MULTI-SCALE MODELING FOR OPTIMAL DESIGN, OPERATION AND INTEGRATION OF POWER GENERATION AND STORAGE SYSTEMS

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Abstract

The demand for energy is expected to increase for the foreseeable future as the human population increases, the average standard of living improves, and electronics and automation find more applications in our daily life. While fossil energy resources are greatly in demand, sustainability concerns have motivated energy generation from renewable and reusable energy resources, and the use of more efficient energy-converting and energy-consuming systems. Consequently, for the past decade there have been major advances in harvesting energy from renewable and reusable resources and in improving the efficiency of energy-consuming and energy-converting systems. This paper focuses on these advances in renewable power generation and storage systems, highlighting how multi-scale first-principles mathematical modeling can contribute to systematic optimal design, operation, and integration of these systems. It puts in perspective how multiscale mathematical modeling has contributed to advances in solar cells, fuel cells, flow batteries and rechargeable batteries, and in the integration of these systems with power grids.

Keywords

Mathematical modeling, Power generation, Power storage, Renewable energy, Dye sensitized solar cell

Introduction

The growing demand for energy is driven mainly by population and income growth. By 2030, the world population is projected to reach 8.3 billion (vs. 7.3 billion in July 2016), implying that an additional one billion energy consumers will be created. Concurrently, world total income in 2030 is expected to be roughly 100% higher than the 2011 level. These changes translate into a 2030 world primary energy consumption estimate that is 36% higher than the 2011 level (BP Energy Outlook 2030, 2013).

This increasing demand for energy and growing awareness of the sustainability drawbacks of using fossil fuels (Daoutidis et al., 2016) have created a lot of interest in energy generation from renewable and reusable energy resources, and in the use of more efficient energy-converting and energy-consuming systems. As discussed by Smalley (2005), the world's energy needs can be completely met sustainably (the "terawatt challenge") by having six 100 km by 100 km solar generation areas at 10% conversion efficiency in strategic locations around the earth.

However, because of the highly intermittent nature of renewable energy resources (such as sunlight and wind), the integration of these power generating systems into utility power grids leads to degradation of power quality, unless compensating power storage systems are used. To supply power continuously using renewable energy systems, these systems must be integrated with energy storage systems. Thus, the problem of efficiently and practically harvesting energy from renewable resources is not separable from that of efficiently storing it.

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This paper focuses on renewable power generation and storage systems, and how first-principles (FP) mathematical modeling can contribute to systematic optimal design, operation and integration of these systems. It puts in perspective how mathematical modeling has contributed to advances in solar cells, fuel cells, flow batteries and rechargeable batteries, and in the integration of these systems with power grids.

Power Generation

In 2014, globally a total of 22,433 TWh power (electricity) was produced from coal (38.9%), gases (22%), hydroelectric (16.8%), nuclear (10.8%), petroleum (4.8%), and others (6.7%) [Figure 1]. The other sources include biomass and waste (2%), geothermal (0.9%), solar/tide/wave (0.7%), and wind (3.1%). In same year, the U.S. Energy Information Administration (EIA) reported a net U.S. electrical power generation of 4,094 TWh power, which was produced from coal (38.6% vs. 33.2% in 2015), gases (27.8% vs. 33.0% in 2015), nuclear (19.5% vs. 19.5% in 2015), hydroelectric (6.3% vs. 6.1% in 2015), renewables excluding hydroelectric and solar (6.4% vs. 6.7% in 2015), solar (0.4% vs. 0.7% in 2015), petroleum liquids and coke (0.7% vs. 0.7% in 2015), and other (0.3% vs. 0.3% in 2015). Figure 2 highlights how U.S. electricity from renewables has grown from 2006 to 2016. The percent of power produced from renewable resources globally and in the U.S. in 2014 was 23.5% and 13.1%, respectively. Figure 3 shows the past and forecasted trends in world electricity generation by source; it shows that world energy generation from renewable resources is expected to more than double from 2012 to 2040 and be about 29% of total electricity generation in 2040.

While renewable power resources are very attractive from a sustainability point of view, in terms of power grid management, most renewable sources are classified as anti-dispatchable; that is, their power output levels change with time and the grid operator usually has no (or very little) influence over these changes. Thus, they put additional burden on both power and energy management. To be able to compensate for the highly intermittent nature of these energy sources, renewable energy systems should be integrated with other power generation and/or power storage systems.

