COLLABORATION PLATFORM FOR RESEARCH AND DEVELOPMENT OF SOLID OXIDE FUEL CELLS

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ABSTRACT

A scheme for a collaboration platform for the research and development of solid oxide fuel cell (SOFC) systems is proposed. The proposed platform enables users to design introduction scenarios of the SOFC system into the society and promotes interdisciplinary collaborations among SOFC researchers and developers by providing functions for 1) evaluating the environmental impacts of the SOFC system and its manufacturing process; 2) estimating changes in infrastructures, commodity flows among industries, and the social system; 3) failure prevention based on predictive analysis. The systematic structure and basic mechanisms to realize each type of functionality for the holistic design of SOFC systems and the introduction scenarios are described.

INTRODUCTION

Toward the development of a solid oxide fuel cell (SOFC) system that is economically feasible in existing markets for energy systems, research efforts are being focused on a wide diversity of studies covering materials (1), electrochemical (2), systems (3), and fabrication (4) perspectives. However, to assess the potential for a proposed SOFC design to successfully penetrate the energy market, research is required on developing scenarios for introducing SOFC systems that draw the findings from these specific research studies together holistically.

Assessing the effectiveness of a proposed scenario for SOFC introduction to penetrate the energy market requires concurrent evaluations of cost, environmental impact, and performance-related attributes in terms of various aspects of an SOFC system such as cell characteristics, module configurations, system characteristics, manufacturing processes and their facilities, changes in energy infrastructures, effects of replacement of existing energy technologies, and the inter-industry commodity flow changes induced by the newly established fuel cell manufacturing industries. To create an optimal scenario for rapid, profitable, and non-regrettable market penetration of SOFCs, the SOFC system design and evaluation process together with the manufacturing process and market introduction process must be studied from the research and development phase. A critical part of this research and development phase study is the analysis of the reliability of the SOFC over the entire life cycle of the system, including the manufacturing and operation phases, and how to prevent those failures from occurring. We can use the information related to failure mechanisms in SOFCs and related devices acquired through this analysis to design new specifications for more robust systems.
Clearly, the concurrent and interdisciplinary nature of the studies we have described requires collaborations among researchers and developers from a wide range of disciplines. Our goal is to construct an interdisciplinary collaboration platform for holistic design and evaluation at the research and development phase of SOFC systems and other innovative technologies for achieving an environmentally and economically sustainable future society (hereafter “collaboration platform”). Our global image of the platform, the functionalities that are necessary to achieve the goals of the platform, and the systematic structure and basic mechanisms we propose for implementing those functionalities are described in the following sections.

COLLABORATION PLATFORM

Schematic Image

Figure 1 shows a schematic image of the collaboration platform that we are developing. The collaboration platform is envisioned as a tool to help identify paths for achieving an environmentally and economically sustainable future society through the holistic design of innovative technologies. Toward this ambitious goal, we are constructing a prototype collaboration platform focused on SOFC technologies that provide functionalities enabling the following tasks to be conducted concurrently:

- Evaluation of the cell, stack, and system characteristics of the SOFC.
- Evaluation of the manufacturing process of the SOFC.
- Evaluation of the inter-industrial commodity flow changes induced by the introduction of the SOFC and its related industries.
- Predictive failure analysis from the design specifications and identification of failure prevention measures.
- Forecasting of long-term future changes in social systems resulting from introduction of the SOFC.

Figure 1. Schematic of collaboration platform.
In Figure 1, six information service domains are shown interconnected by a data exchange infrastructure. The “simulation” domain of the platform handles all of the simulation-based evaluations of the SOFC characteristics. The “LCA (life-cycle assessment)” domain uses a scenario-based LCA method to evaluate the life-cycle impacts of large-scale introduction of the SOFC system into the energy market, including environmental impacts of SOFC manufacturing processes and commodity flow changes (5). Predictive forecasting of failures that could occur as a result of a given set of system specifications as well as recommendations for specification changes to prevent the occurrence of the identified failures are performed in the “failure forecasting” domain. To facilitate the mechanism of failure forecasting from a given set of design specifications, we have developed a structured markup language for describing design specifications of chemical devices based on the meta-language, XML (eXtensible Markup Language) (6). The regional information parameter sets that represent the social system, such as geographical information, environmental restrictions, and energy demands, will be handled in the “regional information” domain. The “GUI (graphic user interface)” domain provides a standardized, user-friendly environment for flexible support of user interaction with the total integrated platform.

