

CHAPTER II

LITERATURE REVIEW

2.1 Chemical Process Design

The chemical process is the process to transform raw materials into the desired chemical products. Usually the chemical process can split into many minor steps before we get the desired products and each step will connect to another steps to form the full process. Each step of the chemical process consists of different unit and leads to different purpose in each step. Thus, the synthesis of a chemical process or the chemical process design will be necessary. First of all the *flowsheet* of the process must be constructed to represent all of the individual step in the process and their connection. Once the flowsheet has been constructed, a simulation of the process can be initiated to predict behavior of the process when it was constructed. After evaluation of the basic performance has been done, the last procedure will be an optimization of the process to improve the overall performance of on the basis of economy, sustainability and environment.

2.2 Life Cycle Assessment

Life cycle assessment is the tool for facilitating pollution prevention strategies and environmental management to improve the environmental performance of the entire products/process life cycle. LCA is a “cradle-to-grave” approach for assessing industrial systems. The word “cradle-to-grave” means the life cycle of one product/process is started from raw materials gathered from the earth to products produced and end at disposal of the used products (which all materials return to the earth.). Therefore, LCA enables the estimation of the cumulative environmental impacts resulting from all stages in the product life cycle including impacts not considered in more traditional analysis such as raw material extraction, transportation, waste disposal, etc. Life cycle of product and input/output material is shown in Figure 2.1.

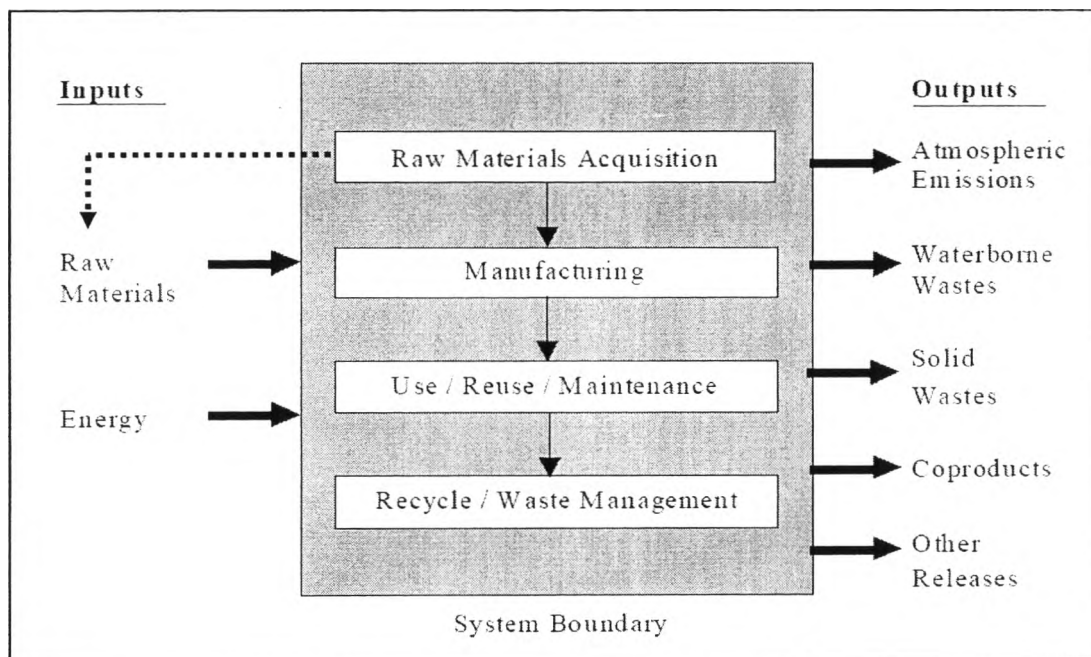


Figure 2.1 Life cycle and input/output material for one product/process.

2.2.1 LCA Components

The LCA is a systematic process consists of four main stages. The first one is goal definition. followed by inventory analysis, impact assessment and end at interpretation.

2.2.1.1 *Goal Definition and Scoping*

Goal definition and scoping is the stage to define the purpose and method of the project, also describe and identify the system boundaries, product, process or activity in the life cycle. In this stage, the items that must be determined are the type of information needed, how accurate the results must be and how the results should be interpreted and displayed.

