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# Identification, Optimization and Control with Applications in Modern Technologies

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Armin Rund, Kati Sternberg, Hans Josef Pesch, Kurt Chudej

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# Optimal Control of a Large PDAE Molten Carbonate Fuel Cell Model

Armin Rund\*, Kati Sternberg, Hans Josef Pesch, and Kurt Chudej

Lehrstuhl für Ingenieurmathematik, Universität Bayreuth, D-95440 Bayreuth, Germany

Molten carbonate fuel cells are well suited for stationary power production and heat supply. In order to enhance service life time, hot spots, resp. high temperature gradients inside the fuel cell have to be avoided. In conflict with that, there is the desire to achieve faster load changes while temperature gradients stay small. For the first time, optimal fast load changes have been computed numerically. The dimensionless model is based on the description of physical and chemical phenomena. The numerical procedure is based on a method of lines approach via spatial discretization and the solution of the resulting very large scale optimal control problem s.t. a differential-algebraic equation system by a nonlinear programming approach.

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## 1 Description of the Molten Carbonate Fuel Cell Model

A detailed dynamic 2D crossflow model of a molten carbonate fuel cell (MCFC) is used for the numerical computation of fast load changes by optimal control [1, 2, 3]. The mathematical model allows for the calculation of the dynamical behavior of molar fractions  $\chi_{a|c}$  and partial pressures in the pores  $\varphi_{a|c}$  of the gas components  $\text{CH}_4$ ,  $\text{H}_2\text{O}$ ,  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{O}_2$ ,  $\text{N}_2$ , molar flow densities  $\gamma_{a|c}$ , temperatures in gas phases  $\vartheta_{a|c}$  in the anode (a) and cathode (c) gas channel; temperature in solid phase  $\vartheta_s$ , cell voltage  $U_{\text{cell}}$ , and current density distributions  $I_{a|e|c}$ ,  $i_{a|e|c}$  for given cell current  $I_{\text{cell}}(\tau)$ . The abbreviation  $w = (\chi, \vartheta)$  is used. The complete model and numerical simulation results can be found in [3]. Spatial domain is  $\Omega = [0, 1] \times [0, 1]$  with spatial coordinates  $\zeta_1$  and  $\zeta_2$  and boundary  $\Gamma = \Gamma_{\text{in}}^a \cup \Gamma_{\text{out}}^a \cup \Gamma_{\text{in}}^c \cup \Gamma_{\text{out}}^c$ . Time is denoted by  $\tau$ .

Partial differential-algebraic equations with boundary conditions:

$$\frac{\partial \vartheta_s}{\partial \tau} = \kappa_1 \frac{\partial^2 \vartheta_s}{\partial \zeta_1^2} + \kappa_2 \frac{\partial^2 \vartheta_s}{\partial \zeta_2^2} + \psi_1(\vartheta_s, w_{a|c}, \varphi_{a|c}, \Phi_{a|c}^L, U_{\text{cell}}), \quad \frac{\partial \vartheta_s}{\partial z}|_{\Gamma} = 0, \quad (1)$$

$$\frac{\partial w_a}{\partial \tau} = -\gamma_a \vartheta_a \frac{\partial w_a}{\partial \zeta_1} + \psi_2(\vartheta_s, w_a, \varphi_a, \Phi_a^L), \quad w_a|_{\Gamma_{\text{in}}^a} = w_{a,\text{in}}(\tau), \quad (2)$$

$$\frac{\partial w_c}{\partial \tau} = -\gamma_c \vartheta_c \frac{\partial w_c}{\partial \zeta_2} + \psi_3(\vartheta_s, w_c, \varphi_c, \Phi_c^L, U_{\text{cell}}), \quad w_c|_{\Gamma_{\text{in}}^c} = w_{m}(\tau), \quad (3)$$

$$0 = \frac{\partial(\gamma_a \vartheta_a)}{\partial \zeta_1} + \psi_4(\vartheta_s, w_a, \varphi_a, \Phi_a^L), \quad \gamma_a|_{\Gamma_{\text{in}}^a} = \gamma_{a,\text{in}}(\tau), \quad (4)$$

