	
Electricity for natural gas production	UCTE: electricity, medium voltage, production UCTE, at grid <agg>	ecoinvent	Union for the Co-ordination of Transmission of Electricity	2004	
Treatment of used process water	CH: treatment, sewage, to wastewater treatment, class 2 <u-so>	ecoinvent	Switzerland	2000	
Electricity for waste water treatment	RER: electricity, production mix RER <agg>	ecoinvent	Europe	2004	
Recovery and use of precipitated inert	CH: portland calcareous cement, at plant (inverted)	ecoinvent	Switzerland	2001	Use of precipitated lime and gypsum together with mineral matter from

Process	Process name	Source	Geographical scope	Year	Comment
mineral matter and used lime and gypsum	<agg>				chemical demineralization process as calcareous input for cement production. The “CH: portland calcareous cement, at plant” has been inverted to model the avoided burdens
Heat production					
Heat produced from natural gas burning	RER: heat, natural gas, at boiler atm. low-NOx condensing non-modulating <100kW <u-so>	ecoinvent	Europe	2000	
Burning of natural gas	RER: natural gas, burned in boiler atm. low-NOx condensing non-modulating <100kW <u-so>	ecoinvent	Europe	2000	Burning of natural gas to production energy
Production of natural gas boiler	RER: gas boiler <agg>	ecoinvent	Europe	1998	Production of the boiler where natural gas is burned
Natural gas produced	CH: natural gas, low pressure, at consumer <agg>	ecoinvent	Switzerland	2000	
Low voltage electricity	UCTE: electricity, low voltage, production UCTE, at grid <u-so>	ecoinvent	Union for the Co-ordination of Transmission of Electricity	2004	Electricity input for the natural gas burning process
Medium voltage electricity	UCTE: electricity, medium voltage, production UCTE, at grid <u-so>	ecoinvent	Union for the Co-ordination of Transmission of Electricity	2004	
European electricity grid	RER: electricity, production mix RER <agg>	ecoinvent	Europe	2004	Electricity from European grid for production of medium voltage electricity
Construction and final decommissioning of pulverized coal power plant					
Construction and decommissioning of power plant	GLO: hard coal power plant, 500MW <u-so>	ecoinvent	World	1992	
Electricity use for construction and decommissioning	RER: electricity, production mix RER <agg>	ecoinvent	Europe	2004	
Transport of construction materials	RER: transport, lorry >16t, fleet average <agg>	ecoinvent	Europe	2005	
Coal burning and electricity production					
Combustion of coal in power plant to produce thermal electricity	DE: hard coal, burned in power plant <u-so>	Modified, ecoinvent	Germany	2000	The process is modified for air emissions, and removal of SOx, NOx and PM to avoid air emissions. The emissions to air are made coal specific. The subsequent treatment of slag from ash and collection of SOx and NOx is made dependent on the coal input and the efficiency of the collection technology. The thermal energy produced is a function of the higher heating valye of the coal
Electricity production in power plant	DE: electricity, hard coal, at power plant <u-so>	Modified, ecoinvent	Germany	2000	The electricity generated from burning coal (*i.e.* MJ produced per MJ thermal input). The process is adjusted to fit the average pulverized power plant efficiency.
Landfilling of hard coal ash from coal burning					
Landfilling of the coal ash slag	DE: disposal, hard coal ash, 0% water, to residual material landfill <u-so>	ecoinvent	Germany	2000	
Electricity use for landfilling process	RER: electricity, production mix RER <agg>	ecoinvent	Europe	2004	
Transport of coal with truck					
Transport from coal storage with truck	RER: transport, lorry >16t, fleet average	ecoinvent	Europe	2005	Transport with truck from coal storage to power plant and from coal storage to chemical demineralization plant

S11 References for ESI

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