- The National Institute of Health U.S. National Library of Medicine’s ChemIDplus Advanced online chemical inventory

Calculation of Concentration Values of Fluid Entries in Dataset

Concentration values were provided in the dataset as the maximum ingredient concentration in the HF fluid as a percentage by mass (which is the only concentration as a percentage of the HF fluid provided on the FracFocus forms). The total volume of HF injected fluid per well was not provided in the dataset. In order to calculate the volume for each chemical entry, the total volume of HF injected fluid per well was first calculated based on the volume of water used per well and the percentage of water in the total volume of HF fluid, both of which were provided in the dataset. For example, if the total volume of water were 4,000,000 gallons, and 85% of the mass of the HF injected fluid was reported as water, then the total volume of the HF injected fluid was calculated to be 4,705,882 gallons. In the same example, if 0.3% of the mass of the HF injected fluid were hydrochloric acid, then the total volume of the hydrochloric acid would be 14,118 gallons. All additives (except sand) were assumed to have the same density as water. Sand was computed separately as pounds per well assuming 1 gallon of HF fluid = 8.328 pounds.

The total volume of HF injected fluid was computed differently for wells where the percent of water in the HF injected fluid was not provided, even though the total volume of water used was provided (n=275). For example, if 15% of the HF fluid were sand and chemicals, then 85% was assumed to be water. In 258 of these wells, the percent of sand in the HF fluid was also not provided. For these cases, if, for example, 1% of the HF fluid were chemicals, then 99% of the HF fluid was assumed to be water.

was applied to all surfactants in the dataset. If a chemical appeared in the dataset with multiple component types, the dominant purpose was selected. There were several chemicals in the dataset for which each chemical entry was missing the component type in the HF fluid. The component type for these chemicals was labeled “Unknown”. Unknown chemicals were eliminated from the analysis.

Table 2. Price per primary compound for each component type based on Jiang et al., (2011)

Component Type	Primary Compound (from Jiang et al (2011))	2010 Price ($/kg)
Proppant	Silica, quartz sand	0.065
Acid	Hydrochloric acid or muriatic acid	0.18
Friction Reducer	Petroleum distillate	0.90
Surfactant	Isopropanol	0.95
Clay Stabilizer/Controller	Potassium chloride	0.30
Gelling Agent	Guar gum or hydroxyethyl cellulose	2.00
Scale Inhibitor	Ethylene glycol	0.95
pH Adjusting Agent	Sodium bicarbonate or sodium/potassium hydroxide	0.20
Breaker	Ammonium persulfate	0.66
Crosslinker	Borate salts	0.95
Iron Control	Citric acid	0.77
Bactericide/Biocide	Glutaraldehyde	2.20
Corrosion Inhibitor	Formamide	0.95

Both chemicals with CAS numbers and proprietary chemicals without CAS numbers were included in the GHG emissions assessment of chemicals. Of the 181 chemicals with CAS numbers in the dataset, 160 chemicals were included in the analysis. The remaining 21 chemicals were eliminated due to a lack of concentration values (n=18) or an unknown component type (n=3). In addition, approximately 133 proprietary chemicals without CAS numbers were provided in the dataset with concentration va from the GHG emissions assessment due to an unknown component type did have concentration values, and therefore were included in calculating chemical usage statistics detailed in Appendix A along with the 160 chemicals included in the GHG emissions assessment of chemicals (n=163).

In order to compute GHG emissions associated with the production of chemicals in the dataset, the cost of chemicals per well in each EIO-LCA category (i.e., organic, inorganic, or petroleum) were calculated (Table 3). The average chemical mass used per well was calculated by taking the total quantity from all chemical entries for each chemical and dividing by the total number of wells (1,907 wells was used instead of 1,921 due to missing information for 14 wells). Life-cycle GHG emissions factors were then applied to each EIO-LCA category of chemicals to calculate tons per CO2 equivalent (t CO2e) emissions per well (Table 4). The 2010 costs were adjusted to reflect 2002 dollars consistent with the adjustment made by Jiang et al., (2011) for each EIO-LCA category. For example, the cost per well of all inorganic friction reducers was $1,596 (Equation 1).

Equation 1. 1,773 kg/well * $0.90/kg = $1.596 per well

The cost per well of all inorganic chemicals for each component type were calculated and rolled-up together to equal $7,869 in 2002 dollars. According to the Purchaser Model, $1M of inorganic chemical manufacturing produces 2,060 t CO2e. Therefore, $7,869 of inorganic chemicals would generate 16.21 t CO2e per well (Equation 2).

