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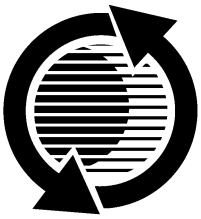

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ABSTRACT

A principal motivation for introducing alternative fuels is to reduce air pollution and greenhouse gas emissions. A comprehensive evaluation of the reductions must include all Life Cycle activities from the vehicle operation to the feedstock extraction. This paper focuses on the fuel upstream activities only. We compare the results and methods of the three most comprehensive existing fuel upstream models in the U.S.A. and we explore the differences and uncertainties of these types of analyses. To explicitly include the impact of uncertainties, we create a new model using the following approaches:

- Instead of using a single value as input, the new model deals with ranges around the most probable value.
- Ranges are discussed and calibrated by an expert network, in terms of their relative probability.
- Probabilistic function techniques are applied to study the impact of the uncertainties on the model output.

The paper also presents the rationale and benefits of using each of the alternative approaches that are discussed and reviewed.

INTRODUCTION AND BACKGROUND

The most realistic and sophisticated way to evaluate the environmental impact of a new technology is to assess the emissions related to all processes in the production chain. This so-called life cycle or full cycle analysis for a new vehicle technology must address the fuel upstream emissions (from the primary resources extraction to the refueling process) together with the vehicle related emissions (Ayres, 1995 and Lee et al, 1995). For each stage in the life cycle (vehicle operation, fuel distribution, fuel production, feedstock transportation and storage, and feedstock extraction and processing) the idea is to assess the water, soil and air emissions for different phases of the project. These phases are Pre-operations (R&D, Site Development and Construction), Operations and Post-operations (Recycling, Decommissioning and Dismantling). For reliable results it is necessary to obtain data from different processes, which necessitates an ongoing data library development. The most detailed life cycle analyses of alternative fuels to date deal with air emissions only and that is also the focus of this paper.

Transportation-related air emissions can be associated with urban air quality in terms of ozone formation, criteria pollutants (non-methane organic gases-NMOG, CO, NOx, SOx and particulate matter-PM) and toxic pollutants (benzene, lead, etc.). Also, it can be associated with global warming and greenhouse gas emissions (CO2, CH4, N2O, CO, CFCs, etc.). The amended ZEV rule (Zero Emission Vehicles), approved by the California Air Resource Board (CARB) in November 1998, highlighted the importance of fuel upstream emissions calculations when it established partial credits for vehicles with low tailpipe emissions that use a cleaner fuel process than gasoline. Several models calculate some of these pollutant emissions for different fuels and different purposes. The most comprehensive models are:

- DeLucchi (1991, 1993 and 1997): Calculated in a spreadsheet (Lotus123), this model focuses on standard greenhouse gas emissions (CO2, CH4, and N2O) and also includes some criteria pollutants (CO, NO2, and NMOG). The criteria pollutants, including SOx and PM10, are calculated with a global perspective, i.e., without separating them into urban area emissions. All calculations are performed based on US national average numbers.
- Greet (1996 and 1999): Calculated in a spreadsheet (Microsoft Excel), this model independently focuses on standard greenhouse gas (CO2, CH4, N2O) and criteria pollutant emissions (NMOG, CO, NOx, PM10 and SOx). It creates a “virtual” urban area for criteria pollutant analysis and uses US national average numbers by default.
- Acurex (1996) (now ARCADIS, Geraghty & Miller): Done in a relational data base environment (Microsoft Access), this model focuses on the photochemical reactivity of NMOG for California's

South Coast Air Basin but also assesses other emissions such as NOx, CO, CO2 and CH4. Local inventory provides the input data.

- Other more specific models are: Darrow (1994) with a US and California case for the year 2000; DTI (1998) for decentralized hydrogen production; and Ogden et al. (1998) with a focus on costs.

These models all calculate the air emissions related only to the operation phase of the life cycle analysis. An exception is DeLucchi's model that includes some air emissions related to the steel and concrete used in the production plants and vehicle assembly. In spite of the large number of studies conducted on the operation phase of the life cycle analysis, it is still difficult to do an analysis for a specific region within the US. The main reason is that national average numbers do not fully describe regional specificity, making it impossible to extrapolate emissions numbers from national to local levels. However, a model that accommodates local analyses can be used to aggregate many local analyses for regional and perhaps national values. Also, a database library including regional details (e.g., California's Central Valley oil, Texas oil, etc.) can be very useful in propagating life cycle analysis use.

