Computer-Aided Modeling Environment for Future Energy Production Systems

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Abstract
There are increasing challenges on energy production systems where traditional energy sources and technologies are causing harm to health and environment, in addition to their high cost. Renewable energy sources and energy conversion technologies are widely investigated to overcome such limitations and to offer clean and cheap energy. However, there is large number of renewable energy sources and possible conversion technologies and production scenarios, which varies based on geographical area, available resources, and energy requirements. It is required to evaluate the different energy production paths with the considerations of life cycle activities and select the most effective scenario. This requires providing automated and intelligent systems that can assist in modeling and evaluating different scenarios of future energy production paths. This paper proposes an integrated modeling framework and computer-aided modeling environment that can be used to analyze different energy production paths in different levels of abstraction. The proposed modeling framework will enable the design and realization of intelligent system for future energy production chain management.
Keywords: energy production chain, production chain modeling, energy systems data modeling

1 Introduction

Energy production is the concern of almost all nations, companies as well as individuals where there is a limited availability in current energy sources, in addition to their harm to health and environment. It is expected that there will be gradual change in energy production and supply where renewable sources will be widely utilized in energy production. The production and use of renewable energy sources involve different processes such as biomass production, transportation, recycling, conversion plants, and distribution. In addition, energy production chain involves energy utilization systems, such as industrial systems, public and social systems, etc. In order to provide flexible management for these interconnected systems, it is essential to design process model that represents the different energy production scenarios and facilitate the design and control of energy production chain operation.

There are widely known energy strategies such as from-waste-to-energy (Chinese et al., 2005), or using renewable energy sources, which includes processing, conversion, and production technologies (Montesa et al., 2005). These energy strategies will be used in the national, organization, and/or individual levels to plan their energy source and technology.

The planning of future energy production chains requires conducting detailed requirement analysis so that requirements from the different views can be considered while realizing the target system. There are different attempts that have been made to analyze energy systems, of different scales i.e. local, national or global. Some of these attempts are data-based while others are model-based approaches. In data-based approaches data are collected from different nodes / sources / systems and methods are applied to analyze and to extract useful knowledge and to decide design issues of energy systems. In model-based approaches, models are developed and used to decide design issues. In data-based approaches, there are different methods that are used to analyze energy systems, for example stochastic methods are used to simulate wind process using real wind data (Nfaoui et al., 2004). In such approach, methods are applied on specific cases, while it was relatively difficult to generalize the solution on other cases or to handle complex energy production chains. Detailed modeling of the underlying or target energy production system requires developing conceptual and abstract level models that can be used as a base to develop more detailed models and evaluate these models in view of different performance indices.

Some of these attempts are focused on specific technology such as wind systems (Sesto et al.,1998), fuel cell (IWV), solar / photovoltaic systems (Sidirasa, et al., 2004), waste treatment via gasification (Calzavara et al., 2005), fermentation (Kheshgi et al., 2005), and other technologies. Due to the variety of these energy paths, and availability of different parameters that affect the selection of optimum energy production scenario, it is essential to provide robust modeling framework to structure related data and acquire domain knowledge that can be used to design intelligent system for energy planning.

System modeling includes different views: (a) domain models, which include data and knowledge models; (b) process models, which include business processes and activities involved in energy production; (c) management models, which includes organizational and operational aspects; and (d) behavioral models which include the definition of the different behaviors that can be used to achieve certain functions (Gabbar et al., 2004).

Although data modeling is one traditional approach that is used to analyze systems, and have been used effectively for decades to realize automated systems. However, it lacks expert views, which are usually defined in domain knowledge, i.e. Ontology. Ontology is the classification of concepts or specification of a conceptualization. Also it is a description (like a formal specification of a program) of the concepts and relationships that can exist for an agent or a community of agents. Due to the importance of domain modeling, this research work proposes practical data and knowledge modeling framework that can be used as part of the system analysis of the target energy planning and management systems. In the next section, background and overview of integrated data and knowledge modeling concepts will be explained.

2 Data & Knowledge Modeling

During the last decade, we have seen an explosive growth in our capabilities to both generate and collect data for engineering systems and other applications. This highlighted the importance of data modeling, which is an essential tool to analyze the underlying system or process as part of the domain modeling.

The modeling process is the abstraction and approximation of the real world i.e. target system while neglecting non-relevant details (Gabbar et al., 2000). Models are represented using set of notations or other representation formats such as graphs, diagrams, formal methods, etc, which are used to express models in understandable format for human, machine and systems. Information engineers develop data models as part of the software engineering lifecycle prior to building database systems. Process systems engineers are also developing data models as part of the concept and deign stages of the target system or process such as chemical or mechanical system or process. Examples of developed data models and their use in constructing database systems are DETHERM (Westhaus, Droge, & Sass, 1999), which holds data of thermodynamic and transport properties. Another example is material conceptual models and its application in process engineering (Yang et al., 2003). Most of these data modeling practices start with conceptual data modeling which identifies concepts and their dependencies and relationships for the underlying problem domain.

Although data models were used successfully to develop different engineering and business systems, however, they couldn't provide the adequate aspects to design intelligent system that can act as human. Data modeling couldn't provide detailed analysis of the underlying problem domain, where aspects of knowledge were not properly modeled, such as: concepts, rules, intentions, skills, experience, etc.

