LIFE CYCLE-BASED AIR QUALITY MODELLING FOR TECHNOLOGY ASSESSMENT AND POLICY APPLICATIONS: THE CONCEPT AND TECHNICAL CONSIDERATIONS

Weimin Jiang*, Steven C. Smyth, Qiangliang Li
National Research Council of Canada, Institute for Chemical Process and Environmental Technology
Ottawa, Ontario, Canada

1. INTRODUCTION

New technologies are being developed to satisfy the material needs of human beings. From a government policy perspective, there is a compulsory need to understand the potential environmental impact of the new and emerging technologies, with air quality impact being one of the most important issues to be addressed.

Up to now, air quality impact associated with new and emerging technologies has been mostly modelled and analysed by two different approaches. A life cycle assessment (LCA) exercise analyses the issue from a whole technology life cycle perspective on a functional unit basis. A typical 3-dimensional (3-D) air quality modelling (AQM) study uses a 3-D air quality model to describe and predict the changes in atmospheric pollutant levels caused by emission changes in certain stage(s) of a technology life cycle, such as exhaust emissions from alternative fuel vehicles.

Although the two approaches have been used for various technology assessment and policy applications, some issues associated with the approaches need to be addressed. To strengthen the scientific basis for technology and policy development, an improved and integrated approach of conducting air quality modelling based on life cycle thinking needs to be developed and implemented. In this paper, we will briefly review the LCA and AQM approaches currently in use. Building on the strengths of the two approaches, we will discuss a new concept of life cycle-based air quality modelling, and some technical considerations and challenges in implementing the concept. SunDiesel, an emerging biofuel made from lignocellulosic materials in biomass, will be used as an example to help explain the concept and some technical considerations.

2. TWO CURRENT APPROACHES IN ANALYSING AIR QUALITY IMPACT OF NEW AND EMERGING TECHNOLOGIES

2.1 Life cycle assessment

LCA is defined by the ISO 14040 standard as "the compilation and evaluation of the inputs, outputs, and potential environmental impacts of a product system throughout its life cycle" (ISO 14040, 1997). In addition to ISO 14040, there is a series of ISO standards related to LCA, which includes ISO 14042, a standard on life cycle impact assessment (ISO14042, 2000).

ISO 14042 defines the concepts of environmental "impact category", "category indicator", and "characterization factor" and lists various requirements and recommendations for these quantities. However, it does not standardize these quantities. In practice, widely used LCA tools, such as GaBi (IKP and PE Europe, 2003) and SimaPro (Goedkoop and Oele, 2004), always contain one or more sets of such quantities for environmental impact characterization. For example, GaBi uses "photochemical ozone creation potential (POCP)" as the characterization factor for the category indicator "tropospheric ozone formation", which is an indicator for the impact category "photo-oxidant formation".

A LCA study contains four phases: 1. Goal and scope definition; 2. Inventory analysis; 3. Impact assessment; 4. Interpretation of results. Definition of system boundary is part of the goal and scope definition phase, and it specifies life cycle stages, from cradle to grave, that need to be considered on a functional unit basis. To analyse the impact of a new biofuel on tropospheric ozone formation, a system boundary can be defined to cover all life cycle stages from biomass feedstock production to final combustion of the fuel on a vehicle km-travelled (VKT) basis. For all the life cycle stages, air emissions corresponding to 1 VKT are assembled, calculated, and allocated in the inventory analysis phase. In the impact assessment phase, the emission of each chemical species is converted to its contribution to an air quality indicator (e.g., " tropospheric ozone

---

**Corresponding author:* Weimin Jiang, National Research Council Canada, Room 233, M2, 1200 Montreal Road, Ottawa, Ontario, Canada K1A 0R6; e-mail: Weimin.Jiang@nrc-cnrc.gc.ca

formation ") by multiplying with a characterization factor (e.g., POCP in the unit of "ethene-equivalent") given in a table. The contributions from all the emitted species are then added together to get a single value for the indicator for each life cycle stage and/or for the whole life cycle. These indicator values are compared with corresponding numbers obtained for a base fuel, such as a petroleum diesel, to show the potential impact of the new biofuel on photo-oxidant formation in the atmosphere.

More details about the LCA approach, including life cycle impact assessment related to air quality, are available in Guinee, 2002.

