

# Section 3

## Modeling Approach

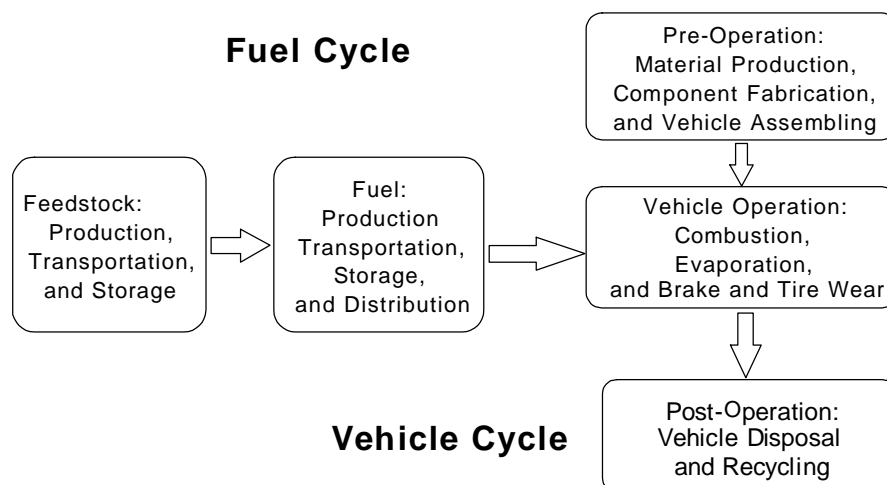
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### 3.1 Fuel Cycles and Their Stages

The use of motor vehicles involves two different energy cycles: production and use of motor fuels (fuel cycle) and production and use of motor vehicles (vehicle cycle). The *fuel cycle* for a given transportation fuel includes the following processes: primary energy (i.e., energy feedstock) production, transportation, and storage (T&S); fuel (i.e., energy source) production, transportation, storage, and distribution (T&S&D); and vehicle operations that involve fuel combustion or other chemical conversions (Figure 3.1). The *vehicle cycle* includes material recovery and fabrication, vehicle production, vehicle operation, and vehicle disposal/recycling. (Note that vehicle operation is included in both the fuel cycle and the vehicle cycle.) The processes that precede vehicle operations are often referred to as upstream activities; actual vehicle operations are referred to as downstream activities.

To evaluate various motor vehicle technologies, both cycles should be considered, because in many cases, use of an alternative transportation fuel or an advanced vehicle technology involves changes in both upstream fuel production activities and in production of materials and vehicles. In energy and emission analyses for consumer goods, researchers often refer to studies of the “cradle to grave” cycle of a product as *life-cycle analysis* (LCA). A so-called *total energy-cycle analysis* (TECA) for transportation technologies includes both the fuel and the vehicle cycles. When TECA results for ICEV-based technologies are separated into three groups — fuel-cycle upstream activities, vehicle production and disposal, and vehicle operations — energy use and emissions from vehicle operations are the largest, those from upstream activities are second, and those from vehicle production and disposal are the smallest. Figure 3.1 presents a flow chart for a total energy-cycle analysis.

The GREET model has been developed to calculate per-mile energy use and emission rates of various combinations of vehicle technologies and fuels for both fuel cycles and total energy cycles. Since the development of GREET 1.0 (which was a fuel-cycle model only), the model has evolved to include three components. The first — the Series 1 component (GREET 1.0, 1.1, 1.2, 1.3, and so on) — calculates fuel-cycle energy use and emissions of light-duty vehicles (passenger cars, vans, and light-duty trucks [LDTs]). This series is the continuation of GREET 1.0. The second — the Series 2 component — calculates vehicle-cycle energy use and emissions of light-duty vehicles. The Series 2 component was developed through Argonne’s effort on total energy-cycle analysis for HEVs. During calculations, the Series 2 model draws data from the Series 1 model to estimate vehicle-cycle energy use and emissions. Energy and emission results of fuel cycle (calculated in Series 1) and vehicle cycle (calculated in Series 2) analyses are combined in Series 2. So, the Series 1 model presents fuel-cycle results only, and the Series 2 model presents both fuel-cycle and total energy-cycle results. Development and use of the Series 2 GREET model will be documented elsewhere.



**Figure 3.1 Flowchart of a Total Energy-Cycle Analysis**

The third component of the GREET model — Series 3 — was developed to estimate fuel-cycle energy use and emissions of heavy-duty vehicles (class 2b to class 8 trucks). The Series 3 model draws data for upstream fuel production activities from the Series 1 model. Development and use of the Series 3 GREET model will be documented elsewhere.

This report documents development and use of the most recent version of the Series 1 model: GREET 1.5. Since 1996, some interim versions (i.e., GREET 1.1, GREET 1.2, GREET 1.3, and GREET 1.4) were developed. Those versions involved some changes in parametric assumptions regarding fuel production and included additional fuels and vehicle technologies. They were used to generate interim results by Argonne and other institutions to evaluate various transportation technologies. No formal documentation for those versions was published. GREET 1.5 includes more than 30 fuel cycles (Table 3.1), involving 13 types of fuel feedstocks (petroleum, NG, flared gas, coal, soybeans, uranium, corn, woody biomass, herbaceous biomass, landfill gases, hydropower, solar energy, and wind) and 14 fuels (conventional gasoline [CG], RFG, conventional diesel [CD], reformulated diesel [RFD], LPG, CNG, LNG, methanol, dimethyl ether [DME], ethanol, hydrogen, Fischer-Tropsch diesel [FTD], biodiesel, and electricity). Because virtually no emissions are associated with electricity generated from hydropower, solar energy, and wind, these cycles are treated together as zero-emission cycles in GREET. These fuel cycles are included in GREET 1.5 essentially because researchers are interested in them and because data regarding fuel production are available. Other cycles may be added to GREET as additional emission and energy use data become available. Detailed technology descriptions and assumptions for these cycles are presented in Section 4.



