Electrochimica Acta 69 (2012) 120–127

Contents lists available at SciVerse ScienceDirect

Electrochimica Acta

journal homepage: www.elsevier.com/locate/electacta

A temperature dependent multi-ion model for time accurate numerical simulation of the electrochemical machining process. Part II: Numerical simulation

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A R T I C L E I N F O

Article history:
Received 5 December 2011
Received in revised form 21 February 2012
Accepted 22 February 2012
Available online 7 March 2012

Keywords:
Thermal properties
Concentration
Current efficiency
Water depletion
Steel

A B S T R A C T

The temperature distribution and shape evolution during electrochemical machining (ECM) are the result of a large number of intertwined physical processes. Electrolyte flow, electrical conduction, ion transport, electrochemical reactions, heat generation and heat transfer strongly influence one another, making modeling and numerical simulation of ECM a very challenging procedure. In part I [1], a temperature dependent multi-ion transport and reaction model (MITReM) is put forward which considers mass transfer as a consequence of diffusion, convection and migration, combined with the electroneutrality condition and linearized temperature dependent polarization relations at the electrode–electrolyte interface. The flow field is calculated using the incompressible laminar Navier–Stokes equations for viscous flow. The local temperature is obtained by solving internal energy balance, enabling the use of temperature dependent expressions for several physical properties such as the ion diffusion coefficients and electrolyte viscosity. In this second part, the temperature dependent MITReM is used to simulate ECM of stainless steel in aqueous $NaNO_3$ electrolyte solution. The effects of temperature, electrode thermal conduction, reaction heat generation, electrolyte flow and water depletion are investigated. A comparison is made between the temperature dependent potential model and MITReM.

1. Introduction

Electrochemical machining (ECM) is an industrial process used to shape metal. A cathode tool and anode workpiece are immersed into an electrolyte solution and subjected to a potential difference, causing electrochemical reactions to occur at the electrode–electrolyte interfaces. At the anode metal is dissolved. Fresh electrolyte solution is continuously pumped through the electrode gap in order to flush the dissolved metal and to remove a large share of the heat generated by the electrochemical reactions.

Despite its advantages and the applicability of ECM in a large number of industrial processes, the design of the ECM process remains a challenge. A multitude of process parameters influence the speed and accuracy of machining so that in practice the design is often achieved by trial and error, which proves to be both costly and time consuming. This clearly shows the need for a better fundamental understanding of the process, such that physical models can be put forward that can be implemented in computer simulation tools. These tools can in turn be employed to more quickly and more precisely design the ECM process parameters and tool shapes.

Simulation of ECM in full detail is an extremely challenging task because of the wide variety of physical processes occurring simultaneously: high velocity laminar or turbulent electrolyte flow, ion transport by diffusion, convection and migration, concurring electrochemical reactions at the electrode–electrolyte interfaces, homogeneous reactions, reaction heat generation, joule heating, gas evolution, heat conduction, natural and forced heat convection, oxide layer formation, pulsed current conditions, capacitive effects, etc. Moreover, all of these processes are strongly influencing one another. For instance the electrolyte flow field affects the temperature distribution, which in turn influences the electrode reaction rate and thus the workpiece shape evolution which once again changes flow field. For this reason, modeling and simulating ECM is a very interesting topic. If the goal of a complete ECM simulation which incorporates all of these aspects is to be achieved, a thorough understanding of the fundamental processes and their interactions is mandatory.

In literature, analytic approaches to tool design have been presented, such as the cos θ method [2,3], the complex variables method [4], exact and approximate quasi-steady-state and locally one-dimensional methods [5] and methods using a Fourier series to represent the workpiece surface [6]. Semi-analytical and numerical techniques include the boundary elements method (BEM) [7,8], the finite difference method (FDM) [9–11], the finite volume method

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doi:10.1016/j.electacta.2012.02.079

(FVM) and finite element method (FEM) [12]. The models used may greatly vary in terms of complexity.

In previous work from the author [13], the potential model (PM), in which no ionic species are modeled in the electrolyte, has been extended with the aim to account for thermal effects. The internal energy balance equation is used for calculating the temperature distribution. Heat is generated in the bulk and in the electrical double layer and a temperature dependent electrical conductivity is used for the electrolyte. The workpiece removal rate is calculated through a temperature dependent reaction current density distribution on the anode surface. The surface evolution in time is calculated using the level set method [14] and boundary displacements are implemented using the elastic body analogy [15]. The heat conduction through the electrodes and the heat produced by electrode reactions were found to play an important role.

Part I of this article presents a more complex model for dealing with ECM simulations [1]. The PM is replaced by the multi-ion transport and reaction model (MITReM) [16], which considers mass transfer as a consequence of diffusion, convection and migration, combined with the electroneutrality condition and linearized polarization relations at the electrode–electrolyte interface. The MITReM is able to deal with concurrent electrode reactions (e.g. metal dissolution vs. oxygen evolution at the anode), such that the current efficiency is inherently part of the model. The model is further extended with temperature and concentration dependent diffusion constants and ECM-specific equations to account for the effects of water depletion at the electrodes [17,18]. Internal energy balance is added to the set of equations such that the temperature field can be calculated. This allows for the inclusion of temperature dependence of several physical parameters and processes into the model. The electrode reaction kinetics, the diffusion coefficients of all ions and the viscosity of the electrolyte fluid are made temperature dependent. In addition, boundary conditions dealing with cooling of the electrodes by natural convection are added.

