Update of the Carbon Fiber pathway in GREET® 2021

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ACRONYMS

AN	Acrylonitrile
CF	Carbon fiber
CFRP	Carbon fiber-reinforced plastic
FCV	Fuel-cell vehicle
GHG	Greenhouse gas
HB	Haber-Bosch
ICEV	Internal combustion engine vehicle
LCI	Life-cycle inventory
MMA	Methyl methacrylate
PAN	Polyacrylonitrile
SA	Strategic Analysis
SMR	Steam methane reforming

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This memo documents updates in the GREET® model for the carbon fiber pathway and the weight-ratio of constituents (resin and fiber) in carbon fiber-reinforced plastic.

1. Introduction

Carbon fiber (CF) has emerged as an important material in vehicle lightweighting to improve fuel economy through its usage as reinforcement in plastics in automotive components (Das 2011; Ghosh et al. 2021; Pradeep et al. 2017; Taub et al. 2019). CF is also used in the outer lining of hydrogen tanks in fuel-cell vehicles (FCVs) (Moradi and Groth 2019), which are an alternative to conventional internal combustion engine vehicles (ICEVs) with zero tailpipe emissions. Yet, the lightweighting capability of CF as well as its suitability for use in alternative energy-powered vehicles are accompanied by its high costs and energy intensity of CF production (Das 2011; Ghosh et al. 2021; Nunna et al. 2019). This makes it critical to quantify the trade-off between the weight reduction via use of CF and the increase in energy use for vehicle production, or even the trade-off between the decrease in greenhouse gas (GHG) emissions and the rise in GHG emissions during production for FCVs over ICEVs. To enable such quantification, both previous and existing GREET models have provided the life-cycle inventory (LCI) for cradle-to-gate production of CF using data provided by (Johnson and Sullivan 2014). This report provides details of changes made to this LCI data for CF production, which have been incorporated in the 2021 GREET update, using more-recent LCI data.

2. Carbon Fiber (CF) Production

(Johnson and Sullivan 2014) describe the entire process of carbon fiber (CF) production as a combination of several steps (flowchart shown in Figure 1), along with the type and quantity of materials (initial and intermediate) and different energy sources used for these steps. The existing GREET 2020 model provides a single life-cycle inventory (LCI) for cradle-to-gate CF production by combining these material and energy flows across multiple steps into a single tabular output. In the updated GREET 2021 model, LCI for production of each of these intermediary materials is provided separately and updated based on available literature. Using these individual LCIs, the final cradle-to-gate LCI for production of CF is calculated and provided to users.