**Table 3.1 Fuel Cycles Included in GREET 1.5**

| Primary Energy Source                 | Fuel                                    |
|---------------------------------------|---|
| Petroleum                             | Conventional gasoline                   |
|                                       | Reformulated gasoline                   |
|                                       | Conventional diesel                     |
|                                       | Reformulated diesel                     |
|                                       | Liquefied petroleum gas                 |
|                                       | Electricity via residual oil            |
| Natural gas                           | Compressed natural gas                  |
|                                       | Liquefied natural gas                   |
|                                       | Liquefied petroleum gas                 |
|                                       | Methanol                                |
|                                       | Dimethyl ether                          |
|                                       | Gaseous hydrogen/<br>central plants     |
|                                       | Gaseous hydrogen/<br>refueling stations |
|                                       | Liquid hydrogen                         |
|                                       | Fischer-Tropsch diesel                  |
|                                       | Electricity                             |
| Flared gas                            | Methanol                                |
|                                       | Dimethyl ether                          |
|                                       | Fischer-Tropsch diesel                  |
| Coal                                  | Electricity                             |
| Uranium                               |   |
| Hydropower, solar energy, and wind    |   |
| Corn: dry milling                     | Ethanol                                 |
| Corn: wet milling                     |   |
| Woody biomass                         |   |
| Herbaceous biomass                    |   |
| Solar energy (via water electrolysis) | Gaseous hydrogen                        |
|                                       | Liquid hydrogen                         |
| Soybeans                              | Biodiesel                               |
| Landfill gases                        | Methanol                                |

### 3.2 Vehicle Types

As stated above, the Series 1 GREET model estimates fuel-cycle energy use and emissions of light-duty vehicles (i.e., passenger cars and LDTs). Heavy-duty trucks (HDTs) are included in the Series 3 GREET model. Table 3.2 lists vehicle types included in the Series 1 and 3 models. Vehicle types are divided between the two models according to the way in which emission standards are set. For passenger cars, Class 1 trucks (commonly called light-duty trucks 1 [LDT1s]), and Class 2a trucks (commonly called light-duty trucks 2 [LDT2s]), emission standards are set by the EPA on a per-mile basis. Vehicle emissions for these vehicle types are measured on *vehicle chassis* dynamometers. For truck Classes 2b–8b and buses (called HDTs), emission standards are set for engines on a per-brake-horsepower-hour basis. Emissions from *engines*, not from vehicles, are measured on *engine* dynamometers. Emissions from HDTs need to be converted into per-mile emissions for use in the models. This conversion step, which is subject to some uncertainties, makes emission calculations for HDTs different than those for passenger cars and LDTs.

For passenger cars and LDTs, GREET 1.5 includes the following technologies: EVs; HEVs; FCVs fueled with hydrogen, methanol, gasoline, ethanol, or CNG; spark-ignition ICEVs fueled with CG, RFG, CNG, LNG, LPG, or ethanol; and compression-ignition ICEVs fueled with CD, RFD, DME, FTD, or biodiesel. Details on the selection of these fuel/vehicle combinations are presented in Section 4.



**Table 3.2 Vehicle Types Included in Series 1 and 3 GREET Models**

| Series 1 GREET Model   |                        | Series 3 GREET Model         |                        |
|------------------------|------------------------|------------------------------|------------------------|
| Vehicle Type           | GVWR <sup>a</sup> (lb) | Vehicle Type                 | GVWR <sup>a</sup> (lb) |
| Passenger cars         | 0 – 6,000              | Class 2b – 4 trucks          | 8,501 – 16,000         |
| Class 1 trucks (LDT1)  | 0 – 6,000              | Class 5 – 6 trucks           | 16,001 – 26,000        |
| Class 2a trucks (LDT2) | 6,001 – 8,500          | Class 7 trucks               | 26,001 – 33,000        |
|                        |                        | Class 8a trucks              | 33,001 – 60,000        |
|                        |                        | Class 8b trucks              | > 60,000               |
|                        |                        | School buses                 | 21,000 – 31,000        |
|                        |                        | Transit and commercial buses | 26,001 – 60,000        |

<sup>a</sup> Gross vehicle weight rating.

### 3.3 Calculation of Energy Use and Emissions of Upstream Stages

#### 3.3.1 Calculation of Energy Use for an Upstream Stage

To estimate fuel-cycle energy use and emissions, GREET first estimates energy use (in British thermal units [Btu]) and emissions (in grams) per million Btu [ $g/10^6$  Btu] of fuel throughput for a given upstream stage. The model then combines the energy use and emissions from all upstream stages for a fuel cycle to estimate total upstream fuel-cycle energy use and emissions. The aggregation takes into account, among other factors, loss of a fuel during the fuel cycle (see detailed discussion in Section 3.3.4). Because fuel-cycle fossil fuel and petroleum consumption, as well as total energy consumption, are of interest, GREET is designed to calculate both of these values as well as fuel-cycle total energy consumption, all at the primary energy level. Energy consumption and emissions of the following fossil fuels are calculated in GREET: petroleum, NG, and coal. Total energy includes fossil energy and renewable energy such as solar energy, wind, and geothermal energy. Therefore, the model can estimate the amount of fossil fuel and petroleum displaced as a result of using alternative transportation fuels and advanced vehicle technologies instead of conventional vehicles fueled with gasoline.

For a given upstream stage, energy input per unit of energy product output is calculated by using the energy efficiency of the stage. By definition, energy efficiency is the energy output divided by the energy input (including energy in both process fuels and energy feedstock). Thus, total energy input is:

$$Energy_{in} = 1/efficiency, \tag{3.1}$$

where

Energy<sub>in</sub> = Energy input of a given stage (say, in Btu per Btu of energy product output from the stage), and



Efficiency = Energy efficiency for the given stage (defined as [energy output]/[energy input] for the stage).

The energy efficiencies of each upstream stage for various fuel cycles are presented in Section 4.

Equation 3.1 calculates total energy input to a process. The total energy input comprises energy feedstock and process fuels. In most cases, energy feedstock includes both a feed for production of a fuel and a process fuel used during production. To calculate emissions, especially emissions of criteria pollutants, the total feedstock input needs to be separated into feed and fuel. Converting feed to a given fuel (which, in most cases, is a chemical process) may or may not produce emissions. Combustion of a feedstock as a fuel certainly produces emissions. The combustion emissions can be estimated by using the amount of fuel burned and the combustion emission factors.

To separate energy feedstock input between feed and fuel, researchers must consider three cases. In the first case, all the energy feedstock input is burned in producing a fuel. An example is electricity generation. In the second case, some (usually a majority) of the energy feedstock input is used as feed in a conversion process to produce a fuel; the remainder, together with any other process fuels necessary for the conversion process, is burned to provide heat or steam for the process. Examples include chemical processes such as production of methanol, hydrogen, DME, and FTD from natural gas. In this case, the total natural gas input needs to be broken down into natural gas used as feed and natural gas used as fuel. Only the natural gas used as fuel is included in combustion emission calculations. In the third case, no chemical processes are involved in production (or transformation) of a fuel. Of the total energy feedstock input, a unit of energy in fuel product output requires a unit of energy in feedstock input. The difference between the energy in the feedstock input and the energy in the energy product is the amount of feed used as the process fuel. Examples include CNG and LNG production. For this case, the following equation is used to estimate the amount of process fuel required:

$$\text{Process Fuels} = 1/\text{efficiency} - 1, \quad [3.2]$$

where

Process fuels = The amount of process fuels required during a given stage to generate one unit of energy for production (say, in Btu per Btu of energy output from the stage), and

Efficiency = Energy efficiency for a given stage (defined as [energy output]/[energy input] for the stage).

