

Article

Chebyshev–Gauss–Lobatto Collocation Method for 1D Diffusion in Holby–Morgan Model of Platinum Degradation

Victor A. Kovtunenکو 1,2 

¹ Department of Mathematics and Scientific Computing, Karl-Franzens University of Graz, NAWI Graz, Heinrichstr. 36, 8010 Graz, Austria; victor.kovtunenکو@uni-graz.at

² Lavrentyev Institute of Hydrodynamics, Siberian Division of the Russian Academy of Sciences, 630090 Novosibirsk, Russia

Abstract

Electrokinetic mechanisms of platinum catalyst degradation in polymer electrolyte membrane fuel cells are represented by platinum ion dissolution and platinum oxide formation. The other primary mechanism of degradation is the diffusion of platinum particles. The governing one-dimensional Holby–Morgan model across the catalyst thickness is described by nonlinear reaction–diffusion equations with Butler–Volmer reaction rates. To approximate properly spatial diffusion, the Chebyshev–Gauss–Lobatto pseudo-spectral collocation method is introduced and tested numerically within implicit–explicit time discretization. The accurate approximation makes it possible to simulate the nonlinear degradation of a platinum catalyst over a long cyclic voltammetry test until it loses its operational capacity.

Keywords: polymer electrolyte membrane fuel cell; platinum catalyst degradation; mathematical modelling; reaction–diffusion system; numerical analysis

MSC: 78A57; 35K57; 65N35

1. Introduction

The electrochemical reactions of platinum (Pt) dissolution and platinum oxide (PtO) film formation govern the loss of electrochemical surface area (ECSA) on platinum catalysts. In turn, the ECSA loss simulated by Accelerated Stress Tests (ASTs) encourages catalyst degradation in Polymer Electrolyte Membrane (PEM) fuel cells, which limits their durability. Developing more durable fuel cells and mitigation strategies remains a crucial challenge for commercialization; the fundamentals can be found in books by Basile et al. [1], Eikerling and Kulikovskiy [2], and Hacker and Mitsushima [3].

The review by Hidayat et al. [4] summarizes recent advancements in PEMFC materials focusing on Catalyst Layers (CLs), membranes, gas diffusion layers, bipolar plates, and peripherals. Despite progress in developing alternatives to platinum as a catalyst, challenges remain in enhancing durability and manufacturing. Yang et al. [5] gave atomic-level insights into the common structural features required for multifunctional catalysis. In Prijatelj et al. [6], a new bimetallic alloyed catalyst degradation model was developed on the basis of the continuity equation and the rate of change of particle radii. Shih and Chen [7] described microwave-assisted synthesis of a platinum-based composite nano-catalyst in direct methanol fuel cells because of their simple construction. Danilov et al. [8] reviewed other promising solutions using protonic ceramic electrochemical cells with thin-film electrolytes, which affects the kinetics of the oxygen reduction and oxygen evolution reactions.



Academic Editor: Miklas Scholz

Received: 16 June 2026

Revised: 22 July 2026

Accepted: 26 July 2026

Published: 28 July 2026

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Electrocatalyst performance has historically been measured in terms of overpotential, which is the potential difference necessary to drive a certain reaction rate. Kumar et al. [9] critically examined limitations of the traditional static descriptors and proposed a dynamic active-site electrocatalytic evolution. Alimbekova et al. [10] established degradation patterns and proposed a predictive model for device lifetime using a galvanostatic method.

Globally, transportation accounts for 30% of all greenhouse gas emissions. In their review, Hegde et al. [11] examined recent researches on platinum catalyst degradation in the context of automotive applications. Studying the durability of CLs in PEMFC buses, Golaghaei et al. [12] developed an electrochemical degradation model that translates driving cycles into voltage profiles based on the Ostwald ripening phenomenon. When various involved parameters were tested, an increase in vehicle speed was the largest contributor to durability; other contributors included vehicle acceleration and deceleration. In contrast, increased fluctuations led to greater degradation. Wang et al. [13] investigated simulated dynamic automotive conditions using both in situ and physical characterisation techniques. In experimental data and model calculations, Pt dissolution and Ostwald ripening in cells with low Pt loading were found to be effectively mitigated by increasing the lower potential limit. Validated against the Toyota Mirai, simulations by Rašić et al. [14] clarified that cold start-up led to a catalyst ECSA degradation rate of two orders of magnitude higher than warm start-up.