Ontology is widely used to express concepts. However, there were misunderstanding of the differences between knowledge in its wide meaning and the ontology. Ontology is explicit formal specifications of the terms in the domain and relations among them (Gruber 1993). Ontology includes: classes (sometimes called concepts), properties of each concept describing various features and attributes of the concept, (called slots or roles), and restrictions on slots (which are facets or role restrictions) (Noy, 1995). It is important to differentiate between domain knowledge and ontology. Ontology editors, such as Protégé, OILEd, and other ontology tools, are originally used to define ontology and classify concepts, and then gradually improved their capabilities to be able to define domain knowledge. That is the reason of having initiatives of developing upper ontology, which is simply the actual ontology that represents concepts. Upper ontology is concepts that are domain independent, which is the original definition of ontology. In other words, by following the original definitions of ontology, the term upper ontology is just a redundant term, which refers to the use of ontology as part of the knowledge modeling of the underlying domain. Hence, ontology modeling and domain modeling are in fact two different practices with completely different targets. It can be understood that the term knowledge modeling includes ontology modeling, and can be used to refer to domain modeling.

In knowledge engineering, all aspects of knowledge are captured and maintained in knowledgebase. This requires performing knowledge modeling or domain modeling. Currently, the most commonly used technology for domain modeling is ontology editors, which can be used to perform domain (or knowledge) modeling.

In general, knowledgebase includes a set of assertions, which is composed of rules and data structures or facts (Wu, 2000; Mineau, 2000). Knowledge modeling is the way to design and construct knowledgebase as part of the development of knowledgebase systems or knowledge management systems. In addition, knowledge modeling is a prerequisite to knowledge discovery and is the base of data mining practices on large data. Knowledge analysis, which is equivalent to data analysis, can be viewed as analysis stage to acquire and structure knowledge including concepts and relations in view of the underlying system or problem domain (Kavakli, 2001).

It is possible and logical to map concept modeling of the underlying problem domain, which is also known as concept stage of process engineering or conceptual design, to the ontology modeling using ontology editor.

It is essential to carry out both data and knowledge modeling as part of the concept, design, and engineering stages of large-scale systems, where data and knowledge models are constructed either in parallel or in sequence and tuned iteratively. The commonly used data and knowledge modeling practices could not provide reliable framework to maintain and synchronize data and knowledge models in unified framework, which caused time and efforts and affected the efficiency and robustness of the underlying system. This problem is escalated when dealing with large-scale systems with different views and interconnected domains. This raised different questions and concerns such as the difference between these two modeling practices, how to integrate them, the representation and tools available, and how to link them to other the engineering activities and systems such as design, simulation, operation, etc.

In this paper, authors present practical data and knowledge modeling approach and propose integrated modeling framework, which is applied to case study of energy production system. The reason energy production system is selected as a case study is due to the current challenges in finding cheap renewable energy sources with less environmental impact. Also energy production system is a complex system that has links to other industrial and social systems, which requires linking the energy related data to domain knowledge and system engineering activities. The proper data and knowledge modeling will enable systems engineers to understand the current practices and analyze future energy production scenarios, which will be reflected to energy production system and other industrial and social systems.

The next section presents the selected case study of energy production system, which is used to illustrate the proposed integrated data and knowledge modeling approach. Data modeling approach will be illustrated in section three. In section four, knowledge modeling will be presented for the selected case study. In the section five, the proposed integrated modeling framework will be illustrated.

3 Energy Production System

In this section, a brief description of the target energy production system will be explained.

3.1 System Overview

Energy production chain starts from the production and preparation of energy sources or feedstock. Energy is then converted into bio-products, energy, or fuel, which are utilized by industrial market or domestic use. Government role comes in the organization and management of regulations and policies for the whole energy production chain. Improvement in the quality and quantity of the energy sources will improve the production of energy, fuel, and/or bio-products; hence will have positive impact on the whole energy production chain (Bryan, 2002; BTAC, 2002). Currently, almost all countries are concerned with energy and renewable energy sources, as well as the analysis of current sources and possible production scenarios and their impacts on social, industry, and government / politics (Johansson, 2004). Such analysis includes different factors such as cost, environment, quality (e.g. exergy), etc. At this stage, the target energy production system has main objective to support the analysis and collection of energy related data and to design practical energy production chain in view of different energy production scenarios.

The target energy production chain includes entities from the different stages of energy processing options.

Figure 1 shows high-level use case model of energy production chain, which shows the main processes involved in the underlying energy production chain. The proposed energy production chain shows the role of energy related R&D to coordinate the different results with the different processes in resources production, treatment, energy conversion, transportation, and utilization. This includes different systems such as public, social, industrial, etc.

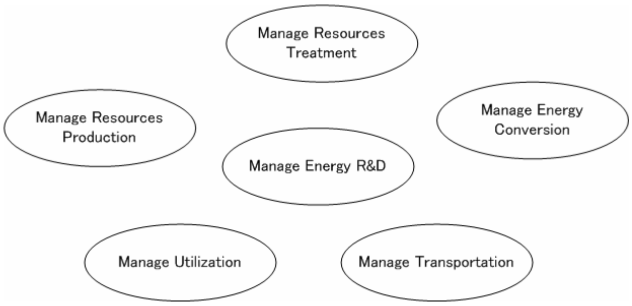

Figure 1. Use Case Modeling of Energy Production Chain

There are different scenarios for energy production, among them the use of biomass and fossil fuels. The case study showed in this example is for biomass-based production chain, which includes of production of feedstock biomass and conversion into electricity, byproducts, and/or fuel. The system analysis of such production chain shows model elements grouped in main packages, for the target energy production system, as follows:

