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Dynamic temperature modeling of an SOFC using least squares support vector machines

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Abstract

Cell temperature control plays a crucial role in SOFC operation. In order to design effective temperature control strategies by model-based control methods, a dynamic temperature model of an SOFC is presented in this paper using least squares support vector machines (LS-SVMs). The nonlinear temperature dynamics of the SOFC is represented by a nonlinear autoregressive with exogenous inputs (NARXs) model that is implemented using an LS-SVM regression model. Issues concerning the development of the LS-SVM temperature model are discussed in detail, including variable selection, training set construction and tuning of the LS-SVM parameters (usually referred to as hyperparameters). Comprehensive validation tests demonstrate that the developed LS-SVM model is sufficiently accurate to be used independently from the SOFC process, emulating its temperature response from the only process input information over a relatively wide operating range. The powerful ability of the LS-SVM temperature model benefits from the approaches of constructing the training set and tuning hyperparameters automatically by the genetic algorithm (GA), besides the modeling method itself. The proposed LS-SVM temperature model can be conveniently employed to design temperature control strategies of the SOFC.

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Keywords: Solid oxide fuel cell (SOFC); Dynamic temperature model; Least squares support vector machine (LS-SVM); Hyperparameter tuning; Genetic algorithm (GA)

1. Introduction

The solid oxide fuel cell (SOFC) is expected to be one of the most promising devices for energy conversion because of its high efficiency, low pollutant emissions and flexible fueling strategies. Possible applications of SOFCs range from vehicular auxiliary power units to stationary power plants [1]. Cell temperature control plays a crucial role in SOFC operation [2,3]. This is because the cell temperature has a significant effect on the electrical characteristics of an SOFC, e.g. the cell voltage and the current density distribution. Moreover, the variation of cell temperature may cause degradation, even damage to the fuel cell due to thermal fatigue or thermal cracking of the cell material. Thus, the average cell temperature should be carefully controlled. In

order to design effective temperature control strategies by using model-based control methods, simple and accurate dynamic temperature models of SOFCs are highly desired.

In recent years, many dynamic physical models of SOFCs based on conservation laws and electrochemical principles have been reported [3–6]. Although these models are useful for the analysis and optimization of SOFCs, in general they are too complex for applying model-based control methods. The complicated phenomena associated with SOFCs easily drive such models to high complexity [7]. Developing simpler data-driven models based on the system identification methodology is an important way to control complex plants [8,9]. Following this line, many data-driven modeling approaches, such as classical system identification, artificial neural networks (ANNs) and fuzzy logic, can be applied to dynamic temperature modeling of SOFCs. The requirements for developing such data-driven temperature models of SOFCs for control purpose can be summarized as:

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Nomenclature
            cell active area (m<sup>2</sup>)
\boldsymbol{A}
            reforming reaction surface area (m<sup>2</sup>)
A_{\rm r}
            anode section area (m<sup>2</sup>)
A_{\rm sh}
AR
            air ratio
b
            bias term
           fitting function coefficients of specific heat capac-
b_0 - b_3
           ity
            specific heat
                                capacity
                                                 of
                                                        gas
                                                                 species
c_p
            (\bar{J} \, \text{mol}^{-1} \, K^{-1})
C_p^{\rm s}
            specific heat capacity of solid part (J kg^{-1} K^{-1})
           prediction error of the kth data point
e_k
E_{\rm a}
            activation energy (J \text{ mol}^{-1})
F
            Faraday's constant (=96,485 \,\mathrm{C} \,\mathrm{mol}^{-1})
h_i
            molar enthalpy (J mol^{-1})
           total change of molar enthalpy for chemical reac-
\Delta H
            tion (J \text{ mol}^{-1})
            average current density (A m^{-2})
J
            coefficient for unit conversion (=10^5 \, \text{Pa bar}^{-1})
k_{\rm p}
                                     reaction
k_{\rm r}
            (=4274 \text{ mol s}^{-1} \text{ m}^{-2} \text{ bar}^{-1})
            WGS reaction constant (=1.2 \times 10^4 \text{ mol m}^{-3} \text{ s}^{-1})
k_{\rm sh}
           kernel function
K
            equilibrium constant of WGS reaction
K_{\rm sh}
M^{\rm S}
            mass of solid part (kg)
n_{\rm e}
            number of transferred electrons
           molar number of species i within SOFC (mol)
n_i
n_{v}, n_{d}, n_{u} maximum lags
           molar flow rate (mol s^{-1}), number of data points
N
p
           pressure (bar)
P_{dc}
            direct current electric power (W)
           rate of reaction i \pmod{s^{-1}}
r_i
Ř
            universal gas constant (=8.314 \,\mathrm{J}\,\mathrm{mol}^{-1}\,\mathrm{K}^{-1})
R_{\rm ohm}
            total cell resistance (\Omega m<sup>2</sup>)
T
            temperature (K)
T_0
            initial temperature (K)
U
            voltage (V)
            fuel utilization
U_{\rm f}
            volume (m<sup>3</sup>)
w
            feature vector
            input vector
\boldsymbol{x}
            molar fraction of species i
x_i
            output value
y
Greek symbols
           Lagrange multiplier
\beta_{an}, \beta_{ca} pre-exponential factors of anode and cathode
           (A m^{-2})
            overpotential (V)
η
            nonlinear mapping
φ
           regularization parameter
γ
           kernel parameter
\sigma_{an}, \sigma_{ca}, \sigma_{elec} electrical conductivity of anode, cathode
            and electrolyte (\Omega^{-1} m<sup>-1</sup>)
            thickness (m)
τ
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number of chemical reactions
ξ
ζ
         number of gases
Subscripts
act
         activation
         anode
         cathode
ca
         concentration
conc
elec
         electrolyte
i
         gas species i
         the jth reaction
k
         sampling instant k, the kth data point
ohm
         ohmic
         steam reforming reaction
         water-gas shift reaction
sh
Superscripts
         fuel cell inlet
         fuel cell outlet
out
ref
         reference condition
         solid part (including the PEN and interconnect)
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- (1) The model should be able to represent the temperature dynamics of an SOFC accurately over a relatively wide operating range, certainly including the design point.
- (2) The model can be conveniently integrated into the whole control scheme of an SOFC.
- (3) The model's performance should be fully tested over the expected operating range.
- (4) The modeling process should be as simple as possible.

Compared with the substantial progress on physical modeling, however, data-driven dynamic temperature models of fuel cells (particularly of SOFCs), which meet all above requirements, are still rare.

Shen et al. [10] presented an application of radial basis functions (RBFs) neural networks to develop a dynamic temperature model of a molten carbonate fuel cell (MCFC) stack. Although satisfactory degree of precision is obtained, the MCFC RBF-NN model has several weaknesses. First, the topology and training strategy of RBF-NNs are determined by experience, which weakens the model's objectivity. Second, RBF-NNs get easily stuck in local extrema. Third, the effect of load disturbance on cell temperature was left out of consideration, which impairs the model's generality. Jurado [11,12] used different Hammerstein models to represent the dynamic characteristics of an SOFC. As the Hammerstein model, which uses a static nonlinear block followed by a dynamic linear block to represent nonlinear systems, is a special type of nonlinear model, these SOFC models still need more tests over a wide operating range. Yang et al. [13] reported a dynamic T-S fuzzy model of a MCFC, which consists of a voltage and a temperature submodel. However, the temperature submodel can only be valid within a relatively narrow temperature range. In addition, the identification procedure

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