Marine power systems, another important application, are significantly affected by nonlinear electrochemical kinetics and extremely wide fluctuations in the propulsion load profile. To increase fuel cells' efficiency and to decrease hydrogen consumption, Elgammal [15] developed a dynamic simulation model based on particle swarm optimization methods. Aliberti et al. [16] examined the potential of fuel cells in advancing the hydrogen-based aviation sector. There, the key performance indicator relies on improving the mass-to-power ratio. In particular, reducing the bipolar plates' mass and increasing the membrane electrode assembly's operating temperature helps to keep the aircraft maximal take-off mass in an appropriate range. For a computer-aided design system for manufacturing processes in aircraft technologies, see Guzev et al. [17].

The durability of water electrolyzers under renewable power, particularly solar photovoltaic (PV) systems, is a critical challenge for green hydrogen production to decarbonise the global energy system. The acidic cell environment requires catalysts of noble metals such as iridium or ruthenium at the anode and platinum or palladium at the cathode, which are scarce and expensive. Al-Mandhari and Ghosh [18] investigated the performance and ageing of a PEM electrolysis stack, including loss of ECSA, under day–night cycles and seasonal variability in contrasting humid climates. Energy management strategies for PV batteries employ classical optimal control approaches that use the first-order optimality condition ensuring stationarity of solutions. Mundu et al. [19] introduced a second-order variational framework based on Jacobi equations aiming at stability and robustness to operating perturbations. They provided a mathematically grounded and practically relevant foundation for energy management in renewable PV and battery storage systems.

Mechanical degradation of catalyst supports, such as porous carbon layers in fuel cells or electrolyzers, is typically modelled within classical continuum plate theory. In the work of Annin and Volchkov [20], the reader can find a review of methods reducing 3D elasticity theory to 2D models of plates and shells. Using the method of variational inequalities, Khludnev [21] analysed the equilibrium of elastic inclusions assuming that they may delaminate from the surrounding matrix. Popova and Efremov [22] modelled local defects as junction points between separate inclusions, characterized by a positive damage parameter. Xi et al. [23] proved the variational solution of the equilibrium problem for an elastic body in contact with a wedge-shaped rigid inclusion. Leonova et al. [24] applied

periodic homogenization to ascertain the effective characteristics of elastic composite material reinforced by curvilinear inclusions. A hyperelastic body containing a crack that crosses the boundary at zero angle was formulated by Furtsev [25] as minimization of an energy functional. The well-posedness of the problem of non-penetrating cracks in nonlinear elastic bodies was studied by Itou et al. [26].

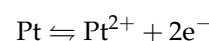
The focus of the current contribution is on diffusion phenomena in the Holby–Morgan model. In general context, diffusion and reaction–diffusion equations explain the macroscopic motion in a mixture arising from random motion of micro-particles. When driven by Brownian motion, particles spread from high-concentration to low-concentration areas in a suitable physical environment. Diffusion is a primary example of a continuous-time stochastic Markov process in mathematics.

In a range of nonlinear diffusion problems, the global existence of solutions is an open problem. When the standard monotone operator theory failed, Bulíček et al. [27] overcame the crucial difficulty by resorting to proper weighted spaces. Alekseev and Pukhnachev [28] proved the global solvability and local uniqueness of a stationary thermal diffusion equation with variable coefficients. Fellner et al. [29] established renormalised solutions and convergence to equilibrium for complex balanced reaction–diffusion systems satisfying an entropy inequality. In vivo dynamical analysis of water diffusion through a skin membrane presents a considerable challenge in biomechanics. Based on experimental observations, Argatov et al. [30] developed a one-dimensional concentration-dependent diffusion model and applied it to evaluate water loss as the central indicator of age-related changes. For heat transfer equations, we refer to Recupero [31] and to Mallikarjunaiah and Bhatta [32] for the finite element model. The Poisson–Nernst–Planck (PNP) system of continuum equations model thermodynamically consistent transport of charged species immersed in a solvent, which is driven by the interaction of diffusion and convection with the electrostatic potential. For cross-diffusion PNP equations describing solvent concentrations, Jüngel and Massimini [33] proved the existence of a global bounded weak solution by using the relative entropy method.