- Feedstock production, which includes all activities related to feedstock (e.g. from residues and crops)
- Processing & conversion, which includes activities required to convert energy into bio-product, fuel, or energy.
- Energy production policies, which includes government activities with the collaboration with industry and R&D to manage energy production policies and regulations
- Energy utilization & distribution, which includes industrial activities for the utilization and distribution of energy products
- Waste treatment, which includes waste management activities
- R&D, which includes all activities related to the discovery of new materials, technologies, techniques related to energy

production, or systems

- Management of the overall energy production, which includes planning, management, and coordination for the different activities within the energy production chain

3.2 Energy Network

What is energy network? Energy is produced and converted into different bio-products, bio-fuel, or bio-energy. There is variety of conversion paths and scenarios, which is defined as energy network. Energy network is continuously expanding and dynamically changing due to many factors such as the progress in R&D and technologies, as well as the changes in market requirements. This requires developing robust data modeling approach that is linked to domain knowledge to support such changes, which is essential for flexible energy production systems. Energy network model elements are grouped in a package called Energy Network. Model elements from energy network package are associated with model elements in other packages such as feedstock production, processing and conversion, etc. The model and management of energy networks will be explained later when addressing knowledge modeling of energy production chains.

4 Data Modeling Framework

The described energy production system shows the general trend in building distributed and integrated global energy production system. Robust modeling of such complex system will enable system engineers to design realistic energy production system. As in most complex systems, system engineer focuses on the core business while analyzing the underlying system. Building blocks are defined in the meta-level, which are used to construct the complete data model. To model such multidimensional systems, operational design modeling methodology (Gabbar et al., 2003) is adopted where data model elements are defined in three major views: structure, behavior, and operation. In our example, energy network is the main focus where it is produced (i.e. in the feedstock production stage), treated (i.e. in the waste treatment stage), converted into different materials (i.e. in the conversion and processing stage), and utilized and distributed (i.e. in the utilization and distribution stage). The following section shows data model framework for energy production chains.

4.1 Data Modeling of Energy Production Chain

Data modeling is performed based on the developed activity models and/or use case models, which reflect the sequence of activities and input / output information in each activity. Such hierarchical use case modeling and/or activity modeling will help system engineer to identify the main groups of the underlying data model.

Data model can be grouped into data sets.

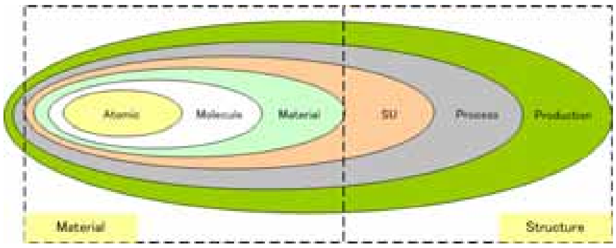

Figure 2. Energy Production Data Abstraction

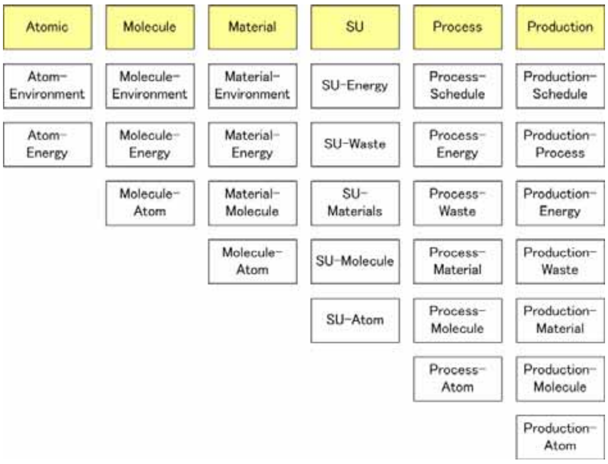

Figure 3. Conceptual View of Energy Production Data Model

Data abstraction of energy production can be viewed in hierarchical levels starting from the atomic level, where atom related data are modeled. Molecule includes atomic level with its composition. Material can be viewed mixture of molecule data in different state as manipulated and processed within structure units (SU's). It includes physical or logical unit to perform physicochemical phenomena, which can be hierarchically decomposed into smaller SU's. Process is composed of sets of SU's organized in topology to produce the final product(s). Production is the managerial layer on top of process, which includes production management such as steady and seasonal timing. Figure 3 shows conceptual view of data models covering from the atomic till the production level. In appendix 2, all detailed data model views are explained.

4.2 Model Views

In this section, different model views will be explained with respect to energy production chains.

4.2.1 Environmental Impacts

Ontology modeling enabled us to define basic environmental objects, which are used as a reference to define all possible impacts that might occur on each environmental object. Within the developed ontology, environmental impacts are classified as: Air, Land, Water, Nature, or Underground. Set of environmental impacts are defined and associated with Air such as Air-pollution. Similarly, there are other environmental impacts that have been defined and associated with Water, such as water-pollution. Water can be associated with any natural resource such as river, sea, lake, rain, etc. These factors are defined for each scope, i.e. atomic, molecular, material, SU, process, and production levels. This enable effective design and planning of energy production scenarios based on environmental impacts. More detailed class definition is required to illustrate more about environmental impacts, specifically on the land, natural and underground. This is kept outside the scope of this paper.

4.2.2 Energy Class

Energy classes include heat and electricity. Energy transformation i.e. heat balance are defined in terms of the basic energy class attributes. Energy class is associated with energy measure (e.g. Watt) and the associated environmental impact class (e.g. Air, water, etc.).

4.2.3 Atomic Class

The atomic level includes the basic classes that represent the base to form molecules, as per table 1.