Photovoltaics

Solar cells are very attractive, as they generate power from sunlight, which is freely available everywhere, making them suitable for local power generation in remote areas. While silicon-based solar cells are still the commercially-dominant photovoltaic technology, new technologies using nanocrystalline materials and conducting polymer films have attracted considerable attention due to their potential lower cost and higher flexibility (Grätzel, 2009; Kojima et al., 2009). Current solar cells are based on organo-metallic perovskites, polymers, oxides nanoparticles sensitized with dye, thin films, quantum dots, extremely thin absorbers, and silicon. Present challenges center around additional cost reduction, enhancement of minority carrier lifetimes, improved photon absorption, greater charge mobility, and ultimately improved efficiency.

One of the most promising photovoltaic technology is perovskite solar cells, which have high light-absorption coefficients with tunable band gaps, high charge carrier mobilities, and very long minority-carrier lifetime leading to long charge diffusion lengths. While the conversion efficiency of perovskite solar cells was just 3.8% in 2009 (Kojima et al., 2009), the efficiency is currently 22.1%. This rapid improvement has led to unanswered questions such as how cell materials operate, how further improvements can

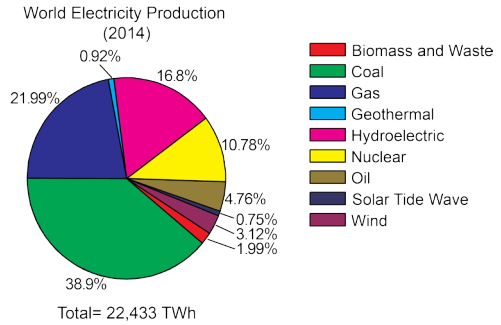

Figure 1: World electricity production from all energy sources in 2014. www.tsWp-data-portal.org

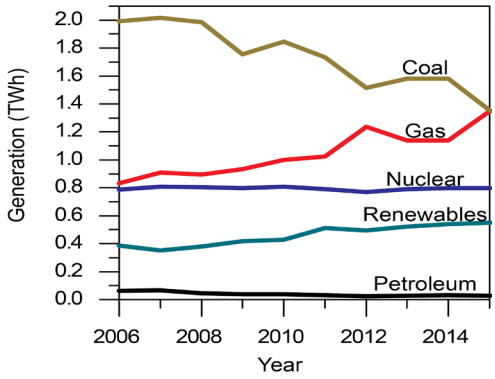

Figure 2: U.S. electricity generation from major energy sources. (U.S. EIA)

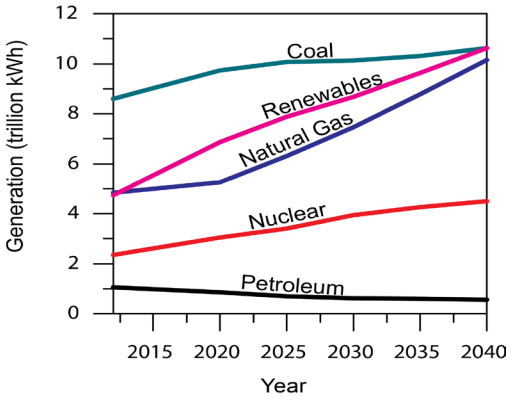

Figure 3: World electricity generation from major energy sources. (U.S. EIA)

be made, and how stability, current-voltage (I-V) hysteresis and chemical degradation due to moisture can be overcome.

Different modeling approaches including FP modeling and equivalent circuit modeling have been used to predict the solar cell behavior. Because of the nonlinear dependence of cell I-V behavior on temperature and irradiance level, nonlinear FP models are needed to predict the cell behavior accurately.

FP electronic-level modeling [density functional theory (DFT)] has provided a better understanding of perovskite solar cells. DFT studies have predicted key solar parameters such as the absorption spectra and bandgap with good accuracy and provided insight into the structural, physical, chemical and electronic properties of these materials (Mosconi et al., 2013; Brivio et al., 2013; Frost et al., 2014).

FP macroscopic models of solar cells are based on macroscopic conservation equations (Bavarian et al., 2014; Smolin et al., 2015). They can predict cell power, I-V behavior, how process parameters (such as the electron diffusion coefficient and the recombination rate constant) influence I-V performance, and how the temporal and spatial variations of charge density and other species concentrations vary within a cell. They can be used to describe cell module characteristics, orientation and geometric characteristics, array-level characteristics, power conditioning unit level characteristics, plant-level characteristics, operations and maintenance characteristics, and so on.