Details of the information to represent the regional characteristics, the format for the design-specification markup language, simulation of the SOFC characteristics, the LCA framework, and basic mechanisms for predictive analyses of failures will be described in the following sections. Graphical user interfaces have been described in the work by Kraines et al. (7) and will be developed further in the future.

**Regional Information**

Because the market penetration of energy systems is strongly influenced by the regional characteristics of the targeted social system, models and databases that express these regional characteristics are necessary (8). For the proposed platform, we use a geographical information system (GIS) database to define the distribution of land use types in the region (7). To assess the effects of the specific mix of centralized and distributed power generation systems for the targeted region, we prepared databases for regional electricity demand, parameters expressing social characteristics (such as regulations, taxes, and interest rates), and parameters governing the energy plans for the region (such as capacity constraints for each power source and energy security considerations). To predict how the penetration of SOFCs into the energy market will occur in the future, we are also developing mechanisms for forecasting the future trends of these regional characteristics.

**Design Specification**

A markup language for describing information on the spatial configurations, the materials used, and the energy distributions and flows in chemical systems was developed using XML (9). We use this markup language to describe the design specifications of the SOFC system that is being considered.

Figure 2 shows how our markup language can be used to describe the design specification of an SOFC system. At the top level, the SOFC system is expressed as an assembly of “apparatus” elements. An apparatus is an expression of a single entity unit, which is generally defined as a space that is clearly delineated by structure entities (described
Information “Structure” and “Fluid” have spatial info. Material - Link to database
Energy - Type - Dimensions
Corresponding spatial position
Quantity - Quantity

Figure 2. Schematic of design specification.

below). Each apparatus is expressed as a group of structure and fluid entities, termed “Structure” and “Fluid,” respectively, that are contained in the apparatus. Each structure and fluid has information on 1) spatial configuration, 2) inventories of materials for structure entities or chemical compositions for fluid entities, and 3) energy types and distributions. The hierarchical nature of XML is suitable for expressing the “part-of” or “contained-in” relationships of the SOFC system components together with the material and energy flowing through the system. In addition, we define information for the connections between 1) two or more structure entities, 2) two or more fluid entities, or 3) a mix of different structure and fluid entities.

Because the design specifications expressed in our markup language adhere to a standard document type definition protocol of XML, we can easily develop computer algorithms that know where to find particular forms of information (10). These algorithms are essential for the realization of the “Phenomena-based simulation” approach described in the next section.

Simulations for the SOFC system phenomena-based simulation. We propose a “phenomena-based simulation” approach as an effective means to realize predictive analysis of failures. In conventional simulations based on identifying the ability of a design to meet a certain function requirement, the model designer must decide what phenomena will be taken into consideration in the model of the target system. Generally, the designer does this by judging the importance of each phenomenon on the system characteristics based on the knowledge that is available. Therefore, a phenomenon that might be found later to lead to failures of the designed item during the benchmark testing phase will not be considered in the design process if the designer is not familiar with the phenomenon, even if it is well known in some other field of study. Consequently, remediation measures must be taken after the costly benchmarking phase rather than during the rather inexpensive and flexible research and development design phase.
A phenomena-based simulation approach could be effective for identifying and preventing failures that result from phenomena not known to the designer during the design phase, alleviating the problem described above in the conventional design process. In the phenomena-based approach, the designer defines only the specifications of the target system. A computer system based on software agent technology (described below) would use the design specifications to discover what phenomena might occur that could lead to failure. The agent-based computer system does this discovery process by accessing expert knowledge and simulation models available to the software system agents (Figure 3). Using agents that can find information on the Internet enables the system to access knowledge and simulation models published on the World Wide Web (11). To handle information on the design specifications more dynamically and flexibly, objects representing the structure and fluid entities described above are automatically instantiated based on design specifications in the markup language.