Table 1. Atomic Level Classes and their Description

C	Carbon
N	Nitrogen
H	Hydrogen
O	Oxygen
S	Sulfur
Cl	Chlorine
Ar	Argon

4.2.4 Atomic – Environmental Impacts

Such relation shows the impacts of different atoms such as carbon, nitrogen, etc. This can be calculated as per international standards, indexes, or as per the underlying domain. Other class models are illustrated in appendix 2, which includes: molecule, SU, Process, Production levels. In addition, energy production and energy feedstock class models are illustrated.

4.3 Energy Production Systems Ontology

While the proposed data models can classify the different levels and scope of the target energy production chain, however, it couldn't answer questions related to different energy conversion technologies, or the different paths in energy production chains. Domain knowledge is essential to explain the different paths in energy networks and the evaluation criteria of each energy production scenario. The development of domain knowledge will enable clear understanding of different paths and the contributing factors and measures for effective planning and flexible production chain operation. In addition, it will help unifying basic concepts and terminologies used within the target energy production system among different parties within the target energy production chain. Protege2000 (Protégé) used to develop the proposed domain knowledge, as shown in figure 4, which shows the screenshot of the developed ontology.

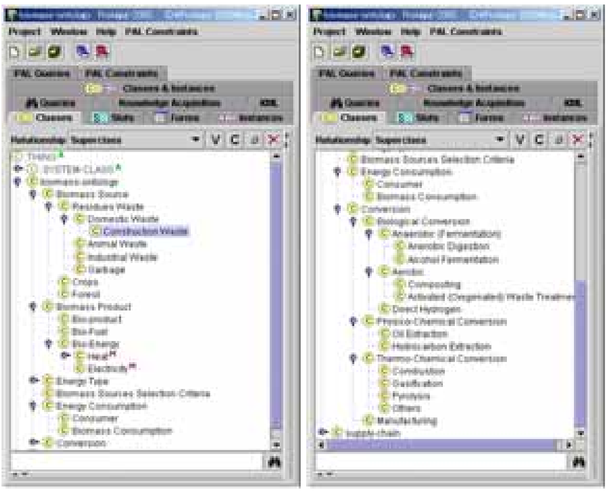

Figure 4. Energy Production Ontology

The integration between the proposed data and knowledge models will enable structuring and management of energy production chain data elements. In addition, the classification of atomic, molecule, material, SP, Process, and Production model elements provided the basis to understand the complete energy production chain and to link nano, micro levels with the macro level model elements for better management and scenario modeling and evaluation of the target energy production chain. Nano level is used to refer to the atomic and molecule level of materials that contribute to energy production. Micro level refers to process level where chemical or fermentation process is used to generate energy. Macro level represents production chain processes including transportation and other social systems. Still the proposed data model requires further development to include all detailed model elements, attributes and define class inheritance and instances for the different model levels, which will be linked to knowledge acquisition system.

5 Computer-Aided Modeling Environment

The proposed modeling framework can be used to model nano, micro and macro level processes and link environmental-related information for more accurate evaluation of different energy production chain paths.

The first part shows computer-aided modeling called CAPE-ModE (Gabbar et al., 2004) proposed to capture process model level, as shown in figure 5. CAPE-ModE can be used to capture process block diagram (i.e. PBD), process flow diagram (i.e. PFD), and piping & instrumentation diagram (i.e. P&ID). In each of these process design levels, process information such as equipment class, associated materials , related environmental impacts, and other life cycle inventory (i.e. LCI) information are captured and linked to each process structure model element. The shown example in the drawing area represents a process of power production plant, which is used to generate energy from oil, coal, or biomass. In such example, LNG (Liquefied Natural Gas), oil, coal, and biomass species are defined in the atom, molecule levels in each structure unit.

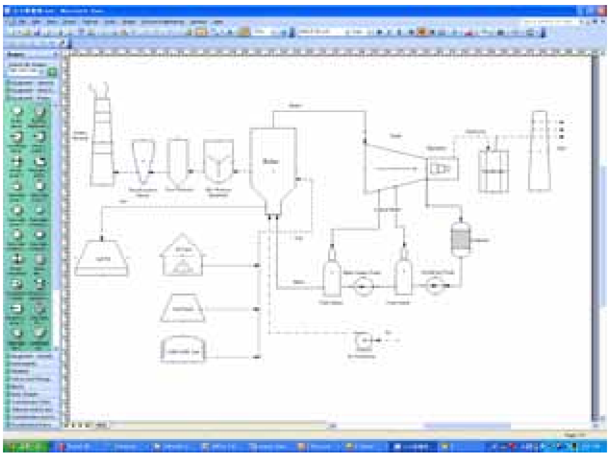

Figure 5. CAPE-ModE showing PFD for Power Production Plant

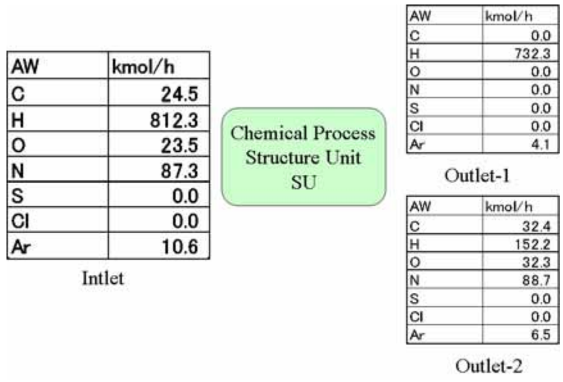

Figure 6. Example of Atom Level Information within CAPE-ModE

The process shows input materials of oil, LNG, or coal to the boiler for burning. The output steam is used to produce energy from dynamo (i.e. turbine). The output of the boiler is cleaned before emission to environment. The overall environmental impact of this process is calculated by calculating the different environmental impacts at each unit from the atom and molecule level. Based on the environmental index value for each atom and molecule level, the overall environmental impact can be calculated. User can simply click on process equipment, such as boiler, to see the associated atom and molecule level information. Figure 6 shows one example of atom level information associated with process equipment SU.