To achieve physical consistency, it is necessary to keep physical quantities positive or bilaterally bounded within certain thresholds. From the standpoint of optimization, this task leads to constrained problems over polyhedral domains. Chok and Petzinna [34] proposed a method based on the logarithmic barrier, which defines a diffusion process that preserves trajectories started in the interior domain, allowing them to remain feasible for all finite times. The preservation of non-negativity of solutions of an evolutionary Partial Differential Equation (PDE), starting with non-negative initial data, for linear problems follows directly from the maximum principle; see, e.g., Fellner and Kovtunen [35,36]. Non-negative solutions in cases where the maximum principle does not hold were studied by Efendiev and Vougalter [37]. For nonlinear PNP equations, Kovtunen and Zubkova [38] guaranteed the balance of total mass and positivity for mass concentrations, forming the Gibbs simplex, within a reduced formulation when employing the positive part of diffusion fluxes. Numerical non-negativity can be achieved by non-local modelling of nonlinear terms within non-standard finite differences; see Mickens [39].

2. Theory

Electrokinetic rate equations to describe platinum catalyst degradation in PEM fuel cells were elaborated by Darling and Meyers [40]. Holby and Morgan [41] reduced subordinate chemical dissolution from the model focusing on the main electrochemical reactions of platinum ion dissolution



and platinum oxide formation



Holby et al. [42] and Li et al. [43] coupled the kinetic model with particle size distribution and approximated it with particle groups. Experimental and theoretical techniques were compared in the work [42] in order to validate the kinetic model. Agravante and Gostick [44], in their review, provided a detailed comparison of Darling–Meyers and Holby–Morgan governing equations, further simplifying assumptions made by the Rinaldo–Stumper–Eikerling model [45] and other models used in the field. Koltsova et al. [46] compared the results of experimental studies. The ECSA loss of the platinum catalyst was found to have a significant impact on overall fuel-cell performance loss. In the simulation [46], the effect of each degradation mechanism on the overall degradation of the platinum catalyst surface of the cathode was studied. See Figure 1 for the schematic illustration of the catalyst degradation process.

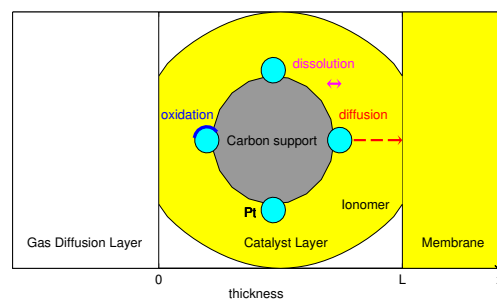


Figure 1. Illustration of the catalyst degradation process.

This study systematically examines the Holby–Morgan electrochemical model for degradation of a platinum catalyst under cyclic voltammetry from a mathematical point of view. Local sensitivity analysis in Kovtunen and Karpenko-Jereb [47] and in Karpenko-Jereb and Kovtunen [48] predicted variance of cycling operating condition, whereas Kovtunen [49,50] collected feasible domain for model parameters. The normal distribution of Pt particles was treated in Kovtunen [51], and in another study by the same author [52], the log-normal distribution was implemented, which is in good agreement with experimental data. Industrial protocols of electric potential of square and triangle wave forms with various upper potential levels were applied to the Holby–Morgan model to model the impact of cycling operating conditions on the durability of fuel cells. The existing Holby–Morgan degradation model is well established and widely used. The novelty of this work’s mathematical contribution consists of developing a pseudo-spectral method for highly efficient numerical computation of its discrete counterpart.