The calculated energy consumption of all process fuels for a particular stage is then allocated to the different process fuels burned during the stage. For example, if  $10^3$  Btu of process fuels is burned to deliver  $10^6$  Btu of fuel throughput from an upstream stage, GREET allocates the  $10^3$  Btu of process fuels into individual process fuels such as diesel, residual oil, and electricity. GREET includes the following process fuels: NG, residual oil, diesel, gasoline,



crude oil, LPG, coal, electricity, and biomass. Allocating the percentages of total energy burned to different process fuels for a given stage is necessary to allow researchers to calculate emissions from the stage; the amount of emissions attributable to fuel combustion depends very much on the type of fuel burned. The allocation process is also necessary for calculating fossil fuel use and petroleum use for each stage.

The shares of process fuels in total fuel use for fuel-cycle stages are different for different fuel cycles and different stages. For existing fuels industries (such as oil, NG, coal, and electric industries), process fuel shares are usually estimated on the basis of historical statistical data on fuel use by fuel type. In these cases, GREET relies primarily on results from Delucchi (1997). For new industries that produce new fuels (such as DME, FTD, and cellulosic ethanol), process fuel shares are assumed in GREET by considering process fuel shares for similar industries and the availability of process fuels.

Although energy efficiencies are used to calculate energy use for most upstream stages according to Equations 3.1 and 3.2, the actual amounts of process fuel and feedstock inputs and product fuel outputs are used to calculate energy use for some stages. For example, in estimating energy use and emissions for production of ethanol from corn, the amounts of corn input (in bushels) and process fuels (in Btu) per gallon of ethanol produced are estimated and entered in GREET. Use of physical units instead of energy use in these cases makes GREET input assumptions more transparent. This applies to ethanol production from corn and biomass, biodiesel production from soybean, and production and transportation of fertilizers, insecticide, and herbicide. Details of inputs and outputs for individual stages are presented in Section 4.

### 3.3.2 Calculation of Emissions for an Upstream Stage

Emissions of VOCs, CO, NO<sub>x</sub>, PM<sub>10</sub>, SO<sub>x</sub>, CH<sub>4</sub>, N<sub>2</sub>O, and CO<sub>2</sub> for a particular stage are calculated in g/10<sup>6</sup> Btu of fuel throughput from the stage. Emissions occurring during a stage include those resulting from the combustion of process fuels and from noncombustion processes such as chemical reactions and fuel leakage and evaporation. Emissions resulting from chemical reactions, fuel leakage, and fuel evaporation are fuel- and stage-specific; they are presented in Section 4, as needed. Emissions from combustion of process fuels for a particular stage are calculated by using the following formula:

$$EM_{cm,i} = \left( \sum_j \sum_k EF_{i,j,k} \times EC_{j,k} \right) \div 1,000,000, \quad [3.3]$$

where

- EM<sub>cm,i</sub> = Combustion emissions of pollutant i in g/10<sup>6</sup> Btu of fuel throughput,
- EF<sub>i,j,k</sub> = Emission factor of pollutant i for process fuel j with combustion technology k (g/10<sup>6</sup> Btu of fuel burned), and
- EC<sub>j,k</sub> = Consumption of process fuel j with combustion technology k (Btu/10<sup>6</sup> Btu of fuel throughput).



$EC_{j,k}$  for a given stage is, in turn, calculated by using the following formula:

$$EC_{j,k} = EC \times Share_{fuelj} \times Share_{techk,j} , \quad [3.4]$$

where

- EC = Total energy consumption for the given stage (in Btu/10<sup>6</sup> Btu of fuel throughput, calculated with Equation 3.1 or 3.2),
- Share<sub>fuelj</sub> = Share of process fuel j out of all process fuels consumed during the stage ( $\sum_j fuel_j = 1$ , see Section 4 for the shares), and
- Share<sub>techk,j</sub> = Share of combustion technology k out of all combustion technologies for fuel j ( $\sum_k tech_{k,j} = 1$ ).

Combustion technology shares (Share<sub>techk,j</sub>) for a given process fuel are influenced by technology performance, technology costs, and emission regulations for stationary sources. Over time, because of increasingly strict emissions regulations, clean-burning technologies will likely be introduced to replace old combustion technologies. In GREET, default technology shares are assumed for each upstream stage. In most cases, for a given combustion technology, GREET has two sets of emission factors: current and future. Current technology factors are used for those emission control technologies that were in place in the early 1990s when the 1990 Clean Air Act Amendment took effect. Future technology emission factors are used for additional emission control technologies employed to reduce emissions further. These technologies are introduced gradually in GREET over time to replace the current technologies. The default shares are based on use of combustion technologies in different fuel industries now and in the near future. To precisely simulate energy use and emissions over a period of time, users of the GREET model need to assess potential use of clean-burning technologies and change the assumed default technology shares accordingly.

Emission factors (EF<sub>i,j,k</sub>) for VOC, CO, NO<sub>x</sub>, PM<sub>10</sub>, CH<sub>4</sub>, and N<sub>2</sub>O for different combustion technologies fueled by different process fuels are primarily derived from the fifth edition of EPA's AP-42 document (EPA 1995). GREET has a sheet called *EF* that contains emission factors for 41 combinations of combustion technologies and fuels. Appendix A (in Volume 2) of this report presents these emission factors.