2.2.1.2 Inventory Analysis or Life Cycle Inventory (LCI)

In this stage, the usage of energy and raw material will be identified and quantified. Collect environmentally relevant information such as atmospheric emissions, waterborne emissions, solid wastes, etc. from the entire life cycle. LCI is one of the important process in LCA. Without an LCI there is no basis existing to evaluate comparative environmental impacts or potential improvements. Results from LCI should be the list containing the quantities of pollutants released to the environment and the amount of energy and material consumed. According to the document named “Life-Cycle Assessment: Inventory Guidelines and Principles” of *United States Environmental Protection Agency* (USEPA) in 1993, LCI can divided into the following four steps:

1. Develop a flow diagram of the processes being evaluated.
2. Develop a data collection plan.
3. Collect data.
4. Evaluate and report results.

2.2.1.3 Impact Assessment or Life Cycle Impact Assessment (LCIA)

After quantification of all input resource and output pollution of the process in the LCI stage, the impact assessment will be conducted. LCIA is the process to evaluate the potential human health and environmental impacts of the environmental resources and releases identified during the LCI. The results of impact assessment should be the ecological and human health effect including resource depletion. ISO has developed a standard for conducting an impact assessment entitled ISO 14042, *Life Cycle Impact Assessment* which consists of seven steps but the first three steps (impact category selection, classification, and characterization) are specified to be the mandatory step to conduct LCIA.

Step 1: Select and Define Impact Categories

In LCIA the impacts are defined as the consequences of environmental release that have effect on human health, plants, and animals, or the future availability of natural resources. For example, an environmental release identified in the LCI may harm human health by causing cancer or increasing global warming. Usually LCIA

will focus on three main impact categories which are human health, ecological health, and resource depletion.

Step 2: Classification

In this step the LCI results will be organized and classified into impact categories for example CO₂ emission will be classified into the global warming category. This example is the simple assignment because CO₂ is the greenhouse gas and can be classified into global warming categories. For LCI item that can classify into more than one impact categories, classification must follow the rule established by ISO 14042. There are two ways to assign LCI results to multiple impact categories.

- Partition a representative portion of the LCI results to the impact categories to which they contribute. This is typically allowed in cases when the effects are dependent on each other.
- Assign all LCI results to all impact categories to which they contribute. This is typically allowed when the effects are independent of each other.

For example, NO_x have an effect on both ozone depletion and acidification at the same time so the entire quantity of NO_x will be classified into both categories (100% to ozone depletion and 100% to acidification). The impacts categories and associated endpoint are shown in Table 1.

Table 2.1 List of impact categories and endpoints that identify the impacts (SAIC, 2006)

Impact Categories		End Point
<u>Global Impact</u>	Global warming	Polar melt, soil moisture loss, longer seasons, forest loss/change, and change in wind and ocean patterns.
	Ozone depletion	Increased ultraviolet radiation
	Resource depletion	Decreased resources for future generations.
<u>Regional Impact</u>	Photochemical Smog	“Smog,” decreased visibility, eye irritation, respiratory tract and lung irritation, and vegetation damage.
	Acidification	Building corrosion, water body acidification, vegetation effects, and soil effects.
<u>Local Impact</u>	Human health	Increased morbidity and mortality
	Terrestrial Toxicity	Decreased production and biodiversity and decreased wildlife for hunting or viewing.
	Aquatic Toxicity	Decreased aquatic plant and insect production and biodiversity and decreased commercial or recreational fishing.
	Eutrophication	Nutrients (phosphorous and nitrogen) enter water bodies, such as lakes, estuaries and slow-moving streams, causing excessive plant growth and oxygen depletion.
	Land Use	Loss of terrestrial habitat for wildlife and decreased landfill space.
	Water Use	Loss of available water from groundwater and surface water sources.

Step 3: Characterization

To characterize the LCI impact the conversion factor call characterization factor will be used this factor commonly referred to as equivalency factors. The purpose of characterization step is to convert LCI results into representative indicators (in term of quantity) of impacts to human and ecological health. Characterization provides a way to directly compare the LCI results within each impact category. For example, characterization would provide an estimate of the relative global warming potential between CO₂, CH₄ and CFC. To characterize indicators the following equation will be used:

$$\text{Inventory Data (from LCI)} \times \text{Characterization Factor} = \text{Impact Indicators}$$

For example, all greenhouse gases can be expressed in terms of CO₂ equivalents by multiplying the greenhouse gases from LCI results by a CO₂ characterization factor and then combining the resulting impact indicators to provide an overall indicator of global warming potential. This calculation method is demonstrated in Example 1.