**Figure 3. Concept of phenomena-based simulation.**

An agent is a software entity or object that has specific goals such as searching for a simulation model that solves a particular phenomenon or contacting a related agent, and can work proactively toward achieving those goals. The agent system for our collaboration platform, in which various agents with respective goals act to achieve those goals by communicating each other, works as follows.

1. An agent that manages the design specification of the SOFC that is being studied finds some spatial or temporal condition in the design, for example, a connection between the cathode gas and the cathode, and judges that some phenomenon might occur there.
2. That agent then sends a request for simulation models that could identify what kind of phenomena might occur and that have the ability to simulate those phenomena.

3. The request is received by specialized search agents that have the ability to find simulation models meeting search criteria as expressed in the initiating agent's request. The search agents do this by comparing the search criteria with metadata provided by agents that manage the simulation models and determining the degree to which the simulation model is appropriate for answering the initiating agent's request.

4. Once an appropriate simulation model is identified and selected for consideration, the necessary input information is obtained from the objects representing the structure and fluid entities, and the simulation is performed.

We succeeded in validating the basic mechanism for the agent system described above using simple models that simulate 1) heat transfer between fluid and solid entities, 2) mass transfer between fluid entities, and 3) heat transfer between solid entities. To realize a more complete phenomena-based simulation system, we are developing a set of metadata tags for enabling identification of the most appropriate simulation models for modeling the particular conditions described by the requesting agent.

**SOFC characteristics simulation.** Although the phenomena-based simulation approach we describe should be effective for identifying possible failures at the design phase, such an approach for studying the market effectiveness of SOFC systems is unlikely to be possible in the foreseeable future. Therefore, we describe here a framework for a more conventional simulation approach that evaluates the effectiveness of a particular SOFC design at penetrating the market for energy systems in a particular social system. This framework will be used in parallel with the phenomenon-based simulation approach described in the previous section.

![Figure 4. Schematic diagram of framework to evaluate SOFC penetration.](image)

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Figure 4 shows a schematic diagram of the market penetration evaluation framework. The framework we propose integrates a power generation mix model and a building energy simulation model with the models and databases in the “regional information” domain. The power generation mix model is a combination of a centralized power system planning and dispatch optimization tool, which optimizes the mix of electricity generation technologies for the power grid of the studied region (12). This power generation mix model makes it possible to evaluate the effectiveness of introducing different combinations of centralized power sources such as a combined cycle of SOFC, gas turbine, and steam turbine (SOFC/GT/ST system), or an integrated coal gasification fuel cell combined cycle system (IGFC).

We use “EnergyPlus,” a building energy simulation software developed by the U.S. Department of Energy (13), to simulate the energy demand in the buildings. EnergyPlus generates hourly profiles of electricity, cooling, and heating demand in the building over the entire year given the building heating and cooling plant configuration, regional weather conditions, building shell configurations, and building use schedules. These results can be used for evaluating the performance of decentralized power sources, such as a system combining a small scale SOFC with a micro gas turbine. Furthermore, the power generation mix model can be used in combination with EnergyPlus to investigate how the introduction of building-scale decentralized systems affects the power generation mix of the grid. To aggregate the results from simulating the energy demands of a single building over all of the buildings in the region investigated, we obtained information on the total numbers of each type and size of the buildings in the region from the GIS database provided in the regional information domain described earlier. Information on the material requirements for implementing the centralized and decentralized SOFC-based energy systems is sent to the LCA domain to evaluate the environmental impacts.

Scenario-Based Life-Cycle Assessment

The environmental aspects of a scenario are key issues to be assessed in this collaboration platform. However, we cannot predict the future market and social situation with sufficient detail to make a full environmental assessment. Life-cycle assessment (LCA) is a tool that measures the potential impacts associated with a unit amount of product or service that occurs over the entire life cycle of the product or service providing entity. Several LCAs of SOFCs can be found in the literature (3, 14, 15).