In the GREET model, SO<sub>x</sub> emission factors for combustion technologies fueled with all fuels except coal, crude oil, and residual oil are calculated by assuming that all sulfur contained in these process fuels is converted into sulfur dioxide (SO<sub>2</sub>). The following formula is used to calculate the SO<sub>x</sub> emissions of combustion technologies:

$$SO_{x,j} = Density_j \div LHV_j \times 1,000,000 \times S\_ratio_j \times 64 \div 32 , \quad [3.5]$$

where

- SO<sub>x,j</sub> = SO<sub>x</sub> (primarily SO<sub>2</sub>) emission factor for combustion of process fuel j (in g/10<sup>6</sup> Btu of fuel j burned);



- Density<sub>j</sub> = Density of process fuel j (in grams per gallon [g/gal] for liquid fuels, grams per standard cubic foot [g/scf] for gaseous fuels such as NG and gaseous hydrogen, or grams per ton [g/ton] for solid fuels such as coal and biomass);
- LHV<sub>j</sub> = Low heating value of process fuel j (in Btu/gal for liquid fuels, Btu/scf for gaseous fuels, or Btu/ton for solid fuels);
- S\_ratio<sub>j</sub> = Sulfur ratio by weight for process fuel j;
- 64 = Molecular weight of SO<sub>2</sub>; and
- 32 = Molecular weight of elemental sulfur.

As the formula implies, SO<sub>x</sub> emission factors for most fuels are determined by the sulfur content of the fuels and not by combustion technologies. However, uncontrolled SO<sub>x</sub> emission factors associated with combustion of residual oil, crude oil, and coal are very high and exceed emission standards. Desulfurization measures have been in place for combustion technologies fueled with these three fuels to reduce SO<sub>x</sub> emissions to acceptable levels. For these cases, SO<sub>x</sub> emission factors for various combustion technologies are derived from the fifth edition of EPA's AP-42 document (EPA 1995).

There are some exceptions to the method of calculating SO<sub>x</sub> emissions described above. Some chemical conversions of feedstocks to fuels or energy require catalysts; these conversions include production of methanol, DME, hydrogen, and FTD from natural gas in plants and production of hydrogen from gasoline, methanol, ethanol, and natural gas on board a fuel-cell vehicle with fuel processors. Sulfur contained in a feedstock can poison catalysts and must be removed from the feedstock before it enters the fuel production units. Desulfurization of feedstocks usually produces solid wastes that contain immobilized sulfur. In these cases, the sulfur contained in the feedstocks used as feed and fuel becomes solid waste, and is not released as emissions. No SO<sub>x</sub> air emissions are assigned for these cases.

In GREET, combustion CO<sub>2</sub> emission factors in g/10<sup>6</sup> Btu of fuel throughput are calculated by using a carbon balance approach. Through the approach, the carbon contained in a process fuel burned minus the carbon contained in combustion emissions of VOCs, CO, and CH<sub>4</sub> is assumed to convert to CO<sub>2</sub>. The following formula is used to calculate CO<sub>2</sub> emissions:

$$CO_{2,j,k} = \left[ Density_j \div LHV_j \times 1,000,000 \times C\_ratio_j - (VOC_{j,k} \times 0.85 + CO_{j,k} \times 0.43 + CH_{4,j,k} \times 0.75) \right] \times 44 \div 12, \quad [3.6]$$

where

- CO<sub>2,j,k</sub> = Combustion CO<sub>2</sub> emission factor for combustion technology k burning process fuel j (in g/10<sup>6</sup> Btu of fuel j burned);
- Density<sub>j</sub> = Density of process fuel j (in g/gal for liquid fuels, g/scf for gaseous fuels, or g/ton for solid fuels);
- LHV<sub>j</sub> = Low heating value of process fuel j (in Btu/gal for liquid fuels, Btu/scf for gaseous, or Btu/ton for solid fuels);





- $C_{ratio_j}$  = Carbon ratio by weight for process fuel j;  
 $VOC_{j,k}$  = VOC emission factor for combustion technology k burning process fuel j (in  $g/10^6$  Btu of fuel j burned);  
0.85 = Estimated average carbon ratio by weight for VOC combustion emissions;  
 $CO_{j,k}$  = CO emission factor for combustion technology k burning process fuel j (in  $g/10^6$  Btu of fuel j burned);  
0.43 = Carbon ratio by weight for CO;  
 $CH_{4,j,k}$  =  $CH_4$  emission factor for combustion technology k burning process fuel j (in  $g/10^6$  Btu of fuel j burned);  
0.75 = Carbon ratio by weight for  $CH_4$ ;  
44 = Molecular weight of  $CO_2$ ; and  
12 = Molecular weight of elemental carbon.

The above formula shows the calculation method for combustion  $CO_2$  emissions by which carbon contained in VOC, CO, and  $CH_4$  is subtracted. On the other hand, VOCs and CO reside in the atmosphere for less than 10 days before decay into  $CO_2$ . In GREET 1.5, the indirect  $CO_2$  emissions from VOCs and CO decay in the atmosphere are considered.

Calculations involved in Equations 3.5 and 3.6 require fuel specifications such as low heating value, fuel density, weight ratio of carbon, and weight ratio of sulfur. Fuel specifications for various fuels are presented in Table 3.3. A sheet containing the information (called *Fuel\_Specs*) is included in the GREET model.

Throughout this report and in default calculations performed by GREET, low heating values (LHVs) are used for all the fuels involved. Some other studies use high heating values (HHVs). The difference between the LHV and the HHV for a fuel is determined by whether energy contained in the water vapor from fuel combustion is taken into account. For stationary combustion processes, some, but not all, of the energy contained in combustion vapor can be recovered in steam and used. For motor vehicles, energy contained in water vapor cannot be practically recovered. Thus, it is more appropriate to use LHV for vehicle applications. However, because heating values are used primarily as conversion factors to derive final results, either LHV or HHV can be used as long as whichever is chosen to be used consistently throughout a study. Inconsistencies occur when data from different studies that use both LHV and HHV are used. The GREET model is designed so the researcher can choose to use either LHV or HHV.

For noncombustion emissions, GREET takes into account the following emission sources. (Details on calculation of noncombustion emissions are presented in Section 4, as needed.)