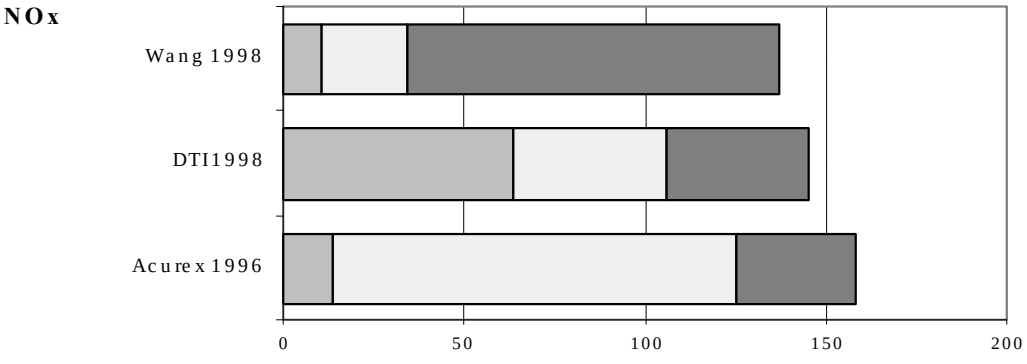
Another important consideration is the availability of these models to other users for comparison purposes. Most of them have summary reports publicly available, which provide some of their input data and also their final results (for specific pathways). However, it is dangerous to use these numbers for a different purpose without being able to check for specific geographical variation and confirmation of the calculation consistency. Without access to the model itself, the basic scientific principle of reproductibility is compromised. An important step in this direction was made by Michael Wang who has made his updated model (Greet 1.5) available on the Internet (since October, 1999) by downloading:

www.transportation.anl.gov/ttrdc/greet

The lack of access to the models explains, in part, the lack of useful and direct comparison among them. Andress (1998) did a qualitative comparison between Greet and DeLucchi's Model for the ethanol fuel cycle, in which some general similarities and differences are addressed. No quantitative comparison was done in Andress' study and the results can be summarized in terms of how they calculate greenhouse gases emissions and make parametric assumptions (determined inside or outside of the models).

Mark (1998) did a comparison among the upstream emission results of three models (Greet, Acurex and DTI) for compressed hydrogen fuel produced in a centralized steam reformation process from natural gas. Figure-1 shows one example of his findings. It is clear from this figure that there is a strong need for better comparative evaluation studies -- since no agreement was found among the models for either the total emissions or their detailed origins.

These variations can be extrapolated to other fuels and other models. Table-1 shows the variation for the local fuel upstream emissions of the existing models for three different fuels. Table-2 shows the same idea for the Vehicle Life Cycle Emissions of CO2. This paper explains some of the reasons for the variations observed in these tables, a primary cause being that these models do not deal with uncertainties at the input data assumption level. Therefore, the sum of the many uncertainties from among all of the different possible input assumptions results in huge differences in the final results. Also included in this paper is a description of a new model which has been developed to better handle these unavoidable uncertainties explicitly, and to accommodate detailed air emissions and energy requirement analysis at the local and regional level.



	Acurex1996	DTI1998	Wang 1998
distribution & compression	33.3	39.3	102.8
production	111.4	42.1	23.8
extraction	13.6	63.6	10.7

g/mmBtu (CH2 delivered - LHV)

Figure 1. Upstream emissions for compressed hydrogen fuel of existing models (source: Mark, 1998).

Table 1. Local fuel upstream emissions.

Local Upstream Emissions (g/gal-eq, HHV)		Gasoline Petroleum	Methanol NG-SR	Hydrogen NG-SR
NOx	DTI (decentral.)	-	-	0.001
	DTI (centraliz)[a]	0	0	4.634
	Acurex	0.324	0.154	0.631 [b]
	Greet 1.5[c]	0.288	0.062	2.664
NMOG	DTI (decentral.)	-	-	0.004
	DTI (centraliz)[a]	10.99	1.176	0.025
	Acurex	1.520	0.573	0.109 [b]
	Greet 1.5	0.528	0.062	0.216
CO	DTI (decentral.)	-	-	0.003
	DTI (centraliz)[a]	0	0.174	0.576
	Acurex	0.143	0.140	0.096 [b]
	Greet 1.5	0.192	0.062	1.008
PM_{10}	Greet 1.5	0	0	0.072
SO_x	Greet 1.5	0	0	0

a: Centralized Plant inside of the basin. Probable cases.
b: LH_2 considered in the Marketing Stage.
c: Based on fuel delivered for Fuel Cell Vehicles (FCV).