In a CL of thickness L (cm), the Holby–Morgan model looks for time-dependent distributions as $x \in [0, L]$ of the platinum ion (Pt^{2+}) concentration $c(t, x) > 0$ (mol/cm³), the platinum (Pt) particle diameter $d(t, x) > 0$ (cm), and the ratio of platinum oxide (PtO) coverage $\theta(t, x) \in (0, 1)$ (1). It validates the nonlinear system of reaction-diffusion equations [43]

$$\begin{cases} \frac{\partial c}{\partial t} - \varepsilon^{1/2} D_{\text{Pt}} \frac{\partial^2 c}{\partial x^2} = \frac{\pi N_{\text{Pt}}}{2\varepsilon V_{\text{Pt}}} d^2 r_{\text{dissol}}(c, d, \theta), \\ \frac{\partial d}{\partial t} = -\Omega r_{\text{dissol}}(c, d, \theta), \\ \frac{\partial \theta}{\partial t} + \frac{2\theta}{d} \frac{\partial d}{\partial t} = \frac{1}{\Gamma} r_{\text{oxide}}(\theta), \end{cases} \quad (1)$$

where the reaction rates r_{dissol} (mol/(cm² s)) and r_{oxide} (mol/(cm² s)) satisfy the following Butler–Volmer equations. The reaction rate of Pt^{2+} dissolution is

$$\begin{cases} r_{\text{dissol}}(c, d, \theta) = \Gamma(1 - \theta) \left(\nu_1 \exp \left[-\frac{H_{1,\text{fit}} + (1 - \beta_1)H_1(d, \theta)}{RT} \right] \right. \\ \left. - \nu_2 \frac{c}{c_{\text{ref}}} \exp \left[\frac{-H_{1,\text{fit}} + \beta_1 H_1(d, \theta)}{RT} \right] \right). \end{cases} \quad (2)$$

In (2), the molar enthalpy difference for dissolution (J/mol) is

$$H_1(d, \theta) = nF(U_{\text{eq}} - V) - \frac{4\Omega}{d}(\gamma_0(\theta) - \Gamma n_2 F \theta V), \quad (3)$$

and the surface tension difference (J/cm²) is

$$\begin{cases} \gamma_0(\theta) = \gamma + \Gamma RT \theta \left(\ln \left[\frac{\nu_2^*}{\nu_1^*} 10^{-2pH} \right] \right. \\ \left. + \frac{2n_2 F U_{\text{fit}} + \omega \theta}{2RT} + \ln \left(\frac{\theta}{2} \right) + \frac{2 - \theta}{\theta} \ln \left(1 - \frac{\theta}{2} \right) \right). \end{cases} \quad (4)$$

The reaction rate of PtO coverage yields

$$\begin{cases} r_{\text{oxide}}(\theta) = \Gamma \left(\nu_1^* \left(1 - \frac{\theta}{2} \right) \exp \left[-\frac{H_{2,\text{fit}} + \lambda \theta + (1 - \beta_2)H_2(\theta)}{RT} \right] \right. \\ \left. - \nu_2^* 10^{-2pH} \exp \left[\frac{-H_{2,\text{fit}} - \lambda \theta + \beta_2 H_2(\theta)}{RT} \right] \right), \end{cases} \quad (5)$$

with the molar enthalpy difference for oxidation (J/mol)

$$H_2(\theta) = n_2 F (U_{\text{fit}} - V) + \omega \theta. \quad (6)$$

The initial conditions are prescribed as

$$c = 0, \quad d = d_{\text{Pt}}, \quad \theta = 0 \quad \text{as } t = 0, \quad (7)$$

with a no-flux boundary condition at the left surface and zero at the right surface of the CL:

$$\frac{\partial c}{\partial x} = 0 \text{ as } x = 0, \quad c = 0 \text{ as } x = L. \quad (8)$$

In the governing relations (1)–(8), R is the gas constant and F is the Faraday constant. The catalyst's structural and kinetic parameters according to the literature [40–43] are gathered in Table 1 for Pt²⁺ dissolution and in Table 2 for PtO formation, and the key operating parameters are indicated in Table 3 and thereafter.

Table 1. The parameters for Pt²⁺ dissolution.

Symbol	Value	Units	Description
ν_1	1×10^4	Hz	dissolution attempt frequency
ν_2	8×10^5	Hz	backward dissolution rate factor
β_1	0.5		Butler transfer coefficient for dissolution
n	2		electrons transferred during dissolution
U_{eq}	1.118	V	Pt dissolution bulk equilibrium voltage
Ω	9.09	cm ³ /mol	molar volume of Pt
γ	2.4×10^{-4}	J/cm ²	Pt [1 1 1] surface tension
c_{ref}	1	mol/cm ³	reference Pt ²⁺ concentration
$H_{1,\text{fit}}$	4.4×10^4	J/mol	partial Pt dissolution activation enthalpy
D_{Pt}	1×10^{-6}	cm ² /s	diffusion coefficient of Pt ²⁺ in membrane

Table 2. The parameters for PtO formation.