- For liquid fuels, VOC evaporative emissions and emissions from fuel spillage during feedstock T&S and fuel T&S&D;
- For petroleum-based fuels, emissions from flaring and venting of associated gas in oil fields and refining-process-related emissions in petroleum refineries;



**Table 3.3 Fuel Specifications**

| <b>Fuel</b>                 | <b>LHV</b> | <b>HHV</b>      | <b>Density</b>  | <b>C ratio<br/>(% by wt)</b> | <b>S ratio<br/>(ppm by wt)</b> |
|-----------------------------|------------|-----------------|-----------------|------------------------------|--------------------------------|
| <b><i>Liquid Fuels</i></b>  | (Btu/gal)  | (Btu/gal)       | (g/gal)         |                              |                                |
| Crude oil                   | 130,000    | 138,100         | 3,200           | 85.0                         | 16,000                         |
| Conventional gasoline       | 115,500    | 125,000         | 2,791           | 85.5                         | 200                            |
| Federal reform. gasoline    | 112,300    | 121,500         | 2,795           | 82.9                         | 30                             |
| Calif. Reform. gasoline     | 113,000    | 122,200         | 2,794           | 83.5                         | 30                             |
| Conventional diesel         | 128,500    | 138,700         | 3,240           | 87.0                         | 250                            |
| Reformulated diesel         | 128,000    | 138,000         | 3,240           | 87.0                         | 050                            |
| Residual oil                | 140,000    | 149,500         | 3,630           | 87.0                         | 5,000                          |
| Methanol                    | 57,000     | 65,000          | 2,996           | 37.5                         | 0                              |
| Ethanol                     | 76,000     | 84,500          | 2,996           | 52.2                         | 0                              |
| Liquefied petroleum gas     | 84,000     | 91,300          | 2,000           | 82.0                         | 0                              |
| Liquefied natural gas       | 72,900     | 80,900          | 1,589           | 74.0                         | 0                              |
| Dimethyl ether              | 68,180     | NA <sup>a</sup> | 2,502           | 52.2                         | 0                              |
| Methyl ester (biodiesel)    | 117,090    | 128,520         | 3,346           | 78.0                         | 0                              |
| Fischer-Tropsch diesel      | 118,800    | 128,500         | 2,915           | 86.0                         | 0                              |
| Liquid hydrogen             | 30,100     | 35,700          | 263             | 0.0                          | 0                              |
| NG liquids                  | 81,460     | 90,500          | NA              | NA                           | NA                             |
| Still gas                   | 128,590    | 142,860         | NA              | NA                           | NA                             |
| <b><i>Gaseous Fuels</i></b> | (Btu/scf)  | (Btu/scf)       | (g/scf)         |                              |                                |
| Natural gas                 | 928        | 1,031           | 20.5            | 74.0                         | 7                              |
| Gaseous hydrogen            | 274        | 324             | 2.4             | 0.0                          | 0                              |
| <b><i>Solid Fuels</i></b>   | (Btu/ton)  | (Btu/ton)       |                 |                              |                                |
| Coal                        | 18,495,000 | 20,550,000      | NN <sup>b</sup> | 60.0                         | 11,100                         |
| Coking coal                 | 20,532,600 | 22,814,000      | NN              | NA                           | 11,800                         |
| Woody biomass               | 17,000,000 | NA              | NN              | NA                           | NA                             |
| Herbaceous biomass          | 15,600,000 | NA              | NN              | NA                           | NA                             |

<sup>a</sup> NA = not available.

<sup>b</sup> NN = not needed.

- For NG-based fuels, CH<sub>4</sub> emissions caused by gas leakage during NG transmission, noncombustion emissions during NG processing, and CO<sub>2</sub> emissions or absorption during production processes from NG to hydrogen, methanol, DME, or FTD;
- For ethanol and biodiesel, NO<sub>x</sub> and N<sub>2</sub>O emissions from nitrification and denitrification of nitrogen fertilizer applied during farming of corn, soybeans, and biomass; and
- For the coal-to-electricity cycle, CH<sub>4</sub> emissions during coal mining and process-related emissions during coal processing.



### 3.3.3 Consideration of Energy Use and Emissions of Upstream Stages for a Fuel Cycle

For a given fuel cycle, vehicle operation is considered a downstream stage; the stages before vehicle operation (production and transportation of feedstock and production and distribution of product fuels) are upstream stages. Upstream energy use and emissions are generated during combustion of process fuels and during production and distribution of the fuel to the consumption site. Energy use and emissions of a given upstream stage are calculated by using the following formula:

$$EM_i = \left( \sum_j (EM_{cm,i,j} + EF_{up,i,j}) \times EC_j \right) \div 1,000,000 \quad [3.7]$$

where

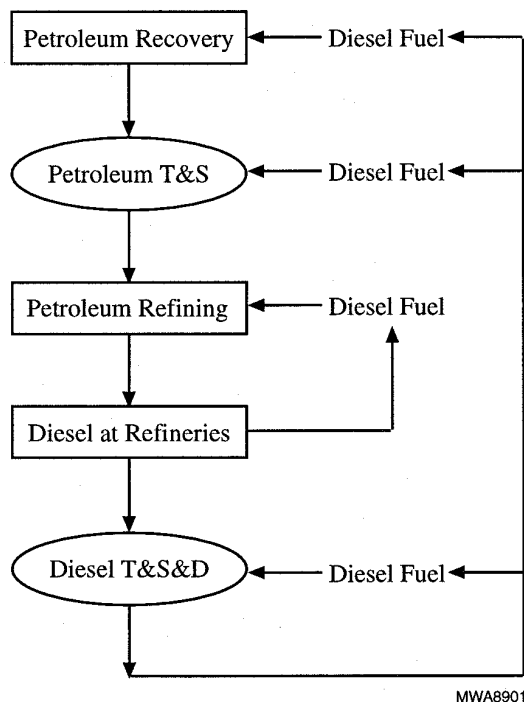
- $EM_i$  = Emissions of pollutant  $i$  in  $g/10^6$  Btu of fuel throughput from a given stage;
- $EM_{cm,i,j}$  = Combustion emissions of pollutant  $i$  in  $g/10^6$  Btu of process fuel  $j$  burned (calculated from Equation 3.3);
- $EF_{up,i,j}$  = Upstream emissions of pollutant  $i$  in  $g/10^6$  Btu of process fuel  $j$  to produce and distribute the process fuel to the stage (considered within GREET through circular calculation programming); and
- $EC_j$  = Energy consumption of fuel  $j$  during the stage (calculated from Equation 3.1 or 3.2).

As Equation 3.7 shows, the introduction of  $EF_{up,i,j}$  to the formula causes circular calculations in GREET 1.5. That is, each upstream stage requires use of process fuels for which production could involve the very stage under evaluation. As Figure 3.2 shows, the circular calculations help fully account for upstream energy use and emissions. The figure uses the petroleum-to-diesel cycle as an example. Petroleum recovery, as one stage of the cycle, requires use of diesel fuel, together with other process fuels (not shown in the figure). Production of diesel fuel requires petroleum recovery together with other stages (petroleum T&S, petroleum refining, and diesel T&S&D to oilfields). As the figure shows, other stages require the use of diesel fuel, and together there are four close-loop calculations involved in fully accounting for energy use and emissions associated with upstream activities for diesel fuel. GREET 1.5 was designed to perform circular calculations by means of the iteration calculation feature in Microsoft Excel. This feature allows GREET to draw data to use in one cell from some other cells (which, in turn, draw data from the first cell) for calculations being performed in the particular cell.