Table 2. Vehicle Life Cycle Emissions of CO2.

CO2 Emissions (g/gal-eq, HHV)	Gasoline (RFG)			Methanol (NG-SR)			Hydrogen (NG-SR-CH2)		
	Fuel	Vehic.[a]	Total	Fuel	Vehic.[a]	Total	Fuel	Vehic	Total
Acurex	1,349	8,421	9,770	1,150	7,969	9,119	11,044[b]	0	11,044
Greet 1.5	2,965	8,431	11,396	1,970	7,969	9,939	10,688	0	10,688
DeLucchi (1997)	2,397	8,563	10,960	2,699	8,500	11,199	10,667[c]	0	10,667

a: Calculated from the model assumed Carbon Content in the fuel.
b: LH2 considered in the Market Stage.
c: Since DeLucchi (1997) do not includes production of H2 using NG steam reformation process the Mark (1996) SR data were used to make a composite result.

BASIC METHODOLOGY

What the existing models did very well was to establish the basic methodology for calculating the emissions and energy requirement based on the assumed single-value input data. Basically, for each fuel that is analyzed one can define two different aggregations: the fuel pathway, defining the process involved in specific upstream-connected activities; and the system definition. For example, in the first aggregation, one pathway example is hydrogen fuel delivered as compressed gas at the fuel station, distributed by pipelines from a bulk storage and produced from natural gas (NG) in a centralized steam reformation plant inside of the analyzed area. A similar specific pathway is extended for the NG (feedstock) back to the extraction process.

The second aggregation is related to the system definition. For example, considering only compressed hydrogen fuel for vehicles, some systems may delivery fuel at a pressure of 4000 psi and others at 6000 psi. Each new alternative considered will define a new pathway in a tree configuration. A single change in the system aggregation or in the pathway aggregation will change the final result. Part of the differences in the results of the existing models is related to the difficulty in matching the exact level of aggregation between any two models. The Greet model has some flexibility and permits the analyst to change the system aggregation.

For each process in the pathway the first step is to calculate the total energy consumed by that process by establishing the process efficiency in terms of energy

delivered per energy consumed. These efficiency numbers are in general measured for existing processes since they are important parameters for cost analyses. The next step is to split this total energy consumed by the different fuels involved in the process and then establish an equipment breakdown for each fuel. At the end of this calculation the model calculates the energy consumed per equipment type. Variations of this calculation can be done with some activities like farming where physical units are used (ex: bushels of corn per gallon of ethanol).

An emission factor in terms of grams of pollutant per energy consumed is assumed for each equipment type. The emissions generated by each equipment type are summed to define the process emissions. It is important to include the fuel that participates in a conversion process itself, for example the NG that is transformed into hydrogen in the steam reformation process. The Greet model originally did not consider this point for all NG-related fuels but that has been corrected at the time of this printing (See comments on Table-3).

The total process emissions are calculated by adding the fugitive emissions associated with the process. Fugitive emissions are related to maintenance, equipment malfunctions, spills, leaks, losses at junctions, purges, etc. and they are very hard to establish since they have a sporadic and not localized occurrence. In general, a percentage of the energy consumed by the process is considered lost and therefore added to the energy requirement. The emissions are related with the lost fuel composition: for example, a NG loss will result in CH4, NMOG and perhaps SOx and CO2 emissions. Evaporative emissions from tanks can be calculated based on the vapor pressure of the fuel and based on the tank configuration. Fugitive emission is a very sensitive variable in the hydrocarbon emission calculations.

