Since the transportation sector still relies mostly on fossil fuels, the emissions and overall environmental impacts of the transportation sector are particularly relevant to the mitigation of the adverse effects of climate change. Sustainable transportation therefore plays a vital role in the ongoing discussion on how to promote energy insecurity and address future energy requirements. One of the most promising ways to increase energy security and reduce emissions from the transportation sector is to support alternative fuel technologies, including electric vehicles (EVs). As vehicles become electrified, the transportation fleet will rely on the electric grid as well as traditional transportation fuels for energy. The life cycle cost and environmental impacts of EVs are still very uncertain, but are nonetheless extremely important for making policy decisions. Moreover, the use of EVs will help to diversify the fuel mix and thereby reduce dependence on petroleum. In this respect, the United States has set a goal of a 20% share of EVs on U.S. roadways by 2030. However, there is also a considerable amount of uncertainty in the market share of EVs that must be taken into account. This dissertation aims to address these inherent uncertainties by presenting two new models: the Electric Vehicles Regional Optimizer (EVRO), and Electric Vehicle Regional Market Penetration (EVReMP). Using these two models, decision makers can predict the optimal combination of drivetrains and the market penetration of the EVs in different regions of the United States for the year 2030.

First, the life cycle cost and life cycle environmental emissions of internal combustion engine vehicles, gasoline hybrid electric vehicles, and three different EV types (gasoline plug-in hybrid EVs, gasoline extended-range EVs, and all-electric EVs) are evaluated with their inherent uncertainties duly considered. Then, the environmental damage costs and water footprints of the studied drivetrains are estimated. Additionally, using an Exploratory Modeling and Analysis method, the uncertainties related to the life cycle costs, environmental damage costs, and water footprints of the studied vehicle types are modeled for different U.S. electricity grid regions. Next, an optimization model is used in conjunction with this Exploratory Modeling and Analysis method to find the ideal combination of different vehicle types in each U.S. region for the year 2030. Finally, an agent-based model is developed to identify the optimal market shares of the studied vehicles in each of 22 electric regions in the United States. The findings of this research will help policy makers and transportation planners to prepare our nation's transportation system for the future influx of EVs.

The findings of this research indicate that the decision maker's point of view plays a vital role in selecting the optimal fleet array. While internal combustion engine vehicles have the lowest life cycle cost, the highest environmental damage cost, and a relatively low water footprint, they will not be a good choice in the future. On the other hand, although all-electric vehicles have a relatively low life cycle cost and the lowest environmental damage cost of the evaluated vehicle options, they also have the highest water footprint, so relying solely on all-electric vehicles is not an ideal choice either. Rather, the best fleet mix in 2030 will be an electrified fleet that relies on both electricity and gasoline. From the agent-based model results, a deviation is evident between the ideal fleet mix and that resulting from consumer behavior, in which EV shares increase dramatically by the year 2030 but only dominate 30 percent of the market. Therefore, government subsidies and the word-of-mouth effect will play a vital role in the future adoption of EVs.