An iterative calculation in Excel requires each cell used in the calculation in the GREET model to have a valid value. An invalid value in a cell (say, characters assigned to a numeric value-required cell) can cause a nonrepairable Excel error throughout GREET. Caution must be taken to make sure each cell used in iterative calculations in Excel has a valid value.



### 3.3.4 Aggregation of Energy Use and Emissions of Individual Upstream Stages for a Fuel Cycle



**Figure 3.2 Closed-Loop Calculations of Upstream Energy Use and Emissions in GREET: Diesel Fuel Use in the Petroleum-to-Diesel Fuel Cycle**

The above sections describe calculation of energy use and emissions per  $10^6$  Btu of fuel throughput for each individual upstream stage. The next step is to aggregate energy use and emissions of all upstream stages for a fuel cycle together so that energy use and emissions per  $10^6$  Btu of fuel delivered at the fuel pump can be calculated. In previous GREET versions, the aggregated value was obtained by adding the energy use and emissions from all upstream stages together. That method ignored the potential fuel loss during all stages that follow the stage that is being evaluated.

If there is no fuel loss during upstream activities, calculated energy use and emissions for each stage (in Btu/ $10^6$  Btu or g/ $10^6$  Btu throughput) can simply be added together to obtain total energy use and emissions per  $10^6$  Btu of fuel delivered at

the final stage (e.g., at the fuel pump) —  $10^6$  Btu of feedstock would result in  $10^6$  Btu of fuel. However, if there is a fuel loss (from spillage, evaporation, or leakage), more than  $10^6$  Btu of a fuel in upstream stages is required to obtain  $10^6$  Btu at the final stage (e.g., at the fuel pump). The energy use and emissions calculated for each upstream stage (per  $10^6$  Btu of fuel throughput from the stage) need to be adjusted to the actual amount of fuel needed (greater than  $10^6$  Btu because of the loss) to deliver  $10^6$  Btu of the fuel in the final stage. The adjusted energy use and emissions for all the upstream stages can then be added together.

Delucchi (1997) graphically and mathematically demonstrated how precisely fuel-cycle energy and emissions should be calculated to account for the effects of fuel loss. On the basis of his equation and GREET's method of handling upstream energy use and emissions, the following equation was developed for GREET to account for fuel loss effects:

$$TEM_{up} = \sum_i EM_i \times K_{i-1} \times K_{i-2} \times \dots \times K_1 \times K_0, \quad [3.8]$$



where

- $TEM_{up}$  = Total upstream emissions for a given fuel cycle (in  $g/10^6$  Btu of fuel at fuel pump);
- $EM_i$  = Emissions from stage  $i$ , calculated in GREET by using Equation 3.7 ( $g/10^6$  Btu of fuel throughput from stage  $i$ );
- $K_i$  = Fuel loss factor for stage  $i$  to take into account fuel loss during stage  $i$ ; and
- $i$  =  $i$ th stage. Stages are numbered with the vehicle operation stage being stage 0. In other words, the vehicle operation stage is considered to be stage 0 and  $K_0$  is always equal to one. The next stage above the vehicle operation stage, fuel distribution to fuel pumps, is considered to be stage 1, and so on).

For a given stage, its fuel loss factor ( $K_i$ ) is calculated by using the following equation:

$$K_i = 1 + (1/efficiency_i - 1) \times Loss\_Share_i \quad [3.9]$$

where

- $efficiency_i$  = Energy efficiency of stage  $i$ , which is calculated as fuel output from the stage divided by total energy input to the stage (including feedstock fuel and process fuels); and
- $Loss\_Share_i$  = The share of fuel loss out of total energy inputs for stage  $i$ .

The fuel loss share of total fuel use for many upstream stages is close to or equal to zero. Thus, the fuel loss factor ( $K_i$ ) is close or equal to one in many cases. However, T&S of liquid fuels via vessels and transmission of gaseous fuels via pipelines are subject to fuel evaporation and/or leaks. In most cases, the amount of fuel evaporated and/or leaked is presented in emissions of VOCs or other compounds. In GREET, evaporative and/or leaked fuels, fuel loss shares, and fuel loss factors are considered together. That is, if transportation of a fuel is subject to a large amount of fuel evaporation or leaks, the transportation stage will have a large fuel loss share, and consequently a large fuel loss factor.

Note that the energy use and emissions calculated up to this point are the result of all upstream activities for delivering 1 million Btu of a fuel at the fuel pump.

### 3.3.5 Energy Use and Emissions of Vehicle Operations

Energy use and emissions of vehicle operations are calculated on a per-mile basis. Energy use (in Btu per mile or Btu/mi) is calculated from vehicle fuel economy. Emissions from ICEVs powered by conventional fuels (i.e., CG, RFG, CD, and RFD) are included in the GREET model for two reasons. First, HDTs fueled with diesel or gasoline are used during upstream stages for transportation and distribution of feedstocks and fuels, and their emissions need to be taken into account in calculating overall emissions during these stages. Second, emissions of benchmark light-duty GVVs and diesel vehicles (DVs) are needed for calculating vehicular emissions for both benchmark vehicles and AFVs.



Emissions of VOCs, CO, and NO<sub>x</sub> for benchmark GVs fueled with CG and benchmark DVs fueled with CD are calculated with EPA's Mobile 5b — the current version of EPA's Mobile model (the next version of the Mobile model, Mobile 6, will probably be released by end of 1999). Use of Mobile 5b is intended to estimate actual on-road emissions of motor vehicles. The Mobile 5b outputs are fed into GREET. PM<sub>10</sub> emissions for benchmark vehicles are calculated by using EPA's Part 5 outside of the GREET model. Emissions of SO<sub>x</sub> for both benchmark vehicles and AFVs are calculated inside the GREET model; for these calculations, we assume that all sulfur contained in each transportation fuel is converted into SO<sub>2</sub>, except for fuel-cell vehicles, for which fuel sulfur is assumed to become solid waste. EPA's Mobile model does not estimate vehicular emissions of CH<sub>4</sub> and N<sub>2</sub>O for any vehicle type. CH<sub>4</sub> emissions for benchmark vehicles can be indirectly estimated with Mobile 5b by estimating emissions of total hydrocarbons (THCs) and total nonmethane hydrocarbons (NMHCs); this approach was used in our study. Emissions of N<sub>2</sub>O for benchmark vehicles are estimated in this study on the basis of existing data presented in Delucchi and Lipman (1996), a recent EPA report (EPA 1998c), and other published sources. Finally, combustion CO<sub>2</sub> emissions for all vehicle types are calculated by using a carbon balance approach (carbon contained in the fuel burned minus carbon contained in exhaust emissions of VOC, CO, and CH<sub>4</sub> is assumed to convert to CO<sub>2</sub>). Because of the short residence time of VOCs and CO in the atmosphere (less than 10 days), the carbon contained in VOCs and CO is converted into CO<sub>2</sub> emissions in GREET.