Equation 2. $7,869 per well * (2,060 t CO2e)/$1,000,000 = 16.21 t CO2e per well

[redacted] **emicals in dataset.**

[redacted]	[redacted]
[redacted]	
[redacted]	$96
[redacted]	$123
[redacted]	$1
[redacted]	[redacted]
[redacted]	$28
[redacted]	$1
[redacted]	
[redacted]	$1,596
[redacted]	$1,430
[redacted]	$3,398
[redacted]	
[redacted]	$1,051
[redacted]	$682
[redacted]	$108
[redacted]	
[redacted]	$3
[redacted]	$294
[redacted]	
[redacted]	$2
[redacted]	$10

[redacted]

Table 4. GHG emissions from production and transportation of chemicals

EIO-LCA Category	t CO2e Emissions from Purchasing $1M of Product	Cost per Well (2010 prices)	Cost per Well (2002 prices)	t CO2e per Well
Petroleum	1,260	$ 3,507	$ 3,897	4.91
Organic chemicals	2,540	$ 10,475	$ 9,839	24.99
Inorganic chemicals	2,060	$ 9,138	$ 7,869	16.21
TOTAL		**$ 23,120**		

manufacturing, oil and gas extraction, etc.). The difference in these indirect GHG emissions between the Producer and Purchaser models is from activities associated with transportation to the final consumer. The Producer Model includes transportation to final consumer. The Purchaser Model does not. Therefore, since spending $512,820 to produce sand and $1M to purchase sand generate the same direct sand mining emissions (i.e., the same quantity of sand), purchasing $1M of sand generates 766 t C02e emissions in the production of sand, which excludes any GHG emissions from transportation to final consumer. The production of sand used in the HF fluid per well generates 110 t CO2e per well (Equation 3).

Equation 3. $143,610 per well * (766 t CO2e)/$1,000,000 = 110 t CO2e per well

Table 5. Emission factors from Producer and Purchaser Models for sand

Types of Activities	**t CO2e Emissions from Producing $512,820 of Sand (Producer Model)[a]**	**t CO2e Emissions from Purchasing $1M of Sand (Purchaser Model)[b]**
Direct sand mining activities	312	312
Indirect activities associated with sand mining[c]	454	1,048
Total GHG emissions	**766**	**1,360**

[a] The Producer Model incorporates GHG emissions associated with the production of a product from the extraction of raw materials to the completion of production (i.e., a cradle to gate of factory model).

[b] The Purchaser Model incorporates GHG emissions associated with the production of a product from the extraction of raw materials to the transportation of the product to the final consumer (i.e., a cradle to consumer model).

[c] Emissions from all other sectors impacted by “sand, gravel, clay, and refractory mining” sector (e.g., power generation and supply, cement manufacturing, oil and gas extraction, etc.)

Transportation of Sand and Water

Background – Transportation of Sand

Transportation of Sand – Stage 2: Processing Plant to Transload Station

Through visual inspection of the silica sand formation in Wisconsin, the center of Eau Claire County, WI was selected as the center of WI mining activity and the starting point for the rail trip from WI to PA. Figure 1 shows the areas of WI where sandstones for mining are found, the locations of sand minds (active, proposed, and in development), as well as the starting point for the rail trip from WI to PA. Through visual inspection of the Marcellus Shale formation, the connecting point of Clearfield, Elk, and Jefferson Counties was selected as the center of the Marcellus shale formation and the end point for the rail trip from WI to PA (Figure 2). According to US Silica Holdings, Inc., Canadian Pacific Railway is the only North American Railroad to serve the Marcellus Shale (US Silica, 2012). As shown in Figure 4, Canadian Pacific lines extend southward from Canada (through Buffalo) to the Marcellus Shale. However, due to a lack of evidence confirming that the Canadian route using Canadian Pacific lines was the exclusive route used to transport sand to the PA Marcellus shale, an entirely U.S. route was also considered (Figure 3). The average of the two routes was used in the base case scenario, and the entirely U.S. route and the Canadian route were used in the low-end and high-end scenarios, respectively.