2.2 3-D air quality modelling

3-D air quality modelling systems have been used to study air quality impact of new and emerging technologies. In all relevant 3-D air quality modelling studies that we found, attention has been paid to certain life cycle stage(s) of the new or emerging technologies. For transportation fuel-related studies, analyses were mostly focused on exhaust emissions and their impact on air quality. The exhaust emission changes due to the use of the new fuels were collected, estimated and/or projected. Scenarios that reflect various penetration levels of the fuels were modelled to show the impact of changing exhaust emissions on ambient concentrations of various pollutants at different times and locations.

2.3 Strengths and weakness of the two current approaches

The major strength in the LCA approach is the life cycle thinking process. It considers all major life cycle stages of technologies, and can show impact of the technologies on air quality for each life cycle stage individually and/or the complete life cycle as a whole. However, the approach is necessarily over-simplified in scientific and technical details. It quantifies the impact on a functional unit basis using characterization factor(s), such as POCP in the unit of ethene-equivalent, instead of showing the impact on ambient concentrations of pollutants. It lacks spatial, temporal, and scale information related to technology applications, which is crucial for understanding air quality issues.

The major strengths in the 3-D air quality modelling approach include its scientific and technical details and its reflection of spatial, temporal, and scale information. State-of-the-art 3-D air quality models contain detailed atmospheric chemistry, physics, and transport processes. They also resolve concentrations of pollutants, their precursors, and relevant intermediates spatially and temporally. They can fully reflect technology penetration levels and show the impact of technology application scale on ambient concentrations of pollutants. However, the 3-D air quality modelling exercises that we found only focused on specific stage(s) of the technologies. Most life cycle stages were not considered. This practice may not pose serious problems if the air quality impact is indeed caused by a single stage in the technology life cycle. However, there was normally no information or justification to support such a claim.

3. THE CONCEPT OF LIFE-CYLCE BASED AIR QUALITY MODELLING FOR TECHNOLOGY ASSESEMENT AND POLICY APPLICATIONS

Considering the strengths and weaknesses in the current approaches, a natural advance of the approaches would be to introduce the life cycle thinking into the 3-D air quality modelling practice when technology impacts on air quality need to be analysed. This concept, which we call life-cycle based air quality modelling (lcAQM), integrates the overall LCA framework defined by ISO 14040 with the current 3-D air quality modelling approach. Fig. 1 shows an operational framework that outlines the lcAQM concept.

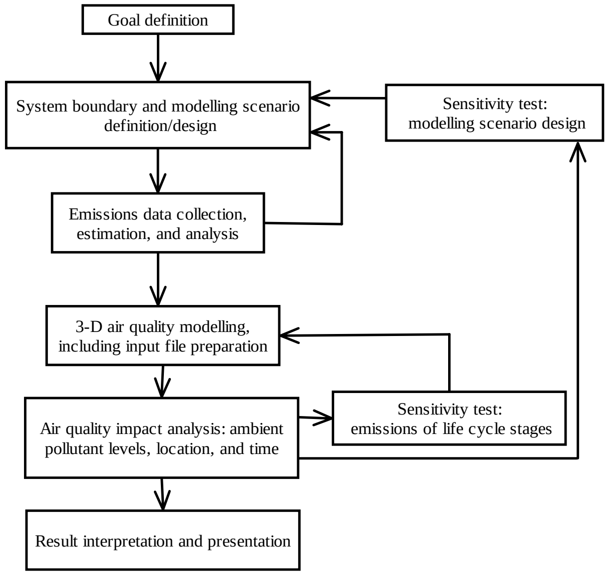

Fig. 1. An operational lcAQM framework for assessing air quality impact of new and emerging technologies.

In the goal definition phase, project objectives and intended audience are explicitly specified.

In the system boundary and modelling scenario definition/design phase, life cycle stages, modelling domain and period, technology application scale and penetration level, as well as locations of emissions sources in all life cycle stages are determined or assumed. The decision on the system boundary could be made through an iterative process based on the availability and significance of emissions, which are determined in the phase of emissions data collection, estimation, and analysis, in each life cycle stage.

Complete 3-D air quality model runs, including input file preparation, are then conducted for the base case and technology scenarios. The results are comparatively analysed to show the impact on ambient air pollutant levels at locations and time of interest, either on the basis of individual life cycle stages or the whole life cycle.

More insight could also be obtained through various sensitivity tests to show the effects of the assumptions used in defining the system boundary and modelling scenarios, and the impact of emissions and emission changes in different life cycle stages.

Finally, the modelling results are interpreted from the perspectives of science processes, emissions characteristics, data limitations, and potential industrial and policy implications.