6 Conclusion

System engineering practices for large-scale systems is based primarily on robust data and knowledge modeling, which are developed based on system requirements. This research paper presented integrated data and knowledge modeling framework, which is proposed to design large scale systems, focusing on energy production chains. Model elements are defined in view of object oriented modeling methodology, which provided systematic way of defining modeling levels, elements, and link to domain knowledge. The modeling practice is used to analyze energy production chains based on renewable energy sources, where they are linked to environmental impacts and production plants. Abstraction view of energy production system is analyzed and modeled using use case and class diagrams. The proposed data and knowledge modeling framework is implemented within computer-aided modeling environment called CAPE-ModE where atom and molecule level information are associated with process level models i.e. PBD, PFD, P&ID. In such energy production system overview, model elements are grouped in packages such as feedstock production, conversion and processing, R&D, utilization & distribution, policies & measures, and production management. The focus in this modeling practice was on the modeling of energy network with respect to environmental impacts, which includes the different paths to produce bio-products / bio-fuels / bio-energy from energy using different processes and conversion technologies. The proposed modeling framework can be used to capture and analyze LCI data associated with energy production chain and can be used to evaluate the different production chain paths / scenarios in terms of environmental impacts. The proposed idea will be applied to capture data in geographical areas and tune simulation models using real time collected data, as integrated with national and local constraints and regulations. The proposed integrated modeling and engineering environment can be used effectively for the planning and management of clean energy production chains.

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Appendix (1) – Energy Ontology

Table 2. Energy Production Options

- energy-ontology
  - Energy Sources Selection Criteria
  - Energy Consumption
    - Consumer
    - Energy Consumption
  - Energy Production
    - Energy Product
      - Bio-Product
        - Bio Chemical Products
          - Fibers
          - Citric & Acids
          - Pesticides
          - Lubricants
          - Surfactants
        - Bio Materials
          - Composite Materials
      - Bio-Fuel
        - Bio-Fuel-Type
          - Solid Fuel
            - Charcoal
          - Liquid Fuel
            - Pyrolysis Liquids
            - Biodiesel
          - Gaseous Fuel
            - Synthesis Gases
              - CO + H2
            - Hydrogen
            - Biogas (Methane + CO2)
            - Methanol
            - Ethanol
        - Fuel Use
          - Transport Fuel
          - Manufacturing Industry
          - Domestic
      - Bio-Energy

- Bio-Energy Type
  - Electricity
  - Heat
- Bio-Energy Utilization
  - Process & Space
  - Power Generation
- Conversion
  - Biological Conversion
    - Anaerobic (Fermentation)
      - Anerobic Digestion
      - Alcohol Fermentation
    - Aerobic
      - Composting
      - Activated (Oxygenated) Waste Treatment
    - Direct Hydrogen
  - Physico-Chemical Conversion
    - Oil Extraction
    - Hydrocarbon Extraction
  - Thermo-Chemical Conversion
    - Combustion
    - Gasification
    - Pyrolysis
    - Others
  - Manufacturing
- Energy Source
  - Residues
    - Domestic Waste
      - Construction Waste
    - Animal Waste
    - Industrial Waste
    - Garbage
  - Crops
  - Forest
  - Marine
- Energy Handling
  - Transportation
  - Collection
  - Processing