Figure 3. WI to PA rail routes used in sand transportation assessment

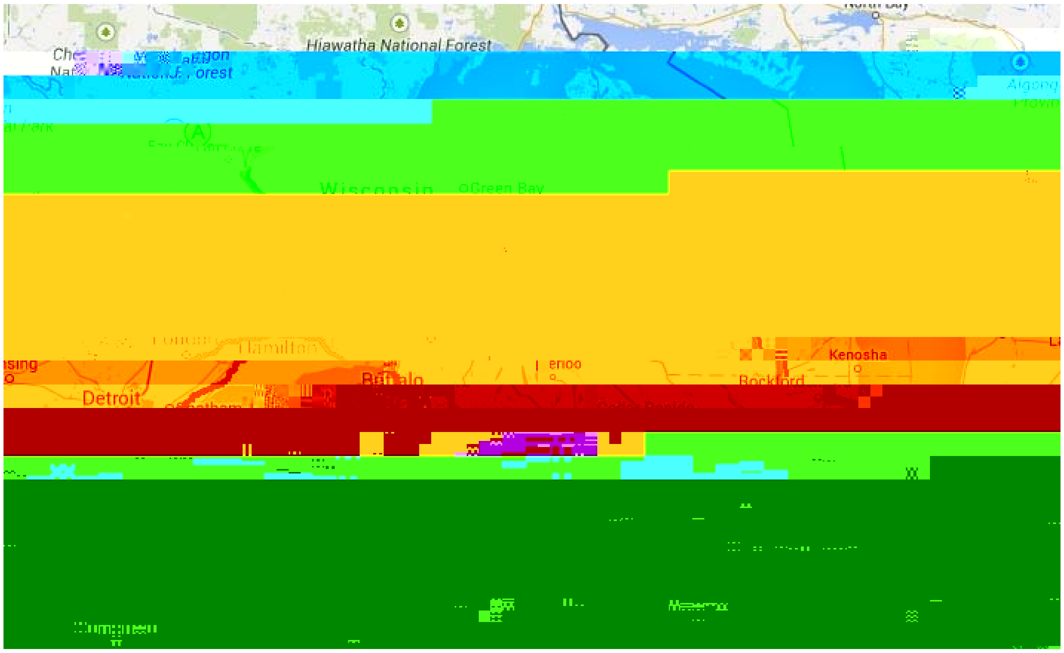
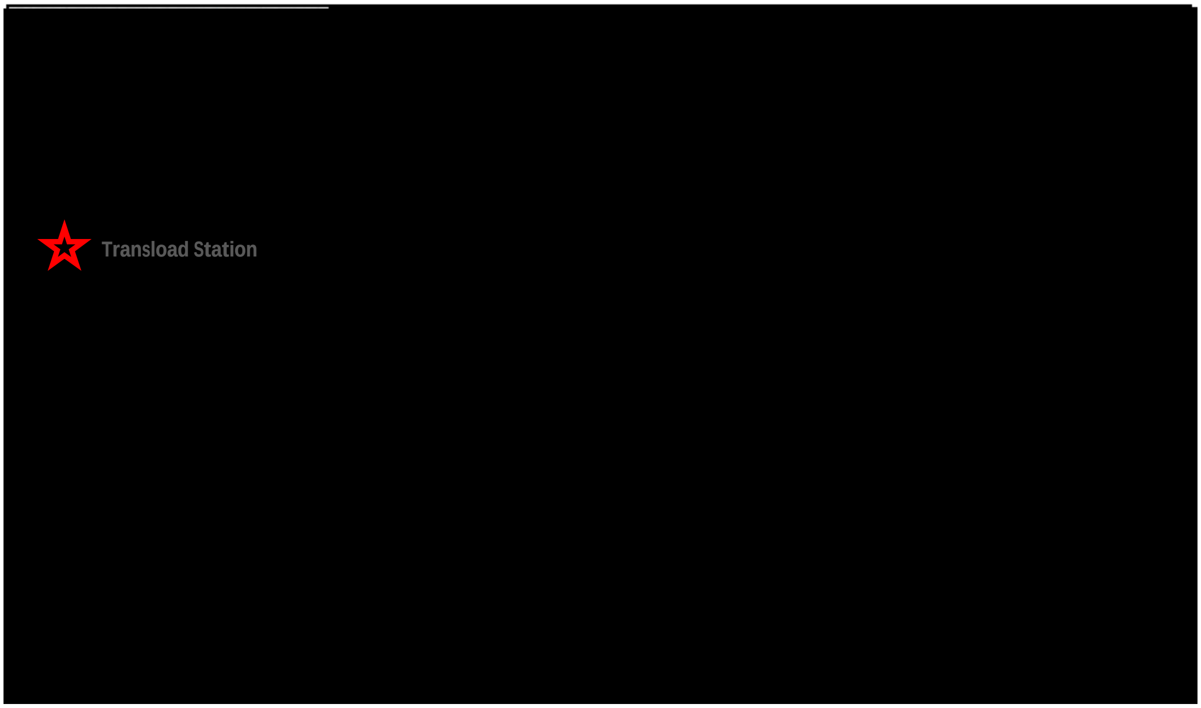