Symbol	Value	Units	Description
ν_1^*	1×10^4	Hz	forward PtO formation rate constant
ν_2^*	2×10^{-2}	Hz	backward PtO formation rate constant
Γ	2.2×10^{-9}	mol/cm ²	Pt surface site density
β_2	0.5		Butler transfer coefficient for oxidation
n_2	2		electrons transferred during oxidation
U_{fit}	0.8	V	PtO formation bulk equilibrium voltage
λ	2×10^4	J/mol	PtO dependent kinetic barrier constant
ω	5×10^4	J/mol	Pt oxide–oxide interaction energy
$H_{2,\text{fit}}$	1.2×10^4	J/mol	partial PtO formation activation enthalpy

Table 3. The parameters of the CL.

Symbol	Value	Units	Description
L	10^{-3}	cm	thickness
T	353.15	K	temperature
pH	0		potential of hydrogen
d_{Pt}	3×10^{-7}	cm	Pt particle diameter
V_{Pt}	1.4×10^{-20}	cm ³	Pt particle density
p_{Pt}	4×10^{-4}	g/cm ²	Pt particle loading
ε	0.02		Pt/C volume fraction
ρ_{Pt}	21.45	g/cm ³	Pt particle density
N_{Pt}	1.3×10^{18}		Pt particle count

This study applies an asymmetric square profile for 40 s electric potential $V(t)$, alternating between voltages of 0.6 (V) for 10 (s) and 0.9 (V) for 30 (s), as recommended by the Fuel Cell and Hydrogen Joint Undertaking (FCH JU).

3. Methods

Advanced space-time discretization of the Holby–Morgan model (1)–(8) is described herein. Let time points $0 = t^0 < t^1 < \dots$ compose intervals of length $\tau^l := t^l - t^{l-1} > 0$ as $l = 1, 2, \dots$. Following time stepping by Ascher et al. [53], implicit–explicit (IMEX) iteration with an intermediate $(l - 1/2)$ time step was introduced in Kovtunen and Karpenko-Jereb [54]:

$$\begin{cases} c^{l-1/2} - w\tau^l \varepsilon^{1/2} D_{\text{Pt}} \frac{d^2 c^{l-1/2}}{dx^2} = c^{l-1} + w\tau^l \frac{\pi N_{\text{Pt}}}{2\varepsilon V_{\text{Pt}}} (d^{l-1})^2 r_{\text{dissol}}(c^{l-1}, d^{l-1}, \theta^{l-1}), \\ c^l = c^{l-1} + \tau^l \varepsilon^{1/2} D_{\text{Pt}} \frac{d^2 c^{l-1/2}}{dx^2} + \tau^l \frac{\pi N_{\text{Pt}}}{2\varepsilon V_{\text{Pt}}} (d^{l-1})^2 r_{\text{dissol}}(c^{l-1/2}, d^{l-1}, \theta^{l-1}), \\ \frac{dc^{l-1/2}}{dx} = \frac{dc^l}{dx} = 0 \text{ as } x = 0, \quad c^{l-1/2} = c^l = 0 \text{ as } x = L, \\ d^l = d^{l-1} - \tau^l \Omega r_{\text{dissol}}(c^{l-1}, d^{l-1}, \theta^{l-1}), \\ \theta^l = \theta^{l-1} + \tau^l \frac{2\Omega \theta^{l-1}}{d^{l-1}} r_{\text{dissol}}(c^{l-1}, d^{l-1}, \theta^{l-1}) + \tau^l \frac{1}{\Gamma} r_{\text{oxide}}(\theta^{l-1}), \end{cases} \quad (9)$$

where the IMEX parameter is set to $w = 0.5$ and initialized at $l = 0$ with

$$c^0 = 0, \quad d^0 = d_{\text{Pt}}, \quad \theta^0 = 0. \quad (10)$$

To solve the Cauchy problem (9)–(10) with nonlinear reaction terms with respect to $c^l(x)$, $d^l(x)$, and $\theta^l(x)$, the 4th-order Runge–Kutta method (RK4) with variable step size τ^l was elaborated in Kovtunen [55]. For the square-voltage FCG JU profile, the time step

is herein set to $\tau^l = 10^{-2}$ (s), which is refined locally to $\tau^l = 10^{-4}$ (s) when the electric potential takes off from $V = 0.6$ (V) to $V = 0.9$ (V) at time 10 (s) during each voltage cycle of 40 (s).