Macroscopic FP modeling of traditional liquid-electrolyte and polymer-electrolyte dye sensitized solar cells (DSSCs) has been studied (Bavarian et al., 2014; Smolin et al., 2015). Combined with experiments, these models provided a better understanding of the processes that occur within DSSCs and helped determine how process parameters affect cell performance (Bavarian et al. 2014). The effects of polymer chemistry and pendant groups on polymer-electrolyte DSSC performance have been studied via modeling (Smolin et al., 2015), leading to the determination of three unique ways that polymer chemistry affects the interfacial DSSC processes and a better understanding of how to improve cell efficiency (Smolin et al., 2015). Also, Wang et al. (2014) developed an FP DSSC model to gain an improved understanding of charge transport via the redox couple in a liquid electrolyte, and theoretically calculated a critical thickness of the TiO_2 electrode for optimal performance.

In addition, macroscopic and microscopic DSSC models have been developed (Andrade et al., 2011; Gagliardi et al., 2011; Nelson, 1999). Also, there have been electronic-level DSSC modeling based on DFT and time-dependent DFT (TD-DFT) (Le Bahers et al., 2011; Labat et al., 2012; Pastore and De Angelis, 2013; De Angelis, 2014). These models have been used to capture snapshots of single processes such as charge injection. Electronic- and molecular-level models have provided a better understanding of the adsorption of novel dyes onto anatase

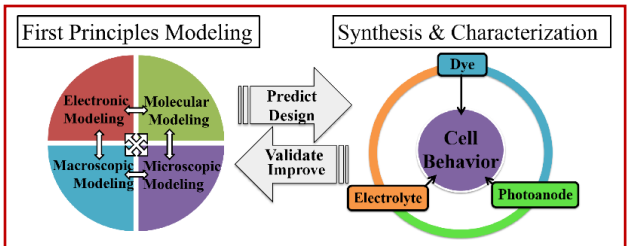

Figure 4: Multiscale modeling of DSSCs and its interaction with cell fabrication and characterization.

TiO_2 and the effects of additives on the conduction band edge of TiO_2, and have predicted optical and electronic properties of novel dyes in liquid-electrolyte DSSCs (Labat et al., 2012; De Angelis, 2014).

Currently, in the area of DSSCs there is a need for a better understanding of how polymer-electrolyte chemistry affects the cell performance; e.g., understanding the interdependences and synergetic effects among DSSC components and processes, which occur at different length and time scales. FP multi-scale modeling (Figure 4) can improve this understanding. It can advance fundamental understanding of materials across length and time scales to elucidate the effects of microstructures and surfaces on the cell performance, predict materials properties and overall cell performance, and provide an understanding of inaccessible but critical interfacial processes that control DSSC performance.

For every type of solar cell, high conversion efficiency is essential for large-scale deployment. Model-based optimization of solar cells allows for calculating the cell optimal design parameters at different irradiances and optimal cell operation conditions, and to find optimal cell integration (with other energy generation and storage systems) conditions and configurations.

Concentrating Solar Power

Concentrating solar power (CSP) technologies use mirrors to reflect and concentrate sunlight onto receivers that collect and convert solar energy to thermal energy. The thermal energy can then be used to produce electricity via a turbine or heat engine driving a generator. As these technologies collect solar energy and convert the energy to thermal energy that can be stored easily, they can provide electricity on demand at an affordable price, even when there is no sunlight. They can also be installed as fossil-fuel backup/hybridization units that allow existing fossil fuel plants to operate cleaner at the same or a lower cost.

CSP technologies have allowed for reducing the cost of solar energy (U.S. DOE SunShot Initiative, 2015), making large-scale dispatchable solar energy systems cost competitive. Indeed, they have already reduced the cost of CSP-generated electricity by about 36%, from 21 ¢/kwh to 13 ¢/kwh, towards achieving the U.S. DOE goal of 6 ¢/kwh.

Mathematical models of the processes involved in the CSP technologies have applications in designing and optimizing each process unit, and optimal integration and operation of these units.

Fuel Cells

A fuel cell converts the chemical potential energy of a fuel to electricity. Fuel cells have been named based on their electrolyte type, which sets their operating temperature range. Commercially-available fuel cells include polyelectrolyte membrane fuel cells (PEMFCs), solid oxide fuel cells (SOFCs), phosphoric acid fuel cells, and molten carbonate fuel cells. Their primary components are an ion-conducting electrolyte, an anode, and a cathode. For brevity, here we limit our focus to SOFCs.