Example 1. Characterization on global warming

Estimate the global warming potential (GWP) of 20 pounds of chloroform and 10 pounds of methane

Solution Chloroform GWP characterization factor value* = 9

Methane GWP characterization factor value* = 21

Chloroform GWP Impact = 20 pounds x 9 = 180

Methane GWP Impact = 10 pounds x 21 = 210

So 20 pounds of chloroform has lower effect on global warming than 10 pounds of methane

*Intergovernmental Panel on Climate Change (IPCC) Model

As we can see in the previous example characterization can put these different quantities of chemicals on an equal scale to determine the amount of impact. Each one has on global warming. All of the commonly use impact categories, representative indicators of impact and description of each characterization factor can be summarized into Table 2.2 as shown below.

Table 2.2 Impact categories and impact characterized detail (SAIC, 2006)

Impact Category	Scale	Examples of LCI Data (i.e. classification)	Common Possible Characterization Factor	Description of Characterization Factor
Global Warming	Global	-Carbon Dioxide (CO ₂) -Nitrogen Dioxide (NO ₂) -Methane (CH ₄) -Chlorofluoro carbon (CFCs) -Hydrochlorofluoro carbons (HCFCs) -Methyl Bromide (CH ₃ Br)	Global Warming Potential	Converts LCI data to carbon dioxide (CO ₂) equivalents Note: global warming potentials can be 50, 100, or 500 year potentials.
Stratospheric Ozone Depletion	Global	-Chlorofluoro carbon(CFCs) -Hydrochlorofluoro carbons (HCFCs) -HalonsMethyl Bromide (CH ₃ Br)	Ozone Depleting Potential	Converts LCI data to CFC-11 equivalents.
Acidification	Regional Local	-Sulfur Oxides (SO _x) -Nitrogen Oxides (NO _x) -Hydrochloric Acid (HCL) -Hydrofluoric Acid (HF) -Ammonia (NH ₄)	Acidification Potential	Converts LCI data to hydrogen (H ⁺) ion equivalents.
Eutrophication	Local	-Phosphate (PO ₄) -Nitrogen Oxide (NO) -Nitrogen Dioxide (NO ₂) -Nitrates -Ammonia (NH ₄)	Eutrophication Potential	Converts LCI data to phosphate (PO ₄) equivalents.

Table 2.2 Impact categories and impact characterized detail (Cont'd)

Impact Category	Scale	Examples of LCI Data (i.e. classification)	Common Possible Characterization Factor	Description of Characterization Factor
Photochemical Smog	Local	Non-methane hydrocarbon (NMHC)	Photochemical Oxidant Creation Potential	Converts LCI data to ethane (C ₂ H ₆) equivalents.
Terrestrial Toxicity	Local	Toxic chemicals with a reported lethal concentration to rodents	LC50	Converts LC50 data to equivalents; uses multi-media modeling, exposure pathways.
Aquatic Toxicity	Local	Toxic chemicals with a reported lethal concentration to fish	LC50	Converts LC50 data to equivalents; uses multi-media modeling, exposure pathways.
Human Health	Global Regional Local	Total releases to air, water, and soil.	LC50	Converts LC50 data to equivalents; uses multi-media modeling, exposure pathways.
Resource Depletion	Global Regional Local	-Quantity of minerals used -Quantity of fossil fuels used	Resource Depletion Potential	Converts LCI data to a ratio of quantity of resource used versus quantity of resource left in reserve.
Land Use	Global Regional Local	Quantity disposed of in a landfill or other land modifications	Land Availability	Converts mass of solid waste into volume using an estimated density.
Water Use	Regional Local	Water used or consumed	Water Shortage Potential	Converts LCI data to a ratio of quantity of water used versus quantity of resource left in reserve.

The three steps above are the mandatory step in the LCIA because these three steps are the most difficult and complicated in the LCIA and they will lead to the final goal of LCA. However to finish LCIA, four more steps must be conducted;

Step 4 Normalization

Expressing potential impacts in ways that can be compared

Step 5 Grouping

Sorting or ranking the indicators

Step 6 Weighting

Emphasizing the most important potential impacts.