Aiming at accurate space approximation, this study applies the Chebyshev–Gauss–Lobatto (CGL) pseudo-spectral collocation method, which may achieve exponential convergence. For a natural number $p \geq 2$, let the CL thickness $[0, L]$ be split by Chebyshev collocation points

$$\xi_k := -\cos\left(\frac{\pi(k-1)}{p}\right), \quad x_k := \frac{L}{2}(1 + \xi_k), \quad k = 1, \dots, p+1, \quad (11)$$

with end points $x_1 = 0$ and $x_{p+1} = L$. Lagrange polynomials of degree p

$$\ell_k^p(x) := \prod_{m \neq k} \frac{x - x_m}{x_k - x_m}, \quad k = 1, \dots, p+1, \quad (12)$$

validate the interpolation property

$$\ell_k^p(x_m) = \begin{cases} 1 & \text{if } m = k, \\ 0 & \text{if } m \neq k. \end{cases}$$

The solution ansatz in the polynomial basis

$$c^l(x) = \sum_{k=1}^{p+1} c_k^l \ell_k^p(x), \quad d^l(x) = \sum_{k=1}^{p+1} d_k^l \ell_k^p(x), \quad \theta^l(x) = \sum_{k=1}^{p+1} \theta_k^l \ell_k^p(x) \quad (13)$$

fully discretizes Equations (9) and (10) in the form

$$\begin{cases} c_k^{l-1/2} - w\tau^l \varepsilon^{1/2} D_{\text{Pt}} \sum_{n=1}^p S_{kn} c_n^{l-1/2} \\ = c^{l-1} k + w\tau^l \frac{\pi N_{\text{Pt}}}{2\varepsilon V_{\text{Pt}}} (d_k^{l-1})^2 r_{\text{dissol}}(c_k^{l-1}, d_k^{l-1}, \theta_k^{l-1}), & c_{p+1}^{l-1/2} = 0, \\ c_k^l = c_k^{l-1} + \tau^l \varepsilon^{1/2} \sum_{n=1}^p S_{kn} c_n^{l-1/2} \\ + \tau^l \frac{\pi N_{\text{Pt}}}{2\varepsilon V_{\text{Pt}}} (d_k^{l-1})^2 r_{\text{dissol}}(c_k^{l-1/2}, d_k^{l-1}, \theta_k^{l-1}), & c_{p+1}^l = 0, \\ d_k^l = d_k^{l-1} - \tau^l \Omega r_{\text{dissol}}(c_k^{l-1}, d_k^{l-1}, \theta_k^{l-1}), \\ \theta_k^l = \theta_k^{l-1} + \tau^l \frac{2\Omega \theta_k^{l-1}}{d_k^{l-1}} r_{\text{dissol}}(c_k^{l-1}, d_k^{l-1}, \theta_k^{l-1}) + \tau^l \frac{1}{I} r_{\text{oxide}}(\theta_k^{l-1}), \end{cases} \quad (14)$$

subjected to the initial condition

$$c_k^0 = 0, \quad d_k^0 = d_{\text{Pt}}, \quad \theta_k^0 = 0. \quad (15)$$

In (14), the stiffness matrix

$$S_{kn} := \sum_{m=2}^{p+1} D_{km} D_{mn} \quad (16)$$

is built from the matrix of derivatives (see Gheorghiu [56])

$$D_{mn} := \frac{2}{L} \begin{cases} \frac{\alpha_m (-1)^{m+n}}{\alpha_n \zeta_m + \zeta_n} & \text{if } m \neq n, \\ -\frac{\zeta_m}{2(1-\zeta_m)^2} & \text{if } m = n = 2, \dots, p, \\ \frac{2p^2 + 1}{6} & \text{if } m = n = 1, \\ -\frac{2p^2 + 1}{6} & \text{if } m = n = p + 1 \end{cases} \quad (17)$$

where $\alpha_m = 1$ as $m = 2, \dots, p$, and $\alpha_1 = \alpha_{p+1} = 1$. The Neumann boundary conditions at $x_1 = 0$ are incorporated in S by means of the identities

$$\sum_{n=1}^{p+1} D_{1n} c_n^{l-1/2} = 0, \quad \sum_{n=1}^{p+1} D_{1n} c_n^l = 0.$$