FP macroscopic modeling has been used to study steady-state and dynamic behavior of fuel cells, design the cells, investigate control strategies, and design experiments (Bavarian et al., 2010). Current challenges are to reduce cost by primarily reducing and/or replacing the use of Pt, improve catalytic activity in both the anode and cathode, and make the systems more robust.

A SOFC (or a PEMFC) can have one (stable), three (two stable and one unstable) or five (three stable and two unstable) steady states depending on the operating conditions (Bavarian et al., 2010). Steady-state multiplicity leads to hot spots in SOFCs and wet spots in PEMFCs that are of critical importance in the operation of the cells. Using macroscopic models, the presence of steady-state multiplicity in proton-conducting and co-ionic conducting SOFCs has been shown (Bavarian and Soroush, 2012; Bavarian et al., 2013). The multiplicity is due to the exponential dependence of the electrolyte ion-conductivity on temperature and a positive feedback between temperature and the rate of heat generation in the cells.

The type and level of details included in a mathematical model of a fuel cell depend on the application of the model. For real-time applications, the model equations should be solvable in real-time. In fuel cell modeling the art is not to include every complexity but to include enough details to predict the variables of interest accurately enough. Accounting for every complexity in fuel cell modeling leads to the development of very complex, multi-time-scale, multi-dimensional models that are computationally expensive to solve (Bavarian et al., 2010).

Fuel cells are inherently multi-time-scale nonlinear systems. The multi-time-scale nature is a consequence of the involvement of processes with significantly different response times (Bavarian et al., 2010). Electronic components of a fuel cell have the fastest responses, while the thermal processes in a fuel cell usually have the slowest responses. The existence of the significantly different time constants, e.g., from 1 *ms* to 10,000 *s*, in a fuel cell makes the governing dynamic equations very stiff. However, it allows one to simplify the models systematically based on the time scale of interest (Bavarian et al., 2010).

Fuel cell optimization is conducted to obtain optimal operating conditions and design specifications, especially when these systems are integrated with fuel processing systems and/or are used together with other power generating and storage systems. The design of fuel cells is a challenging task due to several physical phenomena that should be optimized simultaneously to achieve efficient fuel cell operation. Fuel cell design is a multi-objective, multi-variable problem. More details can be found in (Soroush and Chmielewski, 2013).

Power Storage

Energy storage systems are typically categorized into two groups in terms of their use in power and energy management. Those used in power management include rechargeable batteries, flywheels, flow batteries, and capacitors, and those used in energy management include pumped hydro storage, compressed air energy storage, and thermal energy storage. We discuss only rechargeable batteries and flow batteries herein. A survey of other storage systems can be found in (Soroush and Chmielewski, 2013).

Rechargeable Batteries

A battery has one or more electrochemical cells. Each cell has an electrolyte, a positive electrode (anode), and a negative electrode (cathode). The key process in a rechargeable battery is a reversible electrochemical reaction that collect electrons in one direction and release electrons in the other direction. Rechargeable batteries respond very rapidly to load changes and usually have very low standby losses and high energy efficiency (60–95%). They have a short lead time, are able to withstand sitting, and are modular (Soroush and Chmielewski, 2013). However, they have small power capacity, low energy densities, high maintenance costs, a short cycle life, and a limited discharge capability. The most common battery systems are lead acid, lithium ion, nickel cadmium, sodium sulfur, sodium nickel chloride, and flow batteries such as vanadium redox and zinc bromine batteries (flow batteries are dealt with in a separate section in this article).

Li-ion batteries are currently the most common type of energy storage in consumer electrons and have been widely studied. They have potential applications in the transportation sector (such as electric vehicles) and in load leveling of the power grid, which is critical because of intermittent nature of renewable power sources such as wind and solar. Major current challenges for Li-ion batteries are how to improve power density and cycle life.

Within a Li-ion battery, multiple processes occur over different time and length scales, such as charge transfer, charge carrier and mass transport within the bulk of material, across interfaces, as well as structural changes and phase transformation induced by concentration change of Li (Meng and Arroyo-de Dompablo, 2009).