4. TECHNICAL CONSIDERATIONS FOR CONDUCTING LIFE CYCLE-BASED AIR QUALITY MODELLING

In conducting lcAQM studies for technology assessment or policy applications, special technical considerations need to be paid to the system boundary definition and modelling scenario design, as well as emissions data collection, estimation, and analysis. In this section, we discuss these technical considerations, and use SunDiesel as an example to illustrate the concept and considerations.

4.1 Goal definition

As an example, we want to study the potential impact of large scale production and application of SunDiesel as a transportation fuel on air quality in Canada and the U.S. from a whole life cycle perspective. The results are to be used by the policy community in the decision making process regarding biofuel development.

4.2 System boundary definition

4.2.1 General consideration

To define system boundaries, sufficient knowledge about the chemical, physical, and engineering processes in different life cycle stages of technologies need to be acquired. Attention needs to be paid to the processes in those life cycle stages where emissions of air pollutants or their precursors could be significant. A reasonable system boundary should try to include all these processes. However, capital equipment production may not need to be included within the system boundaries due to its normally long-term life span.

4.2.2 Consideration for the SunDiesel case

SunDiesel is a synthetic diesel fuel introduced by Choren Industries GmbH in Germany (Rudloff 2005). It is made from cellulose, hemicellulose, and lignin, which are major components of a wide variety of biomasses, such as wood residues, switchgrass, etc. SunDiesel is produced from biomass through two major chemical processes: gasification of biomass to produce syngas, and the Fisher-Tropsch (FT) synthesis to convert syngas to SunDiesel. SunDiesel can be used directly to replace petroleum diesel as a transportation fuel.

Fig. 2 shows the overall life cycle of SunDiesel as a transportation fuel.

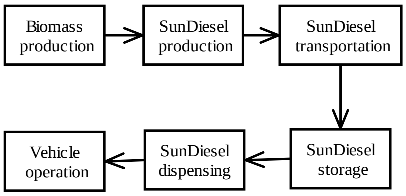

Fig. 2. Life cycle of SunDiesel as a transportation fuel.

Each life cycle stage shown in Fig. 2 may contain multiple processes. For example, for a biomass that needs fertilizer and herbicide for its production, the biomass production stage includes processes shown in Fig. 3.

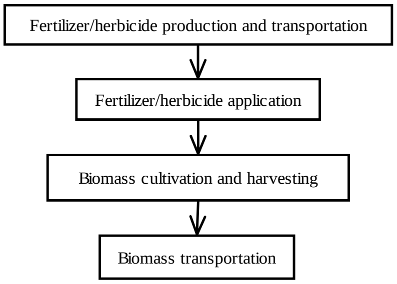

Fig. 3. Processes in the biomass production stage.

The SunDiesel production stage can be more complicated, depending on the processes used to convert biomass to SunDiesel. Fig. 4 shows an energy self-sufficient process model that we assembled based on the publicly available information about the Choren process (Li et al., 2006).

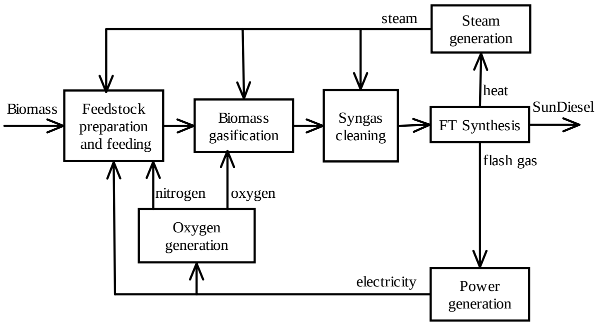

Fig. 4. Processes in the SunDiesel production stage.

The system boundary, as outlined by Figs. 2, 3, and 4, contains all major processes in the life cycle that could generate meaningful air emissions.

4.3 Modelling scenario definition and design

4.3.1 General consideration

In defining and designing modelling scenarios, the air quality modelling domain and time period need to be selected to serve the defined goal of the study. Assumptions regarding the possible locations and timing of industrial and agricultural operations in different life cycle stages need to be made carefully based on detailed analysis of available information. Uncertainties caused by the assumptions can be further analysed through sensitivity tests. In addition, projections of technology application scales and penetration levels should also be done by considering economic and environmental realities and requirements as well as the policy environment supporting the technology development.