In GREET, vehicular VOC emissions include exhaust, evaporation, running loss, resting loss, and refueling emissions, all of which are estimated with Mobile 5b. Vehicular PM emissions include exhaust, tire wear, and brake wear emissions, all of which are estimated with PART 5. Emissions of other pollutants are exhaust only.

In the GREET model, vehicular emissions of VOC, CO, NO<sub>x</sub>, PM<sub>10</sub>, CH<sub>4</sub>, and N<sub>2</sub>O from spark-ignition vehicles fueled with alternative fuel (SI-AFVs) are calculated by applying SI-AFV emission reduction rates to benchmark GV emissions. Emission reduction rates of SI-AFVs relative to those of benchmark GVs are estimated by using testing data for AFV emissions from different studies. (See Section 4 for assessment of AFV emissions reduction rates.)

Vehicular emissions of VOC, CO, NO<sub>x</sub>, PM<sub>10</sub>, CH<sub>4</sub>, and N<sub>2</sub>O from compression-ignition vehicles fueled with alternative fuels such as DME, FTD, and biodiesel (CI-AFVs) are calculated by applying CI-AFV emission reduction rates to those of benchmark DVs.

Energy consumption (in Btu/mi) is calculated by using the fuel economies of benchmark vehicles and AFVs. Benchmark GV fuel economies used in GREET are from the GV fuel economies predicted by DOE's EIA. The fuel economy for benchmark DVs is calculated by applying a fuel economy improvement rate — usually, conventional CI DVs can achieve a 10% improvement in gasoline-equivalent fuel economy over GVs, and CIDI DVs can improve fuel economy by 35%. The fuel economy of SI-AFVs is estimated by applying SI-AFV fuel economy changes (relative to SI GV fuel economy) to SI GV fuel economy. For CI-AFVs, the fuel economy is estimated by applying CI-AFV fuel economy changes (relative to CI DV fuel economy) to CI DV fuel economy. Fuel economy changes by DVs and AFVs are presented in



Section 4. Fuel economies calculated for each vehicle type in GREET are gasoline-equivalent fuel economies.

### **3.3.6 Total Fuel-Cycle Energy Use and Emissions for a Combination of Fuel and Vehicle Type**

Section 3.3.4 presents calculations of upstream energy use and emissions in Btu and  $g/10^6$  Btu of fuel delivered at the fuel pump. Section 3.3.5 presents calculations of energy use and emissions in Btu and  $g/mi$  traveled by each vehicle type. (Note that energy use by vehicles is calculated for total energy, fossil energy, and petroleum.) Now, energy use and emissions of upstream stages and downstream vehicle operations can be combined by converting upstream energy use and emissions from the per- $10^6$  Btu basis to the per-mile basis. The conversion is accomplished by dividing upstream energy use and emissions by vehicular per-mile energy use, which is calculated from vehicle fuel economy. Note that in the GREET model, the total energy use (not fossil energy use or petroleum use) by vehicles is used to convert the per- $10^6$  Btu upstream results into per-mile results in order to avoid potential under-accounting of energy use by vehicles fueled with nonfossil or nonpetroleum fuels.

GREET's fuel-cycle results are presented on a per-mile basis. That is, the model estimates total fuel-cycle energy use and emissions for each mile traveled according to vehicle type fueled with a given fuel. In this regard, GREET is similar to Mobile — both GREET and Mobile estimate per-mile rates, rather than total energy use and emissions of a fleet of vehicles in a given year. To estimate the total emissions or energy use (often called emission and energy inventory), GREET per-mile results can be input into some vehicle stock and usage models.

Because per-mile upstream energy use and emissions are the per-million Btu energy use and emission result divided by Btu-per-mile fuel use (which is directly determined by vehicle fuel economy), vehicle fuel economy is one of the most significant factors in determining total fuel-cycle energy use and emissions.

### **3.3.7 Total and Urban Emissions for Five Criteria Pollutants**

For the five criteria pollutants (VOC, CO,  $NO_x$ ,  $PM_{10}$ , and  $SO_x$ ) included in the GREET model, both the location and the amount of emissions are important, because these pollutants usually pose localized air pollution problems. ( $SO_x$  causes acid rain and poses other regional air pollution problems.) To account for the importance of emission locations, GREET is designed to estimate total emissions and urban emissions for the five criteria pollutants.

The term “total emissions” refers to total fuel-cycle emissions occurring everywhere, at every stage of a fuel cycle (calculated as described in the above sections). “Urban emissions” occur only within the boundaries of a given metropolitan area. GREET calculates urban emissions on the basis of these boundaries. The boundaries of an air control district can be used as the boundaries of an urban area in order to use the results from GREET to analyze air quality implications in an area. Readers should keep in mind that GREET estimates total and urban emission *rates*, not total and urban emission *inventory*. The estimated urban emission rates and estimated urban activity level from some other transportation activity models are needed in order



to estimate the urban emission inventory that will occur with introduction of a transportation fuel or technology. Estimation of emission inventory is beyond the scope and capability of GREET. Ideally, urban emissions can be further disaggregated into grids of an urban area, and grid-specific emissions can be then used in air quality models to simulate air quality impacts of emissions that result from introducing an AFV. Separation of emission rates into total and urban rates in GREET is a simple, first step to provide some general idea of the differences in population exposure of emissions generated from a given fuel cycle.

Emissions from vehicle operations can occur within or outside of urban areas, depending on where vehicles are introduced and where they travel. In GREET, to calculate emission rates, we assumed vehicle miles traveled (VMT) by an AFV type occur in urban areas. That is, we assumed that AFVs are to be introduced to urban areas to make urban VMT. So, all emissions from vehicle operations are treated as urban emissions. In estimating urban emission inventory from mass introduction of a transportation fuel or vehicle technology, researchers must make assumptions regarding splits of urban VMT and rural VMT and consider only the urban VMT using the fuel or the technology. Wang et al. (1998) provides an example for calculating urban emission inventory with GREET-estimated urban emission rates.