$$0 = \frac{\partial(\gamma_c \vartheta_c)}{\partial \zeta_2} + \psi_5(\vartheta_s, w_c, \varphi_c, \Phi_c^L, U_{\text{cell}}), \quad \gamma_c|_{\Gamma_{\text{in}}^c} = \gamma_m(\tau), \quad (5)$$

$$0 = \psi_6(\vartheta_s, \chi_a, \chi_c, \varphi_a, \varphi_c, \Phi_a^L, \Phi_c^L, U_{\text{cell}}), \quad (6)$$

$$\frac{\partial \Phi_{a|c}^L}{\partial \tau} = \psi_7(\vartheta_s, \varphi_{a|c}, \Phi_{a|c}^L, U_{\text{cell}}, I_{a|e|c}; I_{\text{cell}}). \quad (7)$$

Integro differential-algebraic equations:

$$\frac{dU_{\text{cell}}}{d\tau} = \frac{I_a - I_{\text{cell}}}{c_a} + \frac{I_e - I_{\text{cell}}}{c_e} + \frac{I_c - I_{\text{cell}}}{c_c}, \quad (8)$$

$$I_a(\tau) = \int_{\Omega} i_a(\vartheta_s, w_a, \varphi_a, \Phi_a^L) d\zeta, \quad I_c(\tau) = \int_{\Omega} i_c(\vartheta_s, w_c, \varphi_c, \Phi_c^L, U_{\text{cell}}) d\zeta, \quad I_e(\tau) = \int_{\Omega} i_e(\Phi_{a|c}^L) d\zeta, \quad (9)$$

$$\frac{dw_m}{d\tau} = \psi_8(w_m, \int_{\Gamma_{\text{out}}^a} w_a d\zeta_2, \int_{\Gamma_{\text{out}}^a} \gamma_a d\zeta_2, \int_{\Gamma_{\text{out}}^c} w_c d\zeta_1, \int_{\Gamma_{\text{out}}^c} \gamma_c d\zeta_1, \lambda_{\text{air}}, \vartheta_{\text{air}}, R_{\text{back}}), \quad (10)$$

$$\gamma_m(\tau) = \psi_9(w_m, \int_{\Gamma_{\text{out}}^a} w_a d\zeta_2, \int_{\Gamma_{\text{out}}^a} \gamma_a d\zeta_2, \int_{\Gamma_{\text{out}}^c} w_c d\zeta_1, \int_{\Gamma_{\text{out}}^c} \gamma_c d\zeta_1, \lambda_{\text{air}}, \vartheta_{\text{air}}, R_{\text{back}}). \quad (11)$$

Initial conditions:

$$\vartheta_s|_{\tau=0} = \vartheta_{0,s}(\zeta), \quad w_a|_{\tau=0} = w_{0,a}(\zeta), \quad w_c|_{\tau=0} = w_{0,c}(\zeta), \quad w_m|_{\tau=0} = w_{0,m}, \\ \Phi_a^L|_{\tau=0} = \Phi_{0,a}^L(\zeta), \quad \Phi_c^L|_{\tau=0} = \Phi_{0,c}^L(\zeta), \quad U_{\text{cell}}|_{\tau=0} = U_{0,\text{cell}}. \quad (12)$$

\* Corresponding author: E-mail: armin.rund@uni-bayreuth.de, Phone: +49 921 55 7152, Fax: +49 921 55 7155