Rechargeable battery models range from nonlinear and coupled PDEs to simple linear ODEs. Initial models were chemical models. Control researchers then focused on equivalent-circuit models coupled with simple chemical rate equations. FP modeling and reducing the order and complexity of the models to make them suitable for real-time applications have received a lot of attention (Soroush and Chmielewski, 2013). FP models have been used to

better understand materials behavior. Efforts are currently being made to accelerate material discovery to design new compounds *in silico* using FP calculations (Hautier et al., 2012). Ceder et al. (1998) predicted, via DFT, new electrode compositions in which replacement of the transition metal, M, in layered $LiMO_2$ with Al (Al-doping) would improve voltage. FP models have also been used to understand the rate capabilities, capacity, cycle stability, intercalation voltage, electronic structure, electronic conductivity (power and rate), lithium diffusion, thermal stability, and safety of Li-ion systems (Maxisch et al. 2006; Meng and Arroyo-de Dompablo, 2009). DFT studies of the rate capabilities commonly focus on the activation barriers for Li motion to design materials with better performance.

Macroscopic FP models have also been developed for Li-ion batteries to simulate the electrochemical and thermal behavior of the batteries (Botte et al., 2000). Micro-macroscopic models that incorporate solid-state physics of the electrode material, and interfacial morphology and chemistry have also been developed (Gu et al., 1998). These models can predict the average cell temperature, the temperature distribution inside a cell, and the effects of the environment on battery electrochemical and thermal behavior (Gu and Wang, 2000). Multiscale modeling which models batteries at the pore-level, cell level, and the stack level provide a comprehensive picture of such systems (Wang and Srinivasan, 2002).

An application of battery models is in the estimation of the state of charge and the state of health of batteries from their external voltage and current. The real-time model-based estimation has motivated studies to carefully reduce the order and complexity of FP models and to develop computationally-efficient estimation methods. Another application is in the development of optimal battery-charging policies that minimize battery ageing.

Flow Batteries

A flow battery is a type of rechargeable battery that has a high power storage capacity. It typically has two chemical components dissolved in liquids (electrolytes) and most commonly separated by a membrane, which provides the rechargeability. Electrolytes are regenerated and stored externally in tanks. Various electrolytes such as vanadium redox, uranium redox, zinc bromine, zinc cerium, and polysulfide bromide have been used. Flow batteries have a storage period ranging from seconds to hours, a cycle efficiency of 75 to 85%, and a time-response (from zero to full power) in the order of seconds or less.

Advantages of flow batteries over traditional batteries are their flexible layout due to their separate energy and power components, long cycle life, quick response time, and no harmful emission. But they are more complicated and may require pumps, sensors, control units and secondary containment vessels. Also, their energy densities are generally lower than portable batteries, and they have high initial self-discharge rate. Since flow batteries have much in common with fuel cells and traditional rechargeable batteries, their FP models are based on the same principles.

Macroscopic models based on material balances, transport equations, and electrode kinetic expressions have been proposed at the cell and stack levels. These models can predict current and potential distributions, the optimum resistance of the electrolyte, and provide a better understanding of processes occurring within flow batteries (Weber et al., 2011).

Integration with Grids

As intermittent renewable energy sources are increasingly integrated into power grids, the balance between power supply and demand increases in complexity due to abrupt changes in weather conditions. Effective energy storage and total generation should match to total load precisely on a second-by-second basis (Poullikkas, 2013). Grid power management systems should have access to accurate forecasts of the load and be able to constantly compensate for changes in wind and solar power input over short or long time spans (Dell and Rand, 2001).

Current energy storage systems for grid stabilization and support consist of large installations of lead-acid batteries (Purvins et al., 2013). These can provide only a few minutes of energy, while grid power management requires longer durations of storage in the presence of shifting peak loads and power generated by renewable systems. Thus, reengineering of the storage system is required to handle greater energy to power ratios.

Battery storage systems can support large-scale solar and wind integration in existing power systems, by providing grid stabilization, frequency regulation, and wind and solar energy smoothing (Poullikkas, 2013). Currently, sodium-sulfur-based batteries are preferred for large-scale storage. These batteries have the advantage of high energy density, high charge/discharge efficiency (~80%), long cycle life, and fabrication from inexpensive materials. FP models of rechargeable batteries, flow batteries, photovoltaics, and fuel cells allow for efficient power management in grids and optimal design and integration of the systems (Zachar and Daoutidis, 2015).

Concluding Remarks

This paper put in perspective advances in FP multiscale mathematical modeling of several renewable energy and storage systems and highlighted how these systems can benefit from mathematical modeling. Present research challenges in these areas were listed. It is concluded that mathematical modeling can contribute significantly to the optimal design and operation of power generation and storage systems, as well as optimal integration of power storage and generation systems.

Acknowledgments

This material is partially based upon work supported by the National Science Foundation under the grant CBET-1236180.

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