Fukushima and Hirao (5) proposed a new framework of scenario-based life-cycle assessment that integrates LCA with scenario development. In this framework, a systems approach is taken. In conventional LCAs, comparisons between the environmental impacts allocated to two different products can be made only if both product life-cycle assessments are conducted with the same boundaries. In the scenario-based LCA framework, parameters in a virtual systems model, termed life-cycle model, are changed and the inputs and outputs to the overall system boundaries are assessed through life-cycle impact assessment (LCIA) methodologies. A life-cycle model is virtual in the sense that it includes all of the options to be considered, even options that are currently not available. Therefore, the structure of the life-cycle model does not need to be changed when developing a new scenario. Figure 5 shows a life-cycle model with two life-cycle alternatives. Boxes show processes, and arrows labeled f1-10 indicate flows. Parameters such as the efficiency of a process, the recycling rate, and the flow rate of a substance are changed, and the flows that
are connected to external systems, i.e., f1, f4, f5, f7, f8, f10, are evaluated. Each process can be modeled using a linear or a nonlinear unit model. Stocks of substances can also be expressed. Selection of the boundaries should be consistent with the principle of LCA, i.e., the boundaries should be broad enough that changes outside the boundaries are essentially linear.

![Figure 5. Life-cycle model and systems boundary with two options.](image)

Scenarios are expressed using time series of scenario parameters and fixed parameters. Scenario parameters are parameters that are to be changed during the scenario analysis, while the fixed parameters express the background assumptions that are not changed. The parameter time series sets are combined with a life-cycle model for the complete scenario analysis. A given life-cycle model can be reused for different scenarios that assess different options.

The parameter time series can be obtained from the output of other models in addition to user-specified assumptions and predictions. The scenario-based LCA framework itself does not provide any assumptions and predictions. To assess scenarios for the market penetration of SOFC systems, we combine the scenario-based LCA models with the other models and databases in other domains shown in Figure 1.

**Failure Prevention by Predictive Analysis**

As described above, the conventional model-based design approach can only quantify those behaviors that have already been decided qualitatively when the designer selected the models. For example, the behaviors of designed objects are often predicted by connecting a CAD (Computer-Aided Design) system with other simulation software tools. However, because the designers only include those simulation software tools with which they are familiar, only the phenomena that are well known in the designer’s particular field of expertise can be investigated using this approach.

The design of fuel cell systems requires knowledge from multiple disciplines such as mass and heat transport, fluids, materials, chemical reactions, electrochemistry, and thermodynamics in addition to the basic understanding of fuel cells. Furthermore, there are many options for cell and stack configurations, component materials, system capacity, and
use of exhaust heat that must be considered at the same time. Because fuel cells are a rapidly emerging technology, centralized repositories of fuel-cell design-related knowledge are rare. Therefore, fuel cell designers must acquire and use widely diverse knowledge of the behaviors and failure mechanisms that result from various different design specifications. We aim to construct a support system that helps designers to determine what behaviors and failures should be prevented with no omission.

Model-based failure diagnosis using qualitative physical analyses has been studied as a means for predicting and diagnosing a failure mechanism in a studied artifact or system. This method attempts to infer a potential failure mechanism and possibly the physical phenomena that cause the failure as well. The method uses "object models" to represent the components, functions, and design parameters of the relevant product together with a knowledge base of fault phenomena (16, 17).

The new phenomena-based simulation design approach described earlier can help designers access knowledge that is not available to them locally to forecast and prevent design failures, thereby providing a low-cost alternative to the cost-intensive and time-consuming benchmark testing processes that are conventionally used to obtain empirical knowledge on SOFC design failures. We propose a new design approach where the agent system described in the previous section searches the Internet to discover what phenomena might happen (Figure 6). As explained earlier, software agents in the simulation system are given information on design specifications and operating conditions for the SOFC system to be evaluated, and they use that information to find knowledge of chemical and physical phenomena in the form of simulation models and databases.