4.3.2 Consideration for the SunDiesel case

To understand the potential impact of large scale SunDiesel applications on air quality in Canada and the U.S., we choose to have our domain cover both Canada and the continental U.S. We choose to model the full-year period of 2050, for example, when bio-fuels could become major sources of power for transportation purposes and could substantially reduce our dependency on petroleum oil (NRDC, 2004). Conducting the modelling for the full year would reflect the seasonal nature of biomass production processes.

It is a major challenge to make assumptions on locations of all the major agricultural and industrial operations related to the SunDiesel life cycle. Since we are trying to model a dramatically different future scenario, many factors are considered carefully. For example, detailed landuse coverage maps in Canada and the U.S. are examined in order to decide where the biomass feedstock will come from. Logically, logging wood residues will be assumed to come from forest logging sites, and dedicated energy crops, such as switchgrass, will grow on agricultural land or other suitable land. Assumptions are also made on various other factors, such as energy crop yields, conversion efficiencies from biomass to SunDiesel, and new innovations by farmers to address the needs of food crop, animal feed, and energy crops in an integrated way under appropriate economic and market conditions.

It is logical to assume that future SunDiesel production plants will be located at sites close to the places where raw biomass feedstock will grow or will be collected in order to minimize the cost and environmental impact of biomass transportation. However, competing factors of plant sizes and distances from the biomass growth sites also need to be considered. Large plants can normally achieve higher efficiencies and may generate lower emissions on a unit production basis. However, they will require biomass to be collected from larger areas and will increase the transportation distances of the biomass. This will increase emissions and cost.

4.4 Emissions

4.4.1 General consideration

Availability of emissions data associated with new and emerging technologies is most likely to be scarce and will be a major barrier for lcAQM exercises. Significant efforts are needed to measure or estimate emissions of relevant processes. Timely release of emissions data by relevant companies from their pilot plants will be invaluable to ensure the success of lcAQM projects.

To support lcAQM for technology assessment and policy applications, life cycle thinking needs to be introduced into the emissions inventory development process. Life cycle thinking can help to ensure completeness and self-consistency of emissions data in emissions inventories by cross-checking emissions data within different life cycle stages of technologies of interest, such as biofuels. Emissions inventories currently used by the air quality modelling community can also be strengthened and expanded by incorporating information contained in life cycle inventories (LCI) used by the LCA community. Major commercial LCA software packages, such as GaBi and SimaPro, all contain substantial amount of LCI data, which include detailed emissions data on a functional unit basis for numerous processes, materials, and products. In addition, some commercial LCI databases, such as EcoInvent (Ecoinvent, 2004), also contain very useful emissions data. These data can be used to derive emissions for certain life cycle stages of the technologies of interest. If possible, Canada or U.S.-specific data should be used for North American applications. If North American data are not available, data originating from Europe could be used temporarily with an understanding of uncertainties involved. When LCI data are extracted and used, attention needs to be paid to the chemical speciation of the emissions, especially when both criteria pollutants, such as VOC, and speciated pollutants are available from the same LCI data sets.

One major task in the emissions inventory development for lcAQM studies is to derive spatial surrogates and surrogate ratios that reflect the assumed spatial distributions of emissions sources within all major life cycle stages of technologies. In addition, temporal factors for all the processes involved should be determined by considering different characteristics of operations in different life cycle stages.

To reflect the displacement of old technologies by new or emerging technologies, some emissions sources in the base case scenario need to be removed when the technology scenarios are modelled. Detailed analysis of Standard Industrial Classification (SIC) codes, Source Classification Codes (SCC), or descriptions of emissions sources is needed to ensure that the technology displacement reflected by the emissions data change is as accurate as possible.

4.4.2 Consideration for the SunDiesel case

Emissions for some life cycle stages of SunDiesel can be assembled or derived based on the data available in current emissions inventories and in LCA software packages. For example, GaBi contains NO_x, VOC, SO_2, PM, and heavy metal emissions on a functional unit basis for various processes related to different fertilizers, fuels, and power. Combining these data with our analysis of fertilizer and energy needs for biomass growth, and transportation, storage, and dispensing needs for SunDiesel, we can derive emissions for the following processes in the SunDiesel life cycle shown in Figs. 2 and 3: fertilizer production and transport, fertilizer application, biomass cultivation and harvesting, biomass feedstock transportation, and SunDiesel transportation, storage and dispensing. Emissions of some VOC species are available along with some unspeciated VOC emissions. These data can assist in creating VOC speciation profiles for some life cycle stages of interest. The functional unit-based emissions data can be treated as emissions factors, which can be combined with scales of the processes to generate final emissions data.

