



Feasibility study for SOFC-GT hybrid locomotive power: Part I. Development of a dynamic 3.5 MW SOFC-GT FORTRAN model

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ARTICLE INFO

Article history:

Received 21 January 2012

Received in revised form

10 April 2012

Accepted 12 April 2012

Available online 22 April 2012

Keywords:

SOFC-GT

Locomotive

Diesel

Feasibility

Dynamic Simulation

Cascade Control

ABSTRACT

This work presents the development of a dynamic SOFC-GT hybrid system model applied to a long-haul freight locomotive in operation. Given the expectations of the rail industry, the model is used to develop a preliminary analysis of the proposed system's operational capability on conventional diesel fuel as well as natural gas and hydrogen as potential fuels in the future. It is found that operation of the system on all three of these fuels is feasible with favorable efficiencies and reasonable dynamic response. The use of diesel fuel reformat in the SOFC presents a challenge to the electrochemistry, especially as it relates to control and optimization of the fuel utilization in the anode compartment. This is found to arise from the large amount of carbon monoxide in diesel reformat that is fed to the fuel cell, limiting the maximum fuel utilization possible. This presents an opportunity for further investigations into carbon monoxide electrochemical oxidation and/or system integration studies where the efficiency of the fuel reformer can be balanced against the needs of the SOFC.

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1. Introduction

Long-haul locomotive transportation is one of the most prevalent methods of shipping goods in the United States. An exploratory committee formed in 2002 at the Center for Transportation Research at Argonne National Laboratory, under the guidance of the U.S. Department of Energy, reported that in 1997, 4 billion gallons of diesel fuel were consumed by locomotives in the United States. This amount represents 10% of all diesel used for transportation and 2.3% of all transportation fuels. For the rail operators, this represents an annual cost of \$2 billion, contributing 7% of their total operating expenses [1]. Today, the situation is not much different, as the consumption of petroleum in freight rail represented 2.1% of the total national transportation fuel use in 2005, thereby consuming 571.4 trillion BTUs of fuel [2]. Thus, fuel use for long-haul locomotives is continually of economic interest to both government and industry, and represents a field with much potential for increasing energy independence.

In addition to these motivating factors, the use of diesel fuel in railway applications presents a significant environmental concern. Although the nationally averaged emission signature of locomotives

nationwide appears low (in 2001, locomotive-sourced NO_x was only 5% of the national total), locomotives are responsible for much of the emissions, especially diesel PM, in the areas where they are stationary [1]. At classification railyards, locomotives are responsible for 96% of PM emissions; at intermodal railyards, the contribution is 39% [3]. The general public living near these stationary rail operations is most affected by these emissions, and improvements in locomotive emission signatures can enhance the air quality for this subset of the population. Moreover, in California, rail operations tend to be centered in areas that have difficulty achieving air quality standards due to high source concentration and stagnating meteorological conditions; thus, the additional burden is placed on those living in areas already known to have poor air quality. Current estimates attribute 2980 premature deaths, 5100 cases of acute bronchitis, 62,000 cases of asthma and other respiratory problems, and 830 heart-related hospital admissions per year to goods movement in the Southern California Air Basin [4]. Similar to passenger vehicles and diesel freight trucks, locomotives have thus been assigned a progressively limiting tier-based schedule of emissions standards. This Tier system requires substantial ongoing reductions in the emission of NO_x , CO, hydrocarbons, smoke, and particulates [5].

Satisfying the ever-evolving Tier standards may require investigation of technology beyond the conventional combustion reciprocating engine. Early investment in emerging technologies, such as Solid Oxide Fuel Cells (SOFC), may provide more options

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and enable development of systems with greater environmental benefit. The fuel cell has already been identified as having the capability to replace the entire diesel and electric power system for a locomotive, simply based on economic and performance concerns [1]. Moreover, the proven high efficiency and low emissions signature [6,7] of SOFC-based systems, for both criteria pollutants and greenhouse gases like CO₂, present a compelling opportunity for vast improvement in the overall economic, environmental, and health impacts of freight railroading.

In spite of the fact that fuel cells in general have been considered in the literature for the freight locomotive application, very little work has been presented for the use of the solid oxide fuel cell in particular. Most theoretical studies and the only major demonstration project to-date have focused on utilizing low-temperature proton exchange membrane (PEM) fuel cells [8–14]. Systems assuming on-board power, off-board power with electrified line, and hybridization with large auxiliary battery storage have been investigated [9,11–14]. The last of these is the subject of a substantial demonstration project in the United States as part of a collaborative effort between the Burlington Northern Santa Fe Railway System and Vehicle Projects, LLC [15–17].