Step 7 Evaluating and reporting LCIA results

Gaining a better understanding of the reliability of the results

2.2.1.4 Interpretation

The last stage of LCA after doing LCIA is to evaluate information from the results of the LCI and LCIA, and communicate them effectively. ISO has defined the following two objectives of life cycle interpretation:

- Analyze results, reach conclusions, explain limitations, and provide recommendations based on the findings of the preceding phases of the LCA, and to report the results of the life cycle interpretation in a transparent manner.
- Provide a readily understandable, complete, and consistent presentation of the results of an LCA study, in accordance with the goal and scope of the study.

2.2.2 Calculation Models in LCA

To quantify the impact indicator, many calculation models will be used, from which characterization factor are derived for individual pollutant and so on.

2.2.2.1 Climate Change

Climate change or the global warming is defined as the phenomena that the temperature of the earth surface is rising every year. This phenomenon is caused by the emission of greenhouse gas from human activity and has an effect on human and natural environment. Heijungs et al. (1992) has developed the calculation model on climate change by using the factor called Global warming potential (GWP). GWP is the characterization factor for converting quantity of any greenhouse gas to kg of CO₂ equivalent and use in Equation 1.

$$\text{Climate change} = \sum_i \text{GWP}_i \times m_i \quad (2.1)$$

where m_i is the mass of substance i release in kg. The result is expressed in kg of CO₂ equivalent.

2.2.2.2 Stratospheric Ozone Depletion

Stratospheric ozone depletion refers to thinning of stratospheric ozone layer. This depletion will cause the greater fraction of solar UV radiation reach the earth surface. To calculate the ozone depletion Heijungs et al. has proposed the characterization factor called ozone depletion potential (ODP). Like the GWP, ODP is the characterization factor for converting quantity of any ozone depletion substance to kg of CFC-11 equivalent and use to calculate ozone depletion (Heijungs et al., 1992)

$$\text{Ozone depletion} = \sum_i \text{ODP}_i \times m_i \quad (2.2)$$

where m_i is the mass of substance i release in kg. The result is expressed in kg of CFC-11 equivalent.

2.2.2.3 Human Toxicity

This impact category covers the impact on human health by toxic substance present in environment. Human can receive toxic via the main three compartments which are air, water and soil and the calculation model were developed by Heijungs et al. (1992) to calculate human toxicity in term of 1,4-dichloro benzene equivalent by using human toxicity potential (HTP) as characterization factor.

$$\text{Human toxicity} = \sum \text{HTP}_i \times m_i \quad (2.3)$$

where m_i is the mass of substance i release in kg. The result is expressed in kg of 1,4-DCB equivalent.

2.2.2.4 Ecotoxicity

This impact category has divided into two subcategories which are aquatic toxicity and terrestrial toxicity. Both impact categories use calculation model developed by Heijungs et al. (1992).

- Aquatic toxicity

Aquatic toxicity is focus on the emission of substance that can spread into the water and harm aquatic organism. The calculation model is based on the characterization factor call aquatic ecosystem toxicity potential (ATP) developed by Heijungs et al. (1992).

$$\text{Aquatic ecotoxicity} = \sum \text{ATP}_i \times m_i \quad (2.4)$$

where m_i is the mass of substance i release in kg.

ATP is characterization factor to convert m_i into mass of 1,4-DCB equivalent.

The results is expressed in kg of 1,4-DCB equivalent.

- Terrestrial toxicity

Terrestrial toxicity is focus on the emission of substance that can spread into the soil and harm rodent or other living organism. The calculation model is based on the characterization factor call terrestrial ecosystem toxicity potential (TTP).

$$\text{Terrestrial ecotoxicity} = \sum \text{TTP}_i \times m_i \quad (2.5)$$

where m_i is the mass of substance I release in kg.

TTP is characterization factor to convert m_i into mass of 1,4-DCB equivalent.

The results is expressed in kg of 1,4-DCB equivalent.

2.2.2.5 Photochemical Smog

Photochemical smog is the formation of reactive chemical compound such as ozone reacts with the air pollution in the present of ultra violet ray. This smog can be effect on human health, ecosystem even damage crop. The calculation model for this impact category is also use the characterization factor like before and can calculate by equation below (Heijungs et al., 1992).

$$\text{Photochemical smog} = \sum_i \text{POCP}_i \times m_i \quad (2.6)$$

where m_i is the mass of substance i release in kg.