Measured emissions data for the SunDiesel production processes are not publicly available at the moment. Lack of these real emissions data is a major barrier for conducting lcAQM of SunDiesel as a transportation fuel. Although effort is being spent in estimating the emissions by comparing the compositions and Lower Heating Values of flash gas with other fuels that have emissions data available (Li et al., 2006), great uncertainties still exist for the emissions generated by SunDiesel production. Future release of emissions data associated with the Choren process, other FT processes of diesel production, and flash gas combustion will be very beneficial. In the absence of measured data, methods for estimating these emissions need to be further developed.

One major task in the emissions inventory development for the SunDiesel scenario is to derive spatial surrogate ratios that reflect the assumed spatial distributions of all agricultural and industrial sources within all major life cycle stages. Major considerations in determining these distributions have been discussed at the modelling scenario design step. In addition, temporal factors for all the processes involved in different life cycle stages need to be determined by considering the seasonality of agriculture operations and industrial operational schedules.

In the SunDiesel scenario to be modelled, emissions associated with traditional petroleum fuel life cycles need to be partially removed to reflect the displacement of the fuels by SunDiesel.

4.5 Model implementation and result analysis

Emissions related to the SunDiesel scenario and the base case petroleum fuel scenario can be grouped based on major life cycle stages of feedstock generation, fuel production, fuel transportation, storage, and dispensing, and fuel usage for transportation purposes. Model runs can be conducted with all the emissions included. Sensitivity runs can also be done with or without emissions from certain life cycle stages. The modelled results can then be analysed to reveal the air quality impact of SunDiesel on a basis of life cycle stage or all life cycle stages as a whole.

5. SUMMARY AND DISCUSSIONS

Life cycle-based air quality modelling, or lcAQM, is a concept that introduces life cycle thinking into 3-D air quality modelling practices for analysing the impact of new and emerging technologies on air quality.

When conducting a lcAQM study, special considerations need to be paid to the system boundary definition and modelling scenario design, as well as emissions data collection, estimation, and analysis. A reasonable system boundary definition and modelling scenario design are the foundation for a successful lcAQM study.

To support lcAQM for technology assessment and policy applications, life cycle thinking also needs to be introduced into the emissions inventory development process. Emissions inventories currently used by the air quality modelling community could be strengthened and expanded by incorporating information contained in LCIs used by the LCA community. In addition, spatial surrogates and surrogate ratios need to be developed to reflect the assumed spatial distributions of emissions sources within all major life cycle stages. Temporal factors for all the processes involved should also be determined by considering different characteristics of operations in different life cycle stages.

Availability of emissions data, especially the data for new or emerging technologies themselves, presents the most serious challenge for a lcAQM study, and could be the major barrier to the success of the project. Special attention needs to be paid to measure, collect, and estimate emissions related to these technologies.

6. ACKNOWLEDGEMENTS

The authors would like to thank our colleagues Helmut Roth and Albert Chan for their effort in reviewing and providing helpful comments on this paper. Some results generated by our SunDiesel analysis project funded by Natural Resources Canada are used in this paper.

7. REFERENCES

Ecoinvent, 2004. Code of Practice, Ecoinvent Report No. 2, Swiss Centre for Life Cycle Inventories, Dubendorf, June 2004.

Goedkoop, M., Oele, M., 2004. SimaPro 6 – Introduction to LCA with SimaPro, Pre Consultants, September 2004.

Guinee, J.B., 2002. Handbook on Life Cycle Assessment, Kluwer Academic Publishers, 2002.

IKP University of Stuttgard, PE Europe, 2003. GaBi 4 Manual, IKP of the University of Stuttgart, PE Europe GmbH, Germany, March 2003.

ISO 14040, 1997. Environmental management – life cycle assessment – principles and framework, International Organization for Standardization, Geneva.

ISO 14042, 2000. Environmental management – life cycle assessment – lofe cycle impact assessment, International Organization for Standardization, Geneva.

Li, Q., Jiang, W., Smyth, S., Chan, A., 2006. Modelling and analysis of biomass to SunDiesel process, draft report, Institute for Chemical Process and Environmental Technology, National Research Council of Canada, Ottawa, Ontario, Canada, August 2006.

NRDC, 2004. Growing energy, how biofuels can help end America's oil dependence, Natural Resources Defense Council, 2004.

Rudloff, D.I.M., 2005. Biomass-to-liquid fuels (BtL) made by CHOREN process, environmental impact and latest developments, Beograd 2005 European Automotive Congress, Belgrade, Serbia, May 30–June 1, 2005.