To test the accuracy of the CGL approximation, (11)–(17), it is herein compared with uniform meshing of the CL thickness by $N + 1$ points with equal spacing $h := L/N$. The maximum error during $l = 1, \dots, 4037$ time steps within one voltage cycle, measured as a percentage with respect to the finest mesh of $N = 100$, is depicted in Figure 2 versus the reciprocal of the number of points ($\#points$). The errors in Pt^{2+} concentration c , Pt particle diameter d , and PtO coverage ratio θ are shown through respective plots (a)–(c). There, one line represents uniform meshing by $N = 10, \dots, 90$ (that is $(\#points)^{-1} = 1/N$), and another line is obtained for Chebyshev collocation points as $p = 2, 3, 4$ (that is, $(\#points)^{-1} = 1/p$). Whereas the error in Figure 2b,c is negligible, one concludes from Figure 2a that the 8% threshold for $N + 1 = 11$ of uniform points, which was used in our previous works, is easily improved by only $p + 1 = 3$ of collocation points. Correspondingly, the accuracy for $N + 1 = 101$ uniform points is attained by the use $p + 1 = 5$ CGL basis polynomials.

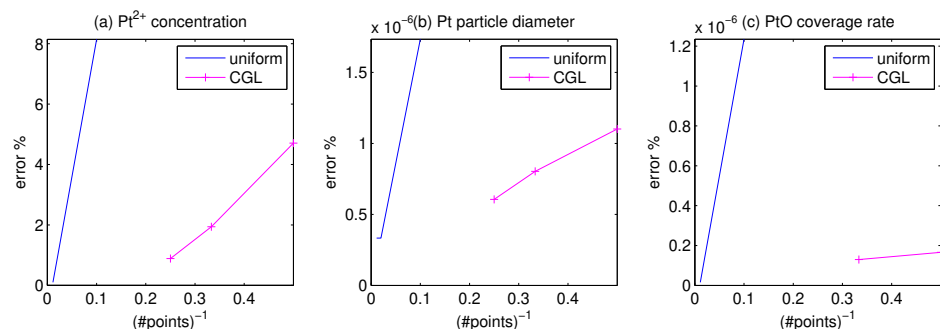


Figure 2. Maximum error within voltage cycle for Pt^{2+} concentration c (a), Pt particle diameter d (b), and PtO coverage ratio θ (c) against reciprocal value of $\#points$.

For convenience, selected numerical values of the error are collected in Table 4.

Table 4. Maximum error within voltage cycle for uniform meshing and for CGL collocation.

#Points	(#Points) ^{−1}	Error c (%)	Error d (%)	Error θ (%)
$N = 10$	$1/N = 0.1$	8.14	1.73×10^{-6}	1.23×10^{-6}
$N = 50$	$1/N = 0.02$	0.89	3.33×10^{-7}	1.37×10^{-7}
$N = 90$	$1/N = 0.01$	0.09	3.33×10^{-7}	1.52×10^{-7}
$p = 2$	$1/p = 0.5$	4.7	1.1×10^{-6}	1.65×10^{-7}
$p = 3$	$1/p = 0.33$	1.93	8.03×10^{-7}	1.29×10^{-7}
$p = 4$	$1/p = 0.25$	0.88	6.05×10^{-7}	1.37×10^{-7}