Having the basic results for each upstream process activity some details should be discussed for the final results:

1. Life cycle circular calculation: The energy requirement and emissions associated with the life cycle of each secondary fuel used in the main pathway calculation must be accounted. Because some processes use a secondary fuel that will be generated using the primary fuel a circular calculation is necessary until the result converges to stability. For example, electricity is used in the NG production and NG can generate electricity so the values used in the first calculation will change in each cycle. Greet and DeLucchi's model uses the circular calculation. Future models should recognize the importance of using this approach.
2. Co-products credits: Since a single process can generate more than one product (with market value) the energy requirement and the emissions generated by the process should be divided among the co-products. Different approaches can be used to split the results such as the energy content, mass, market value or market displacement. For fuel co-products like natural gas liquids (NGL) Greet and DeLucchi's model uses the energy approach. For other kinds of co-products, like food in ethanol production from corn, DeLucchi's uses the co-product displacement approach and Greet gives the option to switch between the displacement approach and a mix of market value and energy approach. Apparently Acurex take no internal co-product credits into account. Wang et al (1997) did a sensitivity analysis to test the importance of using this approach for ethanol calculation. According to this analysis the most significant factor is the co-product credit allocation. Using different co-product credit approaches the authors got results with differences up to 65%.
3. Distance dependence of transportation process: The Greet model uses the same efficiency approach explained above to calculate the energy consumption of transportation processes. It is possible that external calculations were done using national average distances but no references of the calculation procedure or distance used can be found in the model. This is the biggest obstacle in using the Greet model at the local level. Acurex uses a factor in terms of energy per volume transported per mile, and DeLucchi's calculation is in terms of energy per mass per mile.

The differences among the methodology approaches also can be responsible for part of the differences in the results; however, it turns out that the main reason is related with the uncertainties in the data inputs. This is discussed in the next section.

DATA INPUT UNCERTAINTIES

In trying to deal with uncertainties, the existing models present different scenarios that are primarily variations of the system and/or pathway aggregations. However, the possible variation among the input data at the equipment level can be much more critical. In spite of its importance, the variation among the input data is not considered in any existing models. Acurex is the only model that devotes some space to this kind of uncertainty. Their report shows a huge variability of the individual NMOG emissions for the reformulated gasoline case, though the data related to the calculation are unclear.

Table-3 and Table-4 show that there exists an enormous potential for uncertainties at the process level and that some improvement should be made in modeling this factor. The main causes are the normal variation in responses of all systems, aggravated by the fact that, for new technology, these variables are projections into the unknowable future (2010). Also, the tables further explain the differences in the results found by Mark (1998) in the hydrogen case. Closer analyses of other fuels (reformulated gasoline and methanol) results in the same conclusion.

SOLVING THE PROBLEMS

Using Matlab/Simulink software a Fuel Upstream Energy and Emissions Model (FUEEM) has been developed as a complement to the larger fuel cell vehicle model being developed concurrently within the UC Davis Fuel Cell Vehicle Modeling Program (see http://fcv.ucdavis.edu for information about the program). FUEEM incorporates the useful aspects already developed by other models -- such as the basic calculation techniques and the result output format. A graphical user interface is used to allow scenario configurations and geographical analysis flexibility. As a result one is able to generate information about criteria pollutants (NOx, NMOG, CO, SOx, PM10 and PM2.5) and greenhouse gases (CO2, CH4, N2O and total GHG). With the exception of CO2 and total greenhouse gases, which can only be assessed in the total emission form, all the other pollutants can be assessed by geographical occurrence (in the specific area of analysis, or any other urban areas for which input data is available). The total energy requirement can be also summarized in terms of petroleum and/or the fossil fuel requirements.

To explicitly recognize the uncertainties involved in technology forecasting, specific steps have been implemented. The first and most important one is to take special care in generating the input data, since this data defines, and can limit, the quality of the result. To ensure accurate input data, a network of experts was established involving different organizations (US national laboratories, US government agencies, US and

Table 3. Variations on input data used for several studies on the energy requirement calculation for hydrogen production.

HYDROGEN PRODUCTION [a]	GREET [b]	Acurex [c]	Ogden [d]	DTI [e]	Air Products [f]
Efficiency (%)	68	61.1	90	69	75 / 77.6
Energy Share (%)					
Natural Gas	99.8	100	100	97.1	99.5 / 99
Electricity	0.2	-	-	2.9	0.5 / 1.0
Breakdown on NG					
Reformer-Feed Process	-	47.2	82.4	83	90
Reformer-Combustion	100	52.8	17.6	17	10