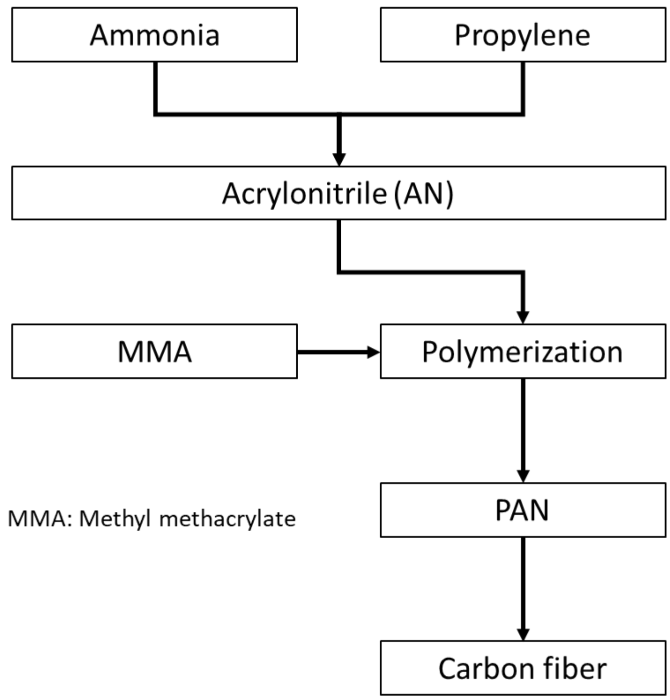

Figure 1. Flowchart for carbon fiber (CF) production

2.1. Production of Ammonia

Typically, ammonia (NH_3) is produced through a two-step pathway: (a) Hydrogen (H_2) production via steam methane reforming (SMR); and (b) Ammonia synthesis via Haber-Bosch (HB) process. In the existing GREET 2020 model, LCI of this conventional ammonia production, as given in (Johnson and Sullivan 2014), is used towards CF production. This LCI is two decades old and is at variance with the most-recent LCI provided for conventional ammonia production in the GREET 2020 model. Also, (Liu, Elgowainy, and Wang 2020) have discussed and analyzed the alternative means of producing ammonia using industrial byproducts and renewable resources. The LCI of this alternative ammonia production (referred to as "*green ammonia*"), and the LCI of total ammonia production, weighted by the shares of conventional and green ammonia production, are given in the existing GREET 2020 model (Wang et al. 2020). The GREET 2021 update utilizes this weighted LCI from GREET1 (for GREET 2021), while enabling the user to modify the share of each production method in total ammonia production and evaluate its effect on overall inventory and impacts. Table 1 shows the energy inputs for both ammonia production methods as reported in GREET 2020.

Table 1: Energy inputs for conventional and green ammonia production

Energy Source	**Energy input (mmBTU/ton of product)**	
	Conventional Ammonia	**Green Ammonia**
Natural gas	31.384	0.000
Electricity	0.404	1.002

2.2. Production of Propylene

Propylene (C_3H_6) is produced through either of steam cracking or petroleum refining processes (Wang et al. 2020). The LCI of CF production in GREET 2020 considers inventory details given in (Johnson and Sullivan 2014), which assumes propylene production to be only through steam cracking. The GREET 2021 update replaces this with the weighted LCI of propylene provided in GREET1, accounting for the shares of steam cracking and petroleum refining methods in overall propylene production and their respective LCIs.

2.3. Production of Acrylonitrile (AN)

Acrylonitrile (AN) is produced primarily via Sohio process (Johnson and Sullivan 2014), where propylene (C_3H_6) and ammonia (NH_3) are used as feedstock inputs and reacted with oxygen to produce AN (C_3H_3N) and water (H_2O). LCI details for AN production in the existing GREET 2020 model are considered from (Johnson and Sullivan 2014). These are extended to the GREET 2021 update as well and are provided separately (detailed in Table 2).

Table 2: Material and energy inputs for acrylonitrile production

Material inputs (ton/ton of product)	
Ammonia	0.48
Propylene	1.17
Energy inputs (mmBTU/ton of product)	
Natural gas	1.197
Coal	0.317
Residual fuel oil	0.034
Electricity	0.344

2.4. Production of Methyl Methacrylate (MMA)

Methyl methacrylate (MMA) is used as co-monomer in the production of polyacrylonitrile (PAN; Section 2.5). For CF production in the existing GREET 2020 model, LCI of MMA production is used from (Johnson and Sullivan 2014) – this is extended to the 2021 update and provided separately for the benefit of GREET users. Table 3 shows the LCI of MMA production.

Table 3: Energy inputs for methyl methacrylate (MMA) production

Energy inputs (mmBTU/ton of product)	
Natural gas	56.686
Coal	5.886
Residual fuel oil	31.560
Electricity	3.715

2.5. Production of Polyacrylonitrile (PAN)

Acrylonitrile (AN) is used as the primary monomer for producing polyacrylonitrile (PAN), along with the use of methyl methacrylate (MMA) as co-monomer, in the weight ratio of 95:5 (PAN:MMA), with the obtained PAN spun into fibers upon its successful polymerization (Johnson and Sullivan 2014). The existing GREET 2020 model uses LCI details for final PAN production (i.e., the sum of polymerization of AN and MMA, filtration, drying of PAN, spinning into fibers, and finishing) from (Johnson and Sullivan 2014). For the GREET 2021 update, material inputs for PAN production are taken from the more-recent LCI provided in (Ghosh et al. 2021), which in turn uses cost-modeling data for CF production from (Nunna et al. 2019). More details on LCI of PAN production are given in Table 4.