Although the PEM systems have shown promise, their operation requires a hydrogen infrastructure, a constraint that may be too limiting at the moment for widespread adoption and which the SOFC can avoid thanks to its fuel-flexible operation. Additionally, the SOFC can be hybridized with a gas turbine (termed an SOFC-GT), allowing for a number of synergistic benefits. Such a system has been shown to potentially operate at efficiencies above 60%, produce virtually zero levels of criteria pollutants, and operate with low noise levels due to the small number of moving parts. The ability to accomplish all of these and operate on the currently used diesel fuel is a capability that is unique to the combination of high-temperature fuel cell with gas turbine.

Since the introduction of the SOFC-GT concept, there has been significant advancement in understanding prototypical systems through work simulating the performance of various designs and exploring detailed considerations such as system integration, control optimization, and drivers and challenges in the expected dynamic response [18–27]. In addition, the available literature is rich with a variety of study methodologies and system design options to develop in-depth understanding of key system-wide dynamic interactions and component limitations as well as identification of preferred system designs. Finally, the SOFC-GT research community has also been able to demonstrate the potential of these systems to be flexible in application, through analyses of systems applied to such varied goals as grid stabilization, Integrated Coal Gasification-Fuel Cell plants, and Distributed Energy Resources [28–30].

However, these prior research works are all based on the designs of SOFC-GT systems for stationary power. With its high fuel-to-electric conversion efficiency, the SOFC-GT is an ideal candidate for stationary power applications, especially large-scale and centralized power. This feature is also attractive in the locomotive application, since the wheels are run by electric traction motors. Still, the combination of the SOFC-GT with this mobile platform has yet to make an appearance in the literature. Mobile SOFC-GT systems have been proposed by Winkler and Lorenz, but for the smaller passenger vehicle platform [31]. There is also some available literature regarding the application of SOFC-GT systems for marine applications [32,33]. As of the time of this publication, there does not seem to be any investigation of the potential for the SOFC-GT hybrid system for the locomotive application.

Significant capital investment in new fueling infrastructure required by PEM solutions can be avoided by taking advantage of the SOFC-GT fuel flexibility. This study has adopted a scenario in

which diesel fuel is the near-term choice, followed by natural gas as a bridging fuel, and finally hydrogen as an end-goal fuel in the future. It is assumed that the two fossil fuels are pre-reformed off board from the locomotive. Thus, this work analyzes the performance of the system when operated on a diesel autothermal reformate, a natural gas steam methane reformate, and humidified hydrogen. Possibilities for on-board reformation will be the subject of future work.

To develop the model, this work builds upon the foundation laid out by the previous studies and aims to provide insight into the unique issues of the SOFC-GT in a large mobile platform. The major issues include the need for fuel processing to accommodate diesel fuel use and the prediction of SOFC degradation due to coke development in the anode. For this reason, the current investigation develops a model of an SOFC-GT system that operates on hydrogen or fuel reformates, but is flexible enough to later incorporate the requirements of the reformer and the undesired but prevalent effects of coking reactions. Because these chemical processes are often complex and include reactions on vastly different timescales, the model was developed with flexible control over numerical algorithms specifically designed for the solution of stiff ODEs in concert with simulation of the remaining pertinent physics in the fuel cell.

Therefore, a novel model framework was developed and implemented in FORTRAN, which leaves open the possibility of incorporation of various numerical schemes for reaction chemistry necessary for investigating the dependency of system performance on fuel choice. In addition, since future versions of the model are projected to incorporate a voltage loss mechanism based on the simulation of coking deposition within the fuel cell, the method of convergence for the current-voltage relationship has been designed to accommodate for more than just the traditional loss mechanisms, which often allows for simplifications in the SOFC model development. This paper presents the development of this model and insights into steady-state fuel dependence.

2. Modeling methodology

2.1. Global solution method

The FORTRAN model developed in this work consisted of a set of modular subsystems based on the analysis of each major component in the system. Each subsystem required iteration to convergence within itself, and in some cases required repeated convergence iteration among subsystems. The schematic of the system modeled in this work is as shown in Fig. 1. It is a simplified model of the extensive system expected to be required of an SOFC-GT powering a locomotive and includes the major components and features required in this application. Namely, the system includes direct linking between the SOFC and gas turbine units, includes an auxiliary combustor before the turbine, includes an air preheater supported by system waste heat, and includes cathode recycle to aid SOFC thermal management. Some balance of plant components are not accounted for in this model (such as fuel pumps, a fuel preheater, and any necessary fuel processing equipment); thus, the performance found in this investigation will be slightly improved compared to a more detailed system model. It is expected that this simplification still provides a reasonable expectation of the system's capabilities.

The overall system model is divided into four major subsystems: the SOFC subsystem, the gas turbine subsystem, the air preheater subsystem, and the controller. The first three of these are closely tied via fluid streams passing through all of these subsystems. Thus, convergence within each subsystem must be matched by global convergence of values shared between subsystems. In order to

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