Figure 4. Railroads in the Marcellus Shale region (Canadian Pacific, 2014)

Transportation of Sand – Stage 3: Transload Station to HF Well

In order to estimate the average distance sand travels from transload station to HF well, the location of each transload station for each independent railroad in PA was identified and mapped out (see Figure 5 for example of an individual railroad map). In order to determine the average distance traveled by truck from a transload station to a HF well, visual inspection and Google Maps Driving Routes were used to identify the furthest points from the nearest transload station in six areas of the PA Marcellus Shale. The mean driving distance was 64 miles (range: 56 – 88 miles). Half the mean driving distance (32 miles) was used as the base case driving distance from transload station to HF well.

Figure 5. Western New York & Pennsylvania Railroad transload stations (Eagan)



Background –Transportation of Water

In the Marcellus Shale, approximately two-thirds of freshwater injected into a new hydraulically fractured well comes from surface water sources (e.g., rivers, ponds, lakes, etc.)

Figure 6: Literature review of water used in HF

Source	Source of Water Withdrawal	% of Injected Water for New Well that is Reused Water	% of Injected Water that Returns to Surface as Flowback Water	% of Flowback Water that is Reused	% of Flowback Water that is Brought to Disposal Site	% of Injected Water Transported to Site that is Brought to a Disposal Site.	Specific to Marcellus Shale?
Mitchell, Small, & Casman (2013)	Almost all water is withdrawn from surface water sources						

Source	Source of Water Withdrawal	% of Injected Water for New Well that is Reused Water	% of Injected Water that Returns to Surface as Flowback Water	% of Flowback Water that is Reused	% of Flowback Water that is Brought to Disposal Site	% of Injected Water Transported to Site that is Brought to a Disposal Site.	Specific to Marcellus Shale?
Penn State Cooperative Extension (2011b)	Permitted surface water sources: ~ 67%; Purchased from public water suppliers: 30%	Freshwater: 90%; Reused water: 10%		75%			Yes
Olawoyin et al (2011)			35%				Yes
Mantell (2011)		~ 10%	~ 10% to 15% recovered in first 10 days; < 200 gallons Per MMCF recovered over life of well.	Chesapeake Energy recycles/reuses nearly 100% of produced water via improved filtering processes			Yes
Jiang et al (2011)	Surface water: 50%; Local treatment plant: 50%		35–40%	30-60% Recycled and reused	40-70%		Yes
Gannett Fleming GFX Freight Solutions (2011)						~ 10-20%	Yes
Clark et al (2011)				95% of flowback assumed to be recycled			Yes
Penn State Cooperative Extension (2010)			13.5%	60%	40%	4%	Yes
Yoxtheimer & Gaudlip (2010)			10% in first 30 days; > 20% over life of well				Yes
NADO (2010)			~ 33%				Yes
Gaudlip et al (2008)	Surface water: 60-70%; Groundwater < 4%		35%				Yes

Transportation of Water: Freshwater to HF Well

Under 25 Pa. Code Chapter 110, the Pennsylvania Department of Environmental Protection ("PA DEP") requires the registration of water withdrawal sources used for HF (PA DEP, 2014a). Data pertaining to registered water withdrawal sources are publically available for download from the PA DEP website. The data include 354 registered withdrawal sources in PA from January 2007 through October 2013 used for HF. Based on the GPS coordinates provided in the PA DEP data, figure 7 displays the spatial distribution of the 354 registered withdrawal sources used for HF throughout the PA Marcellus Shale. Surface water sources and groundwater sources account for 88% (n=311) and 12% (n=43) of the withdrawal sources, respectively.

Figure 7: Location of 354 registered PA withdrawal sources used for HF

To estimate the average driving distance traveled from withdrawal source to HF well, sixteen clusters of HF wells were analyzed in the areas of PA most densely populated with HF wells. Using the locations of the registered withdrawal sources and the registered HF wells, Google Maps Driving Routes were used to determine the furthest driving distance from a withdrawal source to an HF well in each analyzed cluster of HF wells. The mean driving distance was 15.8 miles (range: 7.5 – 27.9 miles). Half the mean (8 miles) was used as the base case driving distance from water withdrawal source to HF well.