POCP is characterization factor to convert m_i into mass of ethylene equivalent.

The results is expressed in kg of ethylene equivalent.

2.2.2.6 Acidification

Acidifications have a wide impact on soil, ground water, surface water, bio-organism, ecosystem and building. The major substances that cause acidification are SO_2 , NO_x and NH_x . Acidification potential is the characterization factor used to calculate this impact category (Heijungs et al., 1992).

$$\text{Acidification} = \sum_i \text{AP}_i \times m_i \quad (2.7)$$

where

m_i is the mass of substance i release (kg).

AP_i is the acidification potential of substance i .

The results Acidification is expressed in H^+ -equivalent.

2.2.2.7 Eutrophication

Eutrophication is the impact of excessiveness of macronutrients such as nitrogen and phosphorous. The excessive of nutrient may cause an undesirable shift in species composition and over elevate biomass production both terrestrial and aquatic. Heijungs et al. has developed the calculation model for this impact category.

$$\text{Eutrophication} = \sum_i \text{EP}_i \times m_i \quad (2.8)$$

where

m_i is the mass of substance i release to air, water and soil (kg).

EP_i is the eutrophication potential of substance i .

The results Eutrophication is expressed in PO_4 -equivalent.

2.3 Program

There are two main programs related with this work which are Microsoft Excel and its subset program Visual basic for application.

2.3.1 Microsoft Excel

Microsoft Excel is one of the programs under the Microsoft Office developed by Microsoft Corporation. This program is electronic work sheet that can use for a variety of purposes such as mathematical, financial, and statistical calculation, creating charts, etc. This program is available for operating system of Microsoft Windows and Mac OS X. The latest version of Microsoft Excel is 2010. The user interface is shown in Figure 2.2 below.

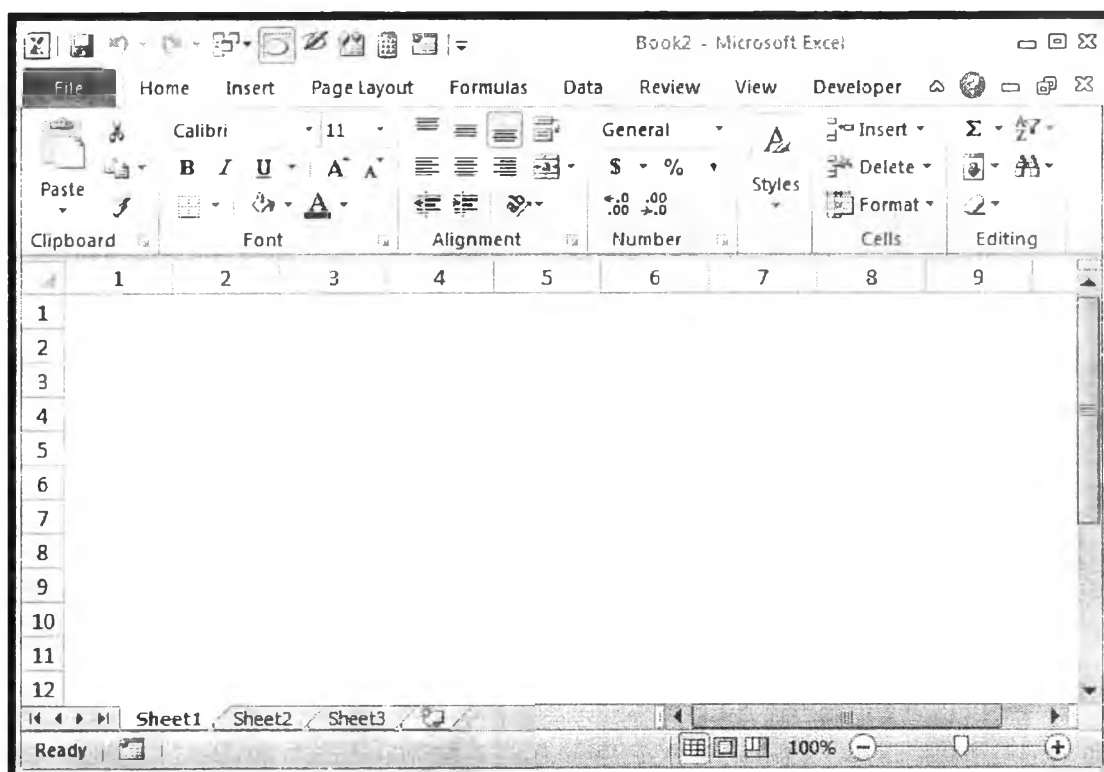


Figure 2.2 User interface of Microsoft Excel ver.2010 program.

