Future energy generation and storage solutions are complex systems, integrating means to capture renewable energy sources, chemical and electrochemical reactors, thermal engines and electric motors. The experimental cost of developing such systems is extremely high. The transition to a model-centric approach, which incorporates experimental results developed across multiple disciplines, and exploits this knowledge in the design, integration and operation of novel energy systems, is thus highly desirable.

Our current research focuses on i) the development of modeling techniques for robust and efficient simulation and optimization of energy generation and storage systems, ii) the development of proactive energy management strategies for buildings and, iii) developing efficient model-based fault detection and isolation schemes.

1. Modeling, Simulation and Optimization of Complex Systems

High fidelity, predictive modeling of energy generation and storage systems requires capturing phenomena (e.g., chemical reactions, material and energy transport and transfer, daily and seasonal variations in renewable energy sources, catalyst deactivation and material ageing) that occur over disparate time and space horizons. The resulting mathematical models are stiff, multi-scale, almost invariably high-dimensional and potentially discontinuous. As a consequence, the formulation (and solution) of rigorous model-based design optimization problems is challenging. Innovative energy system designs are thus at risk of being dismissed due to a lack of economic viability. Numerous opportunities for reducing capital costs and increasing energy efficiency in existing energy systems can be missed as well.

In our work, we rely on systems and control tools to reformulate large-scale, discontinuous differential-algebraic equation (DAE) systems as continuous ordinary differential equation (ODE) systems with favorable numerical properties. This reformulation i) facilitates obtaining steady-state solutions through a computationally efficient time integration and ii) allows the use of recently implemented relaxation-based dynamic optimization algorithms for the fast solution of design optimization problems.

Important applications include air separation through oxygen transport membranes, internal-reforming solid oxide fuel cells and biorefinery processes. We are also working on making this framework available for general use by implementing it in commercial simulators.

2. Proactive Energy Management Strategies for Buildings

Building systems are a leading energy consumer, absorbing more than 60% of the electricity produced in the US every year to fulfill the basic operational objective of ensuring occupant comfort at a minimum cost. Managing the energy use of buildings is thus an important problem with major economic and environmental impact. Human operators and building automation systems are faced with numerous decisions when responding to changes in weather, occupancy and energy costs: Should electricity be purchased from the grid or generated locally? If the latter is true, which (renewable) energy source(s) should be used? When should specific equipment units be started up or shut down? Is it beneficial to sell energy to the grid via net metering? The complexity of these decisions almost invariably leads operators to economically suboptimal solutions. Building energy management thus lends itself naturally to the use of rigorous optimization methods. Applications are, however, limited by the ability to solve large scale problems with both continuous and discrete (e.g., turning equipment on/off) decision variables in a practical amount of time.

We are developing methods for reducing the dimension of the mathematical models of building systems. The resulting reduced models are used to formulate the building operation problem as an *on-line* computationally tractable dynamic optimization over a receding, finite time horizon. Control theory techniques are also used to incorporate the anticipated values of disturbances (e.g., forecasts of weather conditions and electricity prices) in the problem formulation. We are therefore interested in developing a *predictive* rather than *reactive* approach to building energy management, with the goal of significantly improving *tactical*, day-to-day operational decisions, and obtaining important economic benefits in practical applications.

The deregulation of the energy market and the potential for using renewable energy sources also pose important *strategic* questions: What are the benefits of investing in alternative energy sources (e.g., wind, solar)? What are the benefits of implementing energy storage solutions? Will the purchase of energy futures lower operating costs? To address these questions, we are developing a set of tools for strategic decision support aimed at determining optimal capital investment and energy market strategies for next-generation building systems.

3. Fault Detection and Isolation for Multi-Scale Systems

Energy generation and storage systems belong to the broad category of complex, integrated systems. Increasing the complexity of any system (e.g., by increasing the number of subsystems and the strength of their interactions) is typically associated with a propensity to faults and failures. Subsystem interactions tend to amplify the impact of unit-level faults at the system level, with negative effects on the system performance and (potentially) integrity. Model-based fault *detection* relies on a special form of dynamic model (residual generator) for estimating discrepancies (residuals) between the measurements of the system outputs and the corresponding values computed by a system model. If assigning a unique residual combination (or signature) to each fault is possible, system faults can also be uniquely identified or *isolated*
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Fault detection and isolation (FDI) performance is evidently dependent on the dynamics of the residual generator. In the case of multiple time scale complex systems, the fast and slow transients associated with the evolution of the state variables are also present in the dynamics of the residuals. Thus, the detection of the faults whose corresponding residuals vary slowly may not be sufficiently timely; moreover, faults whose signature consists of a combination of several residuals are prone to isolation errors due to the potentially different rates at which these residuals evolve. To address these issues, we are developing FDI algorithms for systems with multiple time scale dynamics. Decomposition techniques are applied to obtain separate models of the dynamics in each time scale, which are then used for residual generation and robust fault detection.