In this second part, the temperature dependent MITReM is used to simulate ECM of steel in aqueous $NaNO_3$ electrolyte solution. Additionally, the effects of temperature, electrode thermal conduction, reaction heat generation, electrolyte flow and water depletion are investigated. Since the model is computationally very heavy, it is important to be able to simplify where possible. Such is for instance the case with the PM which assumes constant concentrations in the electrolyte, making the simulation substantially more manageable in terms of equations and computation speed compared to the MITReM. This is all the more desirable when considering the three-dimensional problem. In order to know whether simplifications are possible and justified, a parameter sensitivity study is performed on the full model. The importance of parameters and their temperature dependence with respect to ECM is studied. In addition, a comparison is made between the temperature dependent PM and MITReM.

2. Theoretical model

A detailed derivation and discussion of the theoretical model and applied boundary conditions can be found in part I of this work [1]. A brief summary is given here for completeness.

2.1. Electrode model

The properties to be solved for in the electrodes are the potential V (V) and temperature T (K), obtained by expressing charge conservation (1) and internal energy balance (2),

$$\vec{\nabla} \cdot \left(\kappa \vec{\nabla} V\right) = 0 \tag{1}$$

$$\vec{\nabla} \cdot \left(k \vec{\nabla} T\right) = 0 \tag{2}$$

Table 1
Diffusion parameters at 25 °C [17,18].

	z_i	D_i^0 (10^{-9} m²/s)	a_i (10^{-4} m³/mol)
Na^+	1	1.33	3.30
NO_3^-	−1	1.90	2.38
H^+	1	9.31	1.00
Me^{z+}	3	1.24	11.4
OH^-	−1	5.26	2.38
H_2O	0	2.00	5.00

with κ (S/m) the electrical conductivity and k (W/m K) the thermal conductivity. Potentials V_c and V_a are applied respectively on the upper cathode and lower anode surfaces. The outer electrode boundaries are cooled by natural convection [19] and the heat flux $\dot{q}$ (W/m^2) leaving the electrodes is calculated as $\dot{q} = h(T - T_{ref})$, with h (W/m^2 K) the heat transfer coefficient and T_{ref} (K) the ambient temperature, taken 25 °C.

2.2. Electrolyte model

For the electrolyte, in addition to the potential U (V) and temperature T, one has to solve for the fluid velocity $\vec{v}$ (m/s), the pressure p (Pa) and the ion concentrations c_i (mol/m^3). If the two-dimensional problem is considered with I the number of ions in the electrolyte solution, there are $I + 5$ unknowns. The system of equations to be solved consists of the electroneutrality condition (3), charge conservation (4), continuity (5) and momentum (6) conservation for viscous incompressible flow, internal energy balance (7) and $I - 1$ ion transport Eq. (8). In this work $I = 6$ (cf. Table 1) and the transport equation for H_2O is skipped.

$$\sum_i z_i c_i = 0 \tag{3}$$

$$\sum_i \vec{\nabla} \cdot (z_i F D_i \vec{\nabla} c_i) + \vec{\nabla} \cdot \left(\sum_i \frac{z_i^2 F^2 D_i c_i}{RT} \vec{\nabla} U \right) = 0 \tag{4}$$

$$\vec{\nabla} \cdot \vec{v} = 0 \tag{5}$$

$$\rho \left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \vec{\nabla} \vec{v} \right) = -\vec{\nabla} p + \mu \Delta \vec{v} \tag{6}$$

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p \vec{v} \cdot \vec{\nabla} T = \vec{\nabla} \cdot \left(k \vec{\nabla} T \right) + P^{bulk} \tag{7}$$

$$\frac{\partial c_i}{\partial t} + \vec{v} \cdot \vec{\nabla} c_i - \vec{\nabla} \cdot (D_i \vec{\nabla} c_i) - \vec{\nabla} \cdot \left(\frac{z_i F D_i c_i}{RT} \vec{\nabla} U \right) = 0 \tag{8}$$

with z_i the valence, F (C/mol) the Faraday constant, D_i (m^2/s) the diffusion coefficient, R (J/mol K) the ideal gas constant, ρ (kg/m^3) the density of the electrolyte, μ (kg/m s) the dynamic viscosity and c_p (J/kg K) the specific heat capacity. P^{bulk} (W/m^3) is the heat generated in the electrolyte bulk solution, obtained from Joule law as

$$P^{bulk} = \left(\sum_i z_i F D_i \vec{\nabla} c_i + \sum_i \frac{z_i^2 F^2 D_i c_i}{RT} \vec{\nabla} U \right) \cdot \vec{\nabla} U.$$

The expression for the diffusion coefficients [17] is temperature and concentration dependent [1],

$$D_i = [D_i^0 \exp(-a_i c_{NO_3^-}) + D_i^{min}][1 + 0.025(T - T_{ref})], \tag{9}$$

with parameters from Table 1.