Storage

Appendix (2) – Energy Production Chain Data Model

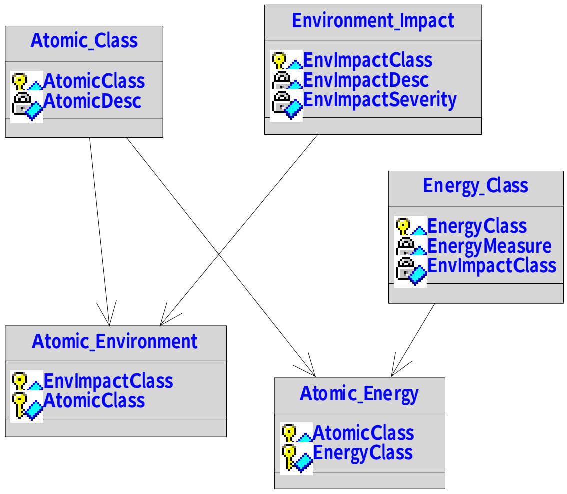

Figure 7. Atomic Level Data Model

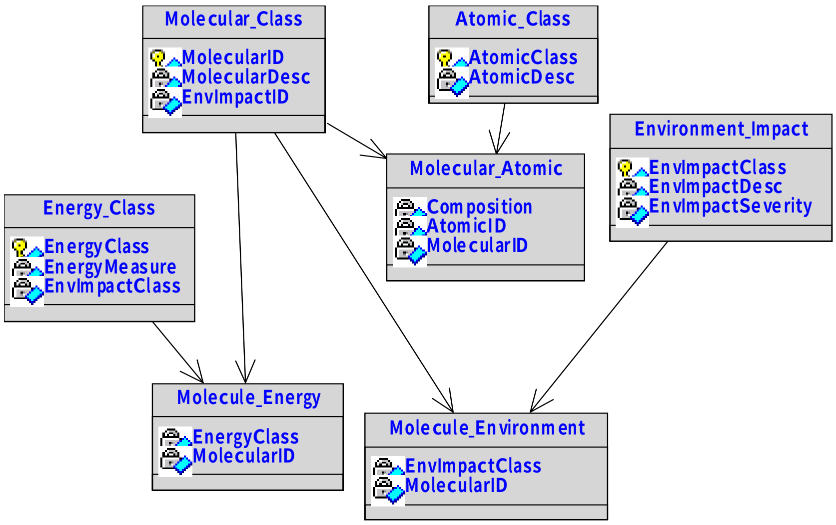

Figure 8. Molecule Level Data Model

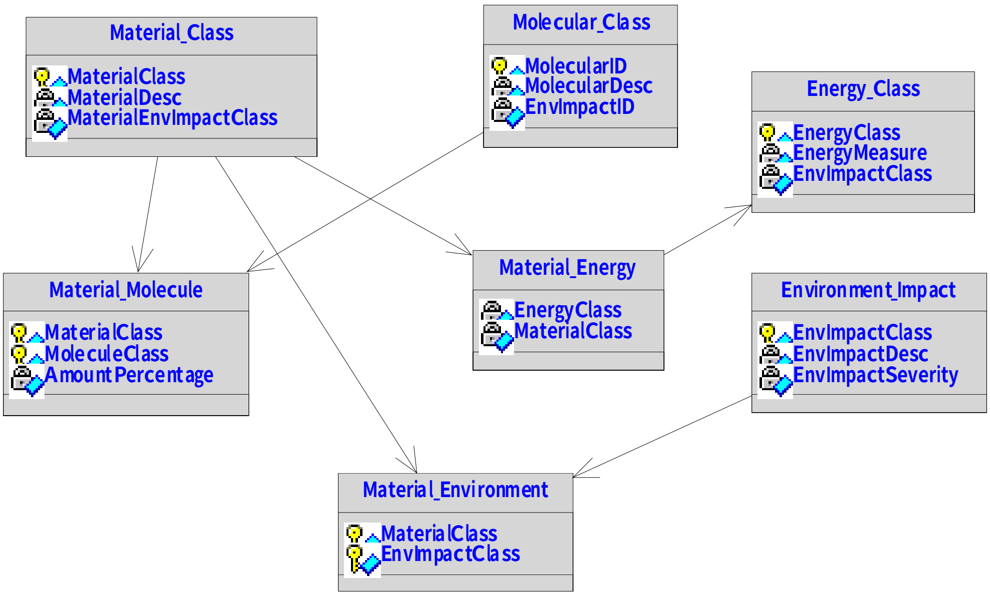