## 2 Optimal Control of a Load Change

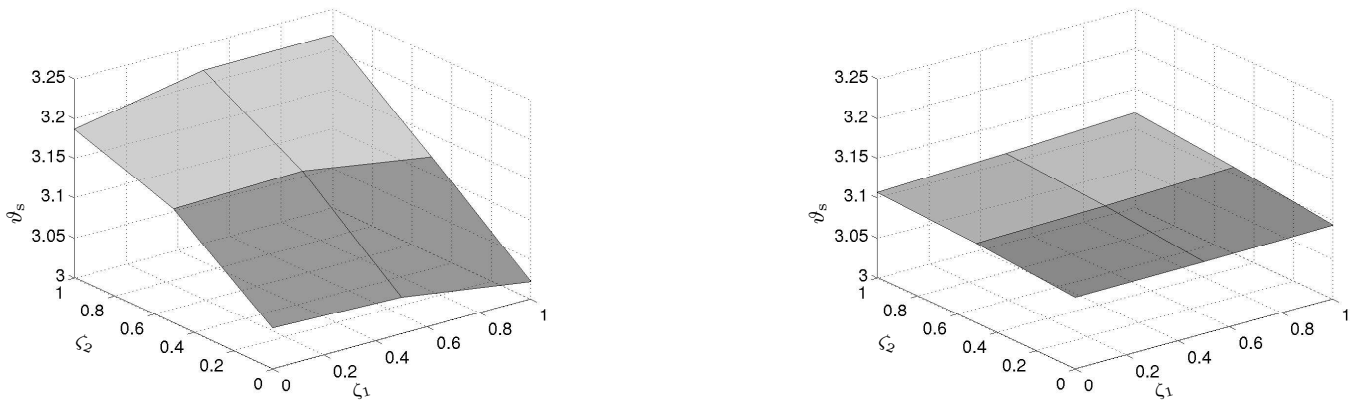
A (possibly discontinuous) change in the input function  $I_{\text{cell}}(\tau)$ , typically a piecewise constant function, is called load change. Load changes are technologically important in the production of electrical current. After a load change the new stationary solution profile should be reached as soon as possible, but large temperature gradients in the solid temperature have to be avoided. Large temperature gradients yield material stress, and reduce drastically the life-time of the very expensive fuel cell. Reaching of the new stationary solution takes approximately 3 hours, if constant boundary conditions are used. A faster approach to the new stationary solution is possible by controlling the boundary conditions as time dependent functions. A logarithmic type grid  $\tau_1 = 0, \tau_2 = 0.1, \tau_3 = 1.1, \tau_4 = 11.1, \tau_5 = 111.1, \tau_6 = 1111.1$  is used, due to the different time scales of the variables. We study a load change from  $I_{\text{cell}} = 0.7$  for  $\tau \leq 0$  to  $I_{\text{cell}} = 0.75$  for  $\tau > 0$ .

We compare two different approaches. In the first approach we solve a sequence of optimal control problems ( $n = 5$ )

$$\left( \min \int_{\tau_k}^{\tau_{k+1}} [U_{\text{cell}} - U_{\text{cell,ref}}]^2 d\tau \text{ s.t. (1-12) with } I_{\text{cell}} = 0.75 \right)_{k=1, \dots, n}, \quad (13)$$

each subproblem with given initial conditions and free final conditions. For  $k = 1$  the initial conditions are the stationary solution for  $I_{\text{cell}} = 0.7$ . For the following subproblems the initial conditions are the final states of the previous problem. In the second approach we only change the cost functional for the last subproblem to

$$\left( \min \int_{\tau_5}^{\tau_6} \int_{\Omega} [\vartheta_s - \vartheta_{s,\text{ref}}]^2 d\zeta d\tau \text{ s.t. (1-12) with } I_{\text{cell}} = 0.75 \right) \quad (14)$$



**Fig. 1** solid temperature  $\vartheta_s$  at time  $\tau_6 = 1111.1$  after the load change, left side: (13) $_{n=5}$ , right side: (13) $_{n=4}$  & (14)

One can see clearly the improved profile of the solid temperature on the right side of Fig. 1. The interplay of all optimal control components  $\chi_{\text{a,CH}_4}|_{\Gamma_{\text{in}}^{\text{a}}}, \vartheta_{\text{a}}|_{\Gamma_{\text{in}}^{\text{a}}}, \gamma_{\text{a}}|_{\Gamma_{\text{in}}^{\text{a}}}, \lambda_{\text{air}}, \vartheta_{\text{air}}, R_{\text{back}}$  is essential for reaching the situation in Fig. 1 on the right side. In contrast, almost the same situation as in Fig. 1 on the left side can be reached with *only one* control component  $\gamma_{\text{a}}|_{\Gamma_{\text{in}}^{\text{a}}}$ . It takes about 36 hours of computer time only to solve subproblem (14).

Additional numerical results for other technologically interesting scenarios can be found in [1] and [3].

## References

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