![Figure 6. Design process for failure prevention by predictive analysis.](image-url)
To realize this predictive analysis approach for failure prevention, we leverage some of the concepts and methods relating to failure prevention and design quality control. In general, FMEA (Failure Mode and Effect Analyses), FTA (Fault Tree Analysis), Design Review, and statistical methods are commonly used for failure prevention. However, we must construct a process of thinking that is optimized for the fuel cell designs. This process will enable designers to predict and prevent failures. The capability of the process to predict and prevent failures depends fundamentally on the quality of failure knowledge accumulation and the effectiveness of utilization of that knowledge, independent of the actual failure prevention method used. We base our method on the Stress-Strength Model proposed by Tamura (18). The Stress-Strength Model is a knowledge structure that enables designers/engineers to cyclopaedically predict possible failures that may occur in designed items through representation of generalized, structured, and modularized knowledge on failure mechanisms.

To predict and prevent potential failures with the model, we must address the following.

1) Deployment of the functions and configurations of SOFCs to express a design for an SOFC as an object model that can be used for prediction of a complex causal chain of failure mechanisms.
2) A method for using the object model described above to extract attributes relating to the occurrence of failure in the designed SOFC.
3) Accumulation of knowledge on failures relating to various design specifications and attributes of an SOFC such as materials, assembly, shapes, and so on.
4) A method for combining fragmented knowledge of physical and chemical phenomena, behaviors, and failures to discover new failure mechanisms in an object design that have not been previously experienced.

The following is an example of how the phenomena-based simulation design approach could aid the design process of an SOFC system. A system designer who wants to assess the feasibility of a particular design for an SOFC system would query the phenomena-based simulation design agent system to find out what would happen in the designed item. For a design for an SOFC system operating at 1000°C, the agent system might identify on the Internet examples of failures that would occur as a result of thermal phenomena and suggest to the designer that a design for lower-temperature operation might be an effective measure to prevent these potential failures. The designer might then test the cathode material, La0.6Sr0.4CoO3-δ (LCS), which has high activity even at low temperatures (19). The agent system would then contact other agents maintaining knowledge bases and simulation models to find information on the use of LCS in the proposed design. Other agents may respond with information on a phenomenon whereby LCS reacts with the electrolyte, YSZ. The agent system would conclude that this would result in the formation of an insulation layer and notify the designer of this potential failure mechanism (20). Based on the problem identified between YSZ and LCS, the designer may test Ce0.8Sm0.2O2-δ (SDC) as an electrolyte. The agent system would consult the simulation model agent that had provided the information on the formation of the insulation layer with YSZ and find that SDC is not reactive with LCS, so no insulation layer is formed. However, the agent system might also find phenomena-based knowledge indicating that SDC is partially reduced on the anode side, leading to expansion of the electrolyte volume and cell breakdown (21). A search on the Internet for expertise related to prevention of this effect might find a suggestion to deposit a very thin layer of YSZ on...
the anode side (22). This expertise could include knowledge that using SDC also avoids an existing problem of cathode performance degradation caused by the evaporation of Cr species in the interconnect material into the cathode (23).

CONCLUSIONS

A scheme for a collaboration platform for supporting comprehensive design and evaluation at the research and development phase of SOFCs is proposed. The proposed platform enables users to 1) evaluate the cell, stack, and system characteristics of the SOFC, 2) evaluate the manufacturing process of the SOFC, 3) evaluate the inter-industrial commodity flow changes induced by the introduction of the SOFC and its related industries, 4) predictively analyze the potential failures from the design specifications and identify failure prevention measures, and 5) forecast long-term future changes in social systems resulting from the large-scale introduction of SOFC energy systems. Six domains were prepared in the platform to achieve these tasks. Basic concepts and mechanisms for design specification, simulations, life cycle assessment, and failure analysis domains were presented. Our platform will promote interdisciplinary collaborations among researchers that support holistic evaluations of SOFC systems in a structured manner.

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