Figure 9. Material Level Data Model

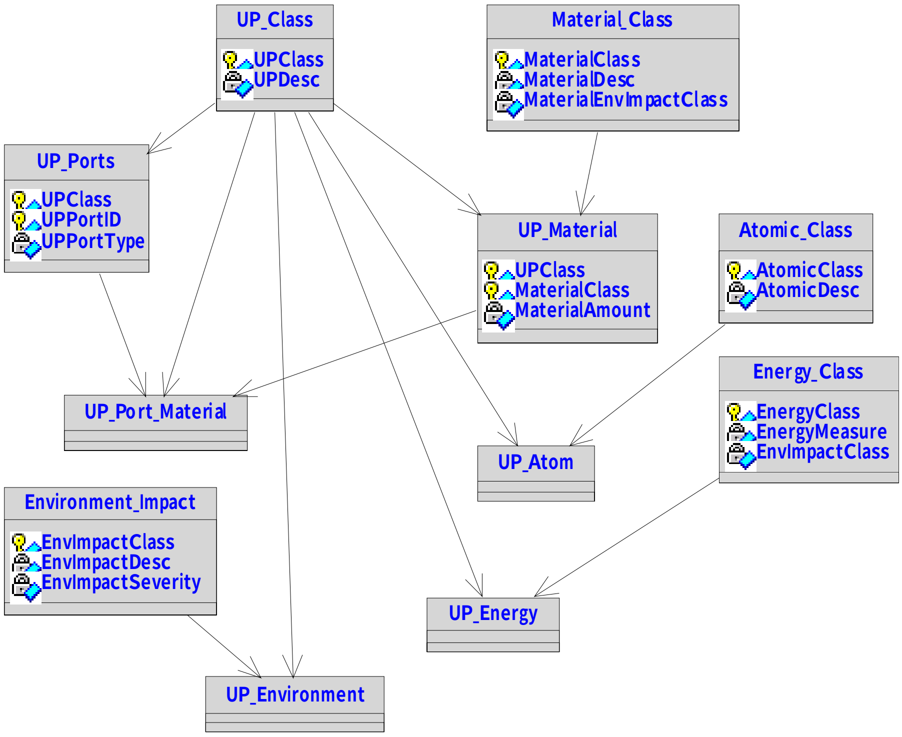

Figure 10. SU Level Data Model

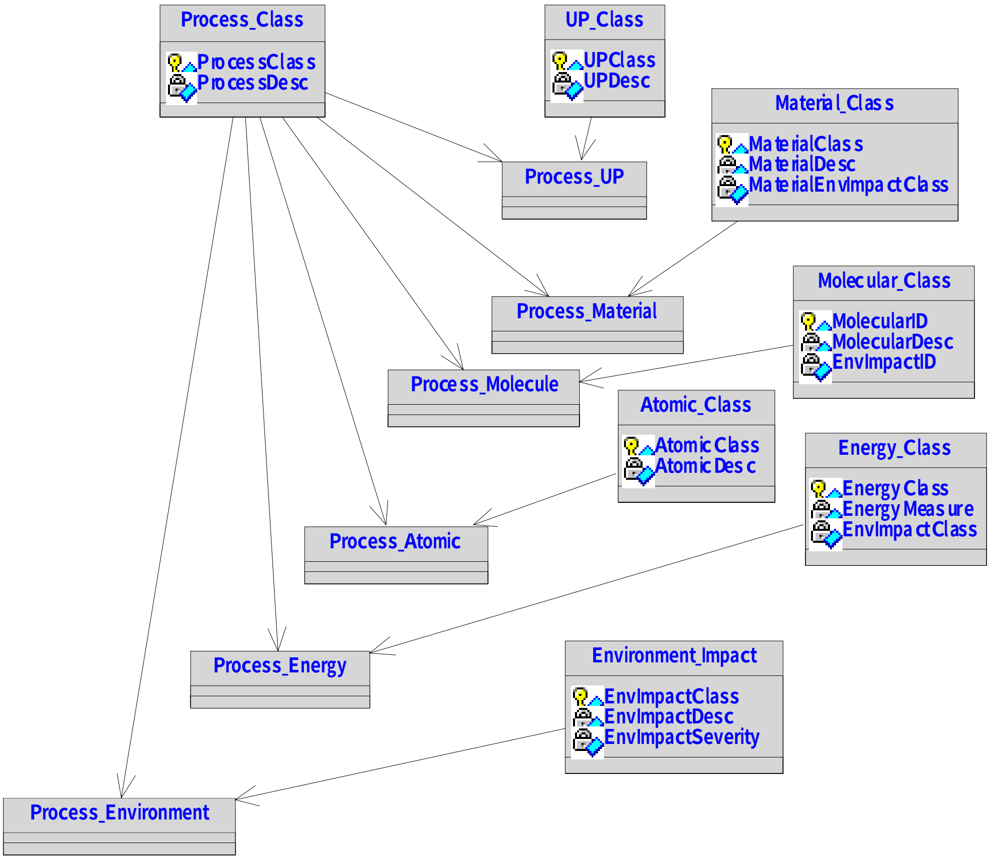

Figure 11. Process Level Data Model

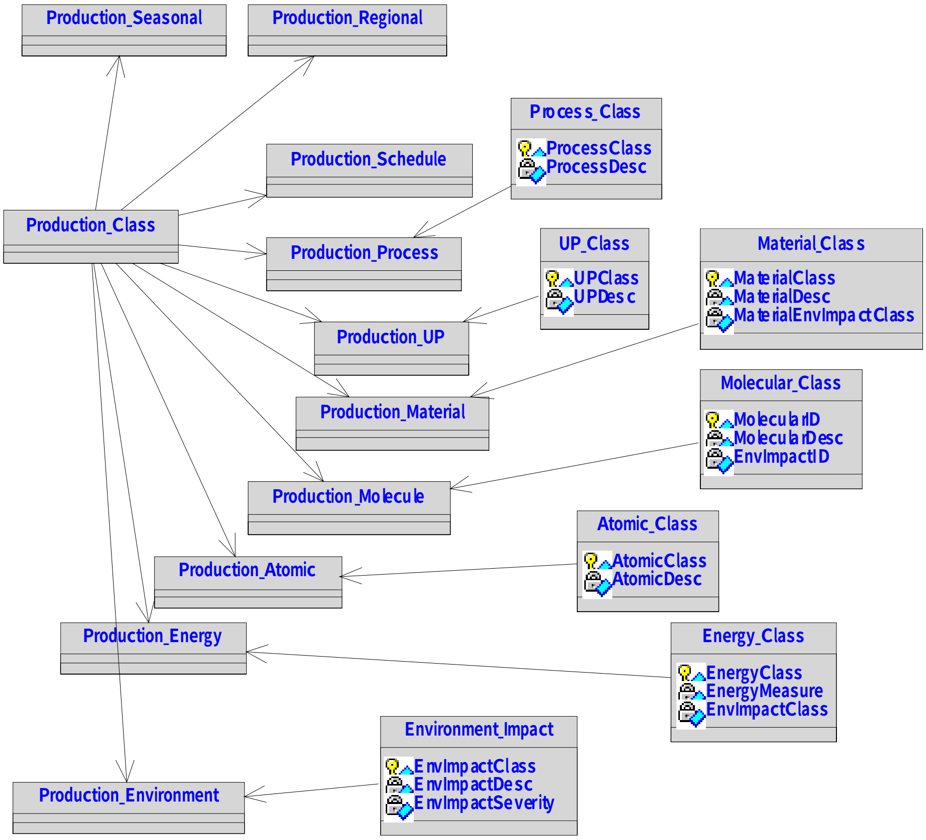

Figure 12. Production Level Data Model