Transportation of Water: Flowback Water

The Pennsylvania Oil and Gas Act requires unconventional well operators to submit production reports which detail each disposal of flowback water per PA HF well. Disposal water data are publically available for download from the PA DEP website. (PA DEP, 2014b) Twelve months of data from July 2012 through June 2013 contain 24,371 reports of the disposal of produced fluid, fracking fluid waste, or drilling fluid waste from 4,929 HF wells. Data include the GPS coordinates of HF wells, disposal methods, names and addresses of waste facilities, and quantities of disposal water. In this 12-month period, unconventional well operators in PA reported 32 million barrels of fluid waste, which is equivalent to 1.76 billion gallons (assuming 1 bbl = 55 gallons).

Assessment of Percentage of Initially Injected Water which Returns to the Surface as Flowback Water

PA DEP fluid waste data were also used to estimate the percentage of initially injected water which returns to the surface as flowback water. For the 4,929 HF wells which reported fluid waste from July 2012 through June 2013, all available PA DEP fluid waste data (from January 2006 through June 2013) were searched to capture every report of fluid waste associated with these wells in order to determine the total quantity of fluid waste per well to date. During this 7.5-year period, the mean quantity of fluid waste reported per well was 1.45 million gallons. Using 1.45 million gallons as the mean volume of returned flowback water per well and 4.29

Table 6. Number of HF wells if FracFocus dataset by natural gas operator

Natural Gas Operator	Wells per Operator	Percentage of Wells by Operator

According to Gannett Fleming GFX Freight Solutions (2011), an average rail car can carry 100 tons of sand, for which four to five trucks are needed to transport sand to HF wells (i.e., 20 – 25 tons per truck) (Gannett Fleming GFX Freight Solutions, 2011). In the Hart et al., (2013) study to assess transportation impacts from frac sand in Wisconsin, it was assumed that each unit train contained 100 rail cars, each rail car carried 100 tons of sand, and each truck carried 25 tons of sand (Hart et al., 2013). In our assessment we also assumed in all scenarios that each train contained 100 rail cars, and the carrying capacity of each rail car was 100 tons of sand. Our average estimate for sand transportation from mine to processing plant assumed each truck to carry 22.5 tons (range: 20 – 25 tons). According to Clark et al., (2011), the terrain in the Marcellus Shale region limits truck carrying capacity to 14.16 tons (Clark et al., 2011). Therefore, our average estimate for sand transportation by truck from transload station to HF well assumed a carrying capacity of 19.58 tons (range: 14.16 – 25 tons).

Regarding the transportation of water in the Marcellus Shale region, trucks to HF wells are said to have a carrying capacity of approximately 5,500 gallons each (22.9 tons) (Gannett Fleming GFX Freight Solutions, 2011). According to Hart et al., (2013), tank trucks can hold 5,465 gallons of water (22.76 tons) (Hart et al., 2013). However, as Clark et al., (2011) determined that the terrain in the Marcellus Shale region limits truck carrying capacity to 3,400 gallons of water (14.16 tons), our average estimate for water transportation by truck assumed a carrying capacity of 18.53 tons (range: 14.16 – 22.9 tons).

[redacted]

The EIO-LCA Purchaser Model incorporates transportation to final consumer. Using an emissions factor of 1,360 t CO2e emissions per $1M of “Sand, gravel, clay, and refractory mining”, the EIO-LCA purchaser model estimates dg]ns

Table 10. Average Estimate of GHG emissions by material, process, and process phase

Material	Process	Process Phase	t CO2e Emissions per Well	g CO2e Emissions per MJ
Chemicals	**Production and Transportation**		**46.1**	**0.014**
Sand	Production		110.0	0.035
	Transportation	Mine to processing plant	49.9	0.016
		WI to PA (Rail)	674.9	0.212
		Transload to HF well	84.9	0.027
	Transportation Total:		809.7	0.255

Seydor, S. M., Clements, E., Pantelemonitis, S., & Deshpande, V. (2012). *Understanding the Marcellus shale supply chain working paper*. Pittsburgh, PA: University of Pittsburgh: Katz Graduate School of Business.

US Silica. (2012, 6/22/2012). *Canadian pacific and U.S. silica holdings, inc. announce multi-year agreement for the transport of frac sand*. US Silica News.

Wisconsin DNR. (2012). *Silica sand mining in Wisconsin*. Madison, WI: Wisconsin Department of Natural Resources.

WRI. (2012). *Waste management of cuttings, drilling fluids, hydrofrack water and produced water*. New York State Water Resources Institute.

Yoxtheimer, D. (2011). *Water management options for Marcellus natural gas development*. Penn State Cooperative Extension.

Yoxtheimer, D., & Gaudlip, T. (2010). Water use and water re-use/Recycli