a: Centralized Steam Reforming Process.
b: From Greet 1.4, only the combustion process is taken into account. It is preserved in this table the values used in the Delphi Process with the FUEEM expert network. In fact, an updated version (Greet 1.5) was released in October 1999 and it uses 73% as the efficiency number for a process without steam exportation and 85% for a process considering steam exportation. For the reformer combustion it assumes 17%.
c: From Table 5-34, calculated using 100,000 Btu NG/lb H2 for feedstock, 52,830 Btu NG/lb H2 for combustion and 61,100 Btu/lb H2 (HHV). For fuel processing it gives the efficiency of 61.1 % that means 61,100 / 100,000. For the boiler (combustion) breakdown 52,830 / 100,000 = 52.8 %. In fact, these numbers do not appear on the report. It appears that the emissions were calculated externally to the model.
d: Ogden et al (1995). The variables were calculated from the Table 6A-5 using 135 Btu-HHV per gram of H2 and 50.29 Btu-HHV per gram of NG.
e: From Table D-1 – Direct Technology Inc. (1998).f: Patel, Nitin (1999). Personal communication and Shahani et al (1998). Calculated from the economics number – 1.18 US$ of NG/Mscf-H2 @ 2.75 US$/MMBtu-NG and 0.03 US$ of Elect./ Mscf-H2 @ 0.045 US$ / kWh-el.

Table 4. Emission factors assumed by existing models to calculate the impact of hydrogen production plants.

EMISSION FACTOR (g/MBtu-NG burned)	Acurex [a]	Mark et al [b]	Greet [c]
	Steam Reformer	**Steam Reformer**	**Industrial Boilers**
NO_x	45.44	31.75	23.339
CO	15.90	15.42	17.614
CH_4	1.33	-	0.128
NMOG	1.33	1.22	0.617

a: From EFAC9.XLS (Acurex, 1996). The numbers were calculated using H2 density of 0.53 lb/100scf and energy content of 32,400 Btu/100scf (HHV). Process efficiency of 61.1 % and 52.8 % of energy share of NG combusted are used on the calculation also. The numbers in the report (grams of pollutant per lb of H2) are: NOx (2.4 g); CO (0.84 g); CH4 (0.07 g) and NMOG (0.07 g).
b: Mark et al (1994) use the following emission factors in terms of grams per MBtu of fuel burned to heat the reformer (mixed with waste gas).
c: From Greet 1.4. The emission factors are related to future devices and they are converted to HHV using the factor of 90%. The Greet 1.5 model is still using the emissions established for industrial boilers and the new values are 35.19 (NOx), 36.99 (CO), 0.99 (CH4) and 2.43 (NMOG).

European universities, NGOs, and oil, methanol and hydrogen industry companies). Based on Porter, et al. (1991), Jones, et al. (1978), and Vose (1996), several techniques have been implemented to generate a consensus on the major input data. The specific techniques employed are Delphi Technique Variants, Nominal Group Process and Committee discussions.

The second step is to set up the model recognizing the uncertainties discussed by the experts. Unlike the existing models – that use single-value scalars as input (and therefore obtain single-value scalars as output) -- the Alpha version of FUEEM uses multi-valued vector representations to bound the probable ranges for input parameters. However, because the output of this approach used in the Alpha version of FUEEM does not explicitly carry the probabilistic importance of the input value within the range, a probabilistic function approach has been introduced in the Beta version of FUEEM. In the Beta version, the possibility of occurrence of each value within the range is established by the expert network, and special numerical routines do the calculation of the output results (assuming the variables are statiscally independent). The results from the Beta version of FUEEM are a pair of vectors (representing the output range and the relative probability of values within the range). These results can then be represented in terms of histograms or “box-plot” of the quartiles and mean. This output is very rich in terms of the information related to the uncertainty of each computed result.

CONCLUSION

The differences in results among the existing models that calculate Life Cycle emissions and energy requirements of fuel for transportation can be interpreted as differences in the fuel pathways and system aggregations used in these models. It can also be related to the fact that none of those models recognize the uncertainties involved in using single-valued inputs for this kind of forecasting.

The Fuel Upstream Energy and Emissions Model (FUEEM) has been developed to explicitly recognize the uncertainties inherent in attempting to forecast future technology attributes and system designs, as well as the inherent uncertainty and unreliability of the input data. FUEEM uses probabilistic functions and relies on an international expert advisory panel to generate a consensus on the critical input parameters, the appropriate range of uncertainty, and to oversee the FUEEM model design. The model tries to avoid the misrepresentation of the accuracy of the results, by introducing probabilistic interpretations to explicitly represent the uncertainties in the results. Also, being an available and flexible tool for different geographical areas, FUEEM will help to spread the application of the Life Cycle Analysis concept.

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