Table 4: Material and energy inputs for polyacrylonitrile (PAN) fiber production

Material inputs (ton/ton of product)	
Acrylonitrile (AN)	0.95
Methyl methacrylate (MMA)	0.05
Energy inputs (mmBTU/ton of product)	
Electricity	11.376

Separately, LCI for PAN production was obtained via personal communication with Strategic Analysis (SA) (James, Houchins, and Huya-Kouadio 2021). While the material inputs provided by SA were in line with literature (Ghosh et al. 2021; Johnson and Sullivan 2014), the difference for SA energy use was only 10% vis-à-vis that used in (Ghosh et al. 2021). This confirms the data for the LCI used here (Table 4).

2.6. Production of Carbon Fiber (CF)

After its production, PAN fiber goes through a series of steps (shown in Figure 2) to obtain the final carbon fiber (CF). While the existing GREET 2020 model uses LCI details for combined sum of these steps from (Johnson and Sullivan 2014), like for PAN, the GREET 2021 update uses the more-recent LCI for CF production from (Ghosh et al. 2021). More details on this LCI are given in Table 5.

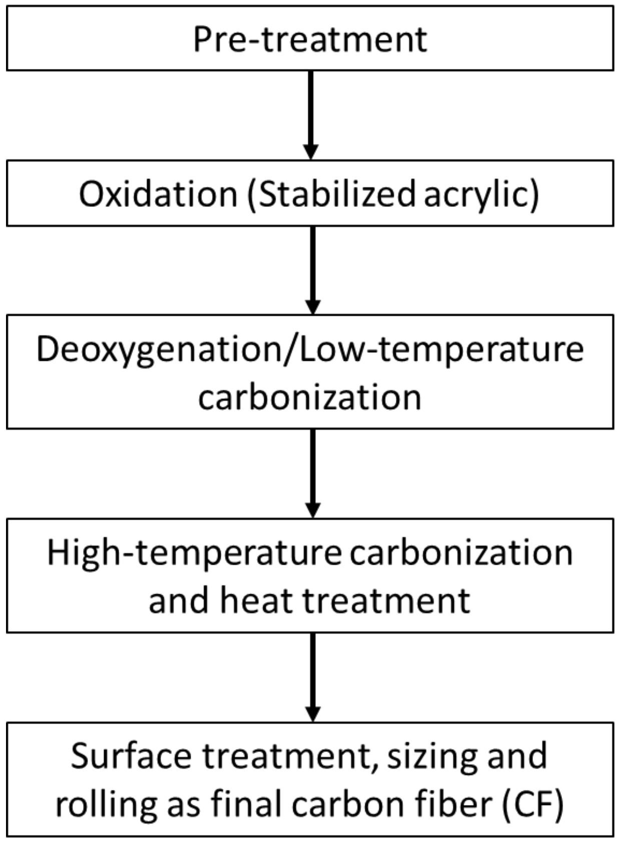

Figure 2: Steps involved in carbon fiber production, based on (Johnson and Sullivan 2014) and personal communication with Strategic Analysis (SA) (James, Houchins, and Huya-Kouadio 2021)

Table 5: Material and energy inputs for carbon fiber (CF) production from polyacrylonitrile (PAN)

Material inputs (ton/ton of product)	
Polyacrylonitrile (PAN)	2.08
Energy inputs (mmBTU/ton of product)	
Natural gas	5.984
Electricity	65.933

As in case of PAN, LCI details for CF production were also obtained via personal communication with Strategic Analysis (SA) (James, Houchins, and Huya-Kouadio 2021) to validate the LCI used here (Table 5). Both material and energy inputs were observed to be in line with literature (Ghosh et al. 2021; Johnson and Sullivan 2014), with the overall difference for total energy use being insignificant (< 1%) between SA (James, Houchins, and Huya-Kouadio 2021) and (Ghosh et al. 2021).

3. Carbon Fiber-Reinforced Plastic (CFRP): Composition

Based on personal communication with Strategic Analysis (SA) (James, Houchins, and Huya-Kouadio 2021), the update in GREET 2021 model modifies the CF-to-epoxy weight ratio to 68:32 for CFRP used in high-pressure vessels.

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