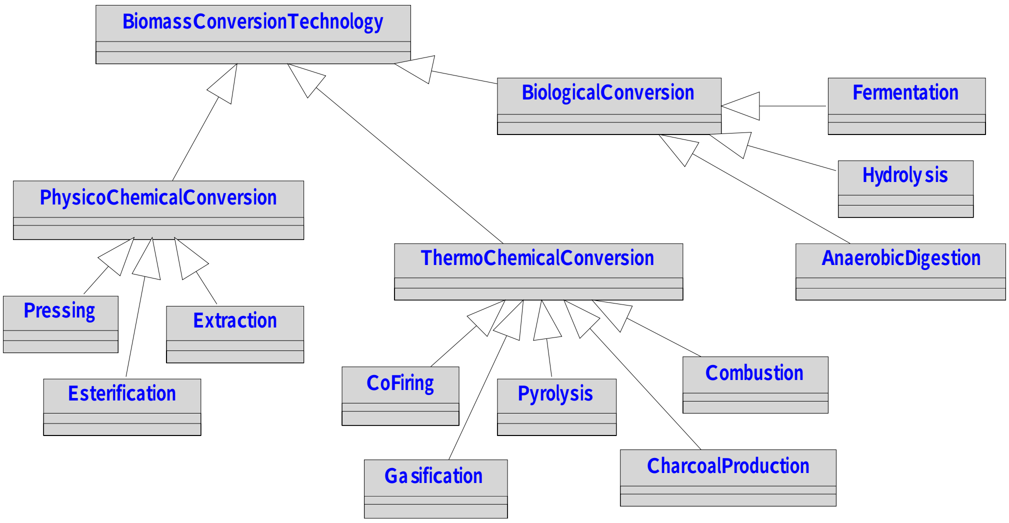

Figure 13. Class Model of Energy Conversion Process

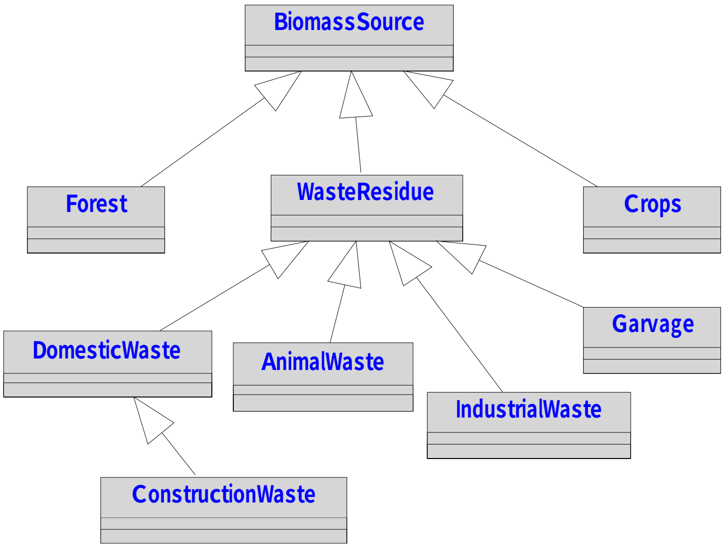

Figure 14. Energy Feedstock Class Model

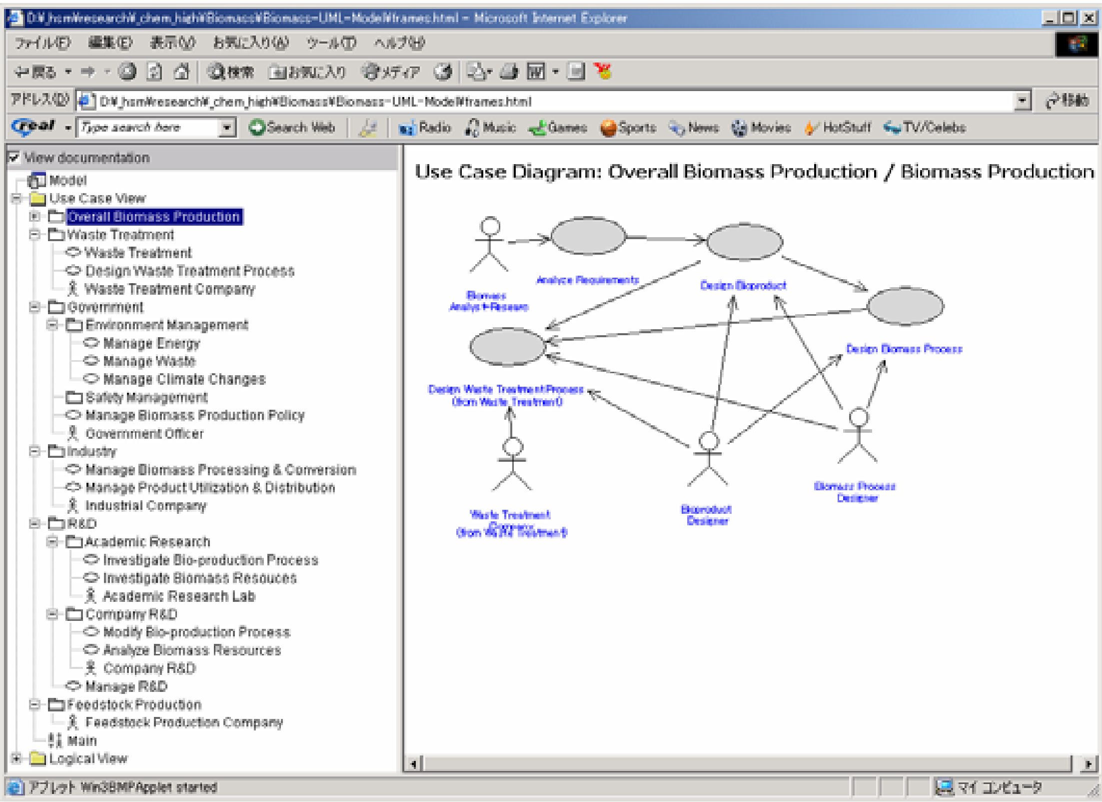

Figure 15. UML Model of Energy Production Chain