Urban emissions of a given upstream stage are determined by facility locations, which are determined by feedstock availability, cost of transporting feedstock, and stationary emission regulations in urban areas. Because feedstocks (petroleum, NG, biomass, etc.) are usually located outside urban areas and because the cost of transporting them is usually much higher than that of transporting fuel (on the basis of the same amount of Btu delivered in the final fuel), upstream stages (except fuel distribution) are often located outside urban areas. Nonetheless, the split of upstream facilities located inside and outside the metropolitan area is fuel-, stage-, and region-specific. In GREET, a default split between urban and nonurban areas is provided for each upstream stage. The default splits were estimates for the United States as a whole. To use GREET to estimate emission rates for a specific area, data regarding the split of facility locations for that area must be collected. For example, to estimate urban emissions of gasoline production from petroleum refineries in Chicago, researchers must know how much gasoline that is consumed in the Chicago area is produced within and outside the Chicago area. Gasoline production within the Chicago area can be estimated on the basis of the capacity of the petroleum refineries located within the Chicago area minus the amount of gasoline shipped out of Chicago by petroleum refineries (net production in Chicago). The amount of gasoline produced outside the Chicago area (for Chicago consumption) can be estimated as the difference between the total gasoline demand and the net gasoline production in the Chicago area.

Direct use of emission rates estimated with GREET for air quality simulations may not be appropriate because emissions occur in different locations (as discussed above) and at different times. For a given quantity of fuel, production (upstream activities) occurs far ahead of consumption (vehicle operations). To accurately simulate air quality impacts, emissions that occurred at different times need to be differentiated; the exception is if a fuel has already achieved equilibrium in terms of production and consumption (i.e., the level of production and consumption stay relatively constant over time), which is not common for new fuels.





### 3.3.8 Summary: Results of Fuel-Cycle Energy Use and Emissions Calculated with GREET

GREET estimates fuel-cycle energy use and emission *rates* in Btu/mi and g/mi by various combinations of fuels and vehicle technologies. To provide clear information on the contribution of each upstream stage to total fuel-cycle energy use and emissions, GREET presents fuel-cycle energy use and emissions in three subcategories: feedstock, fuel, and vehicle operations (see Figure 3.1). The feedstock subcategory includes energy use and emissions associated with recovering, transporting, and storing energy feedstocks; the fuel subcategory includes energy use and emissions associated with producing, transporting, storing, and distributing product fuels; and the vehicle operation subcategory includes energy use and emissions directly related to vehicle operations. GREET presents per-mile energy use and emissions for each subcategory and the share of each subcategory to total fuel-cycle energy use and emissions. By using the estimated per-mile energy use and emissions, GREET then calculates percentage changes in energy use and emissions by alternative transportation fuels and or vehicle technologies relative to baseline GVs fueled with either CG or RFG.

As stated previously, GREET estimates energy use for total energy, fossil energy, and petroleum; total emissions and urban emissions of VOC, CO, NO<sub>x</sub>, PM<sub>10</sub>, and SO<sub>x</sub>; and total emissions of CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O. In the default design of GREET, GHG emissions include CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O. However, GREET is designed for users to include VOC, CO, and NO<sub>x</sub> as GHGs (see the table at the bottom of the *Fuel\_Specs* sheet). If a GREET user considers VOC, CO, and NO<sub>x</sub> as GHGs, the global warming potentials of the three can be provided to GREET, and GREET can automatically use these values to consider the three criteria pollutants as GHGs in GHG emissions calculations.

Besides providing a separate emissions estimate for each of the three GHGs now included in GREET (CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O), GREET combines these three GHGs with their GWPs to estimate CO<sub>2</sub>-equivalent GHG emissions.

GWPs are ratios of potential warming effects of other gases relative to CO<sub>2</sub>. As the Intergovernment Panel on Climate Change (IPCC) acknowledged (IPCC 1996), the GWP is an attempt to provide a simple measure of the relative radioactive effects of various GHG emissions. The index is defined as the cumulative radioactive force between the present and some chosen time horizon caused by a unit mass of gas emitted now, expressed relative to that for CO<sub>2</sub>. Table 3.4 presents GWPs for three GHGs included in GREET.

**Table 3.4 Global Warming Potentials of Greenhouse Gases<sup>a</sup>**

| Gas              | Time Horizon |           |           |
|------------------|--------------|-----------|-----------|
|                  | 20 years     | 100 years | 500 years |
| CO <sub>2</sub>  | 1            | 1         | 1         |
| CH <sub>4</sub>  | 56           | 21        | 6.5       |
| N <sub>2</sub> O | 280          | 310       | 170       |

<sup>a</sup> Source: IPCC (1996).



Other major GHGs include halocarbons and halogenated compounds, aerosols (which, unlike other GHGs, have a cooling effect), and ozone. IPCC did not attempt to estimate GWP for aerosols. It maintained that the calculation of GWPs for VOC, CO, and NO<sub>x</sub> (via the ozone warming effect) is not currently possible because the characterizations of many of the atmospheric processes involved are inadequate. There are large uncertainties in the GWPs already estimated for certain GHGs and a lack of understanding of the mechanism and effects associated with the gases for which GWPs have not been estimated. Some have argued that indirect effects of gases in the atmosphere and in other media should be taken into account in estimating GWPs (Delucchi 1997). Some economists have argued that economic damage indices, instead of GWPs, should be estimated and used for aggregating different GHGs (see Delucchi and Lipman 1996).

In 1997, major industrial countries signed the Kyoto Agreement to set GHG emission reduction goals for individual countries. The Kyoto Agreement adopted the IPCC-recommended GWPs for the 100-year time horizon for each country to use in calculating its baseline GHG emissions and projecting emission reductions. The Agreement included the three major GHGs. To evaluate various climate change mitigation policy options promoted by various governments, it is reasonable to use IPCC-estimated GWPs. So, default GWP values in GREET are those estimated by the IPCC under the 100-year time horizon. No GWP values are assigned to other gases, but GREET allows the user to change GWPs readily.

GHGs such as halocarbons and halogenated compounds are not included in GREET. Although these gases have very high GWPs, their overall contribution to GWP-weighted GHG emissions is small, because use of AFVs and advanced vehicle technologies will probably have little, if any, effect on motor vehicle emissions of these gases. Exclusion of these gases has little effect on changes in GHG emissions of AFVs and advanced vehicle technologies relative to baseline GVs.