2.3.2 Visual Basic for Application Programming

Visual basic for application (VBA) can be accessed by using the Visual Basic icon on the Developer Tab in Microsoft Excel. Clicking that icon opens a window to the Visual Basic editing environment which contain a window for writing code and a sophisticated debugging and code module organization environment as shown in Figure 2.3 VBA enables developers to build user defined functions and automate processes it can also be used to control many aspects of the host application, including manipulating user interface features, such as menus and toolbars.

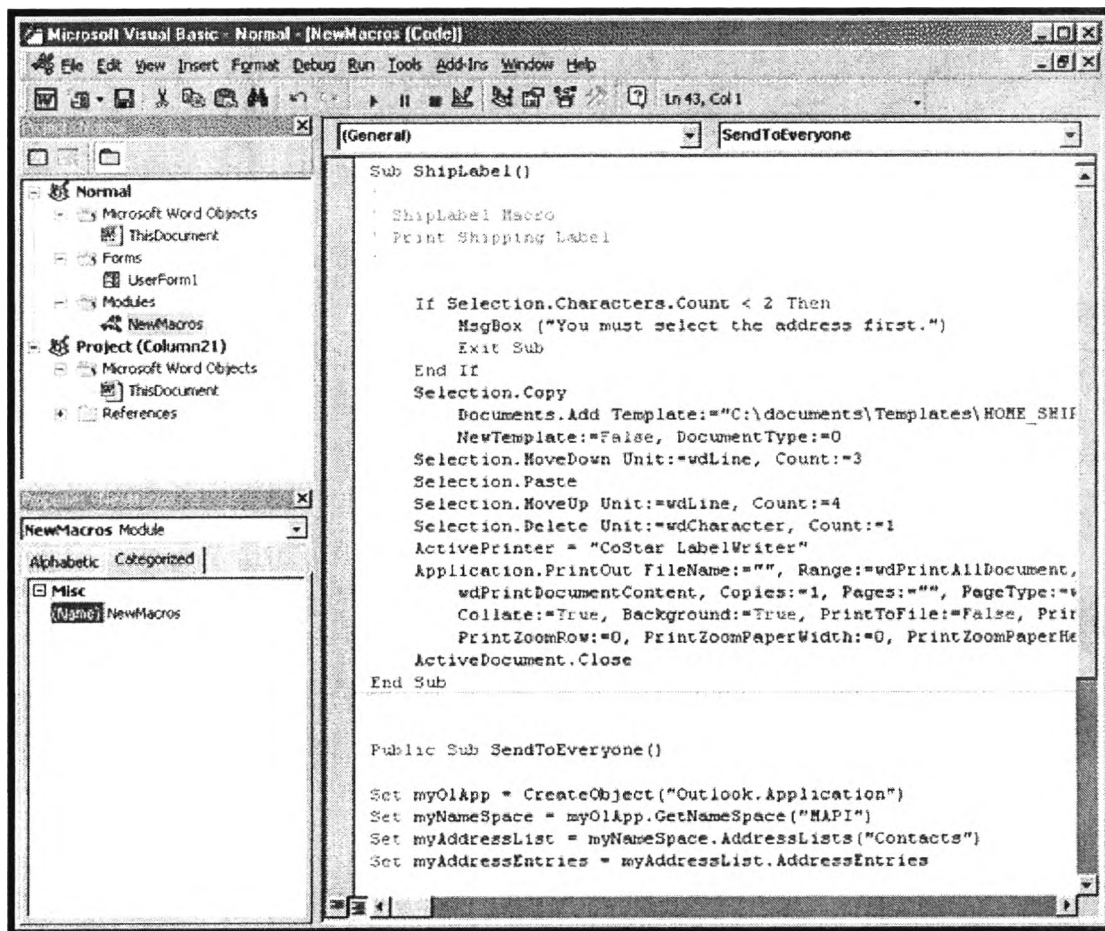


Figure 2.3 Visual basic for application interface.