With the help of (11)–(13), it is possible to approximate the weighted integral mean

$$\tilde{c}^l := \int_0^L \frac{c^l(x) dx}{\pi \sqrt{1 - (\frac{2}{L}x - 1)^2}}, \quad \tilde{d}^l := \int_0^L \frac{d^l(x) dx}{\pi \sqrt{1 - (\frac{2}{L}x - 1)^2}}, \quad \tilde{\theta}^l := \int_0^L \frac{\theta^l(x) dx}{\pi \sqrt{1 - (\frac{2}{L}x - 1)^2}}$$

as the CGL quadrature

$$\tilde{c}^l = \sum_{k=1}^{p+1} w_k c_k^l, \quad \tilde{d}^l = \sum_{k=1}^{p+1} w_k d_k^l, \quad \tilde{\theta}^l = \sum_{k=1}^{p+1} w_k \theta_k^l, \quad (18)$$

where the weights are $w_k := 1/(\alpha_k p)$. These formulas (18) are exact for polynomials of degree $2p + 1$ and will be used in the following evaluation.

4. Results

On every time interval $t \in [t^{l-1}, t^l]$, let Lagrange interpolation polynomials be defined according to (12) as

$$\ell_1^2(t) := \frac{t - t^l}{t^{l-1} - t^l}, \quad \ell_2^2(t) := \frac{t - t^{l-1}}{t^l - t^{l-1}}. \quad (19)$$

Then, using spatial expansion (13), the solution is interpolated piecewise linearly in time as

$$\begin{cases} c(t, x) = \ell_1^2(t) c^{l-1}(x) + \ell_2^2(t) c^l(x), \\ d(t, x) = \ell_1^2(t) d^{l-1}(x) + \ell_2^2(t) d^l(x), \\ \theta(t, x) = \ell_1^2(t) \theta^{l-1}(x) + \ell_2^2(t) \theta^l(x). \end{cases} \quad (20)$$

For one voltage cycle, the numerical solution (19)–(20) is presented in Figure 3 as the triple (c, d, θ) . It is depicted versus time $t \in (0, 40)$ (s) along the catalyst thickness $x \in (0, 10)$, measured in microns (μm). In Figure 3a, the variation in the space variable is observed to be highly significant for Pt^{2+} concentration c due to the diffusion term in the model. Meanwhile, variation along CL is less visible for Pt particle diameter in Figure 3b and PtO coverage ratio in Figure 3c, since d and θ are affected indirectly by c through the reaction term r_{dissol} .

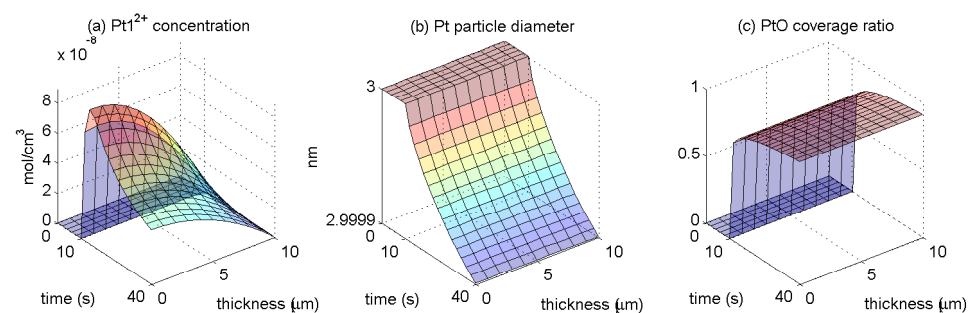


Figure 3. Solution within 1 cycle: Pt^{2+} concentration c (a), Pt particle diameter d (b), and PtO coverage ratio θ (c) against time $t \in (0, 40)$ (s) and thickness $x \in (0, 10)$ (μm).

The weighted integral means over the thickness are defined according to (18) as

$$\begin{cases} \tilde{c}(t) = \ell_1^2(t) \tilde{c}^{l-1} + \ell_2^2(t) \tilde{c}^l, \\ \tilde{d}(t) = \ell_1^2(t) \tilde{d}^{l-1} + \ell_2^2(t) \tilde{d}^l, \\ \tilde{\theta}(t) = \ell_1^2(t) \tilde{\theta}^{l-1} + \ell_2^2(t) \tilde{\theta}^l. \end{cases} \quad (21)$$

For 10 cycles during 6.6 (min), we depict the respective $(\tilde{c}, \tilde{d}, \tilde{\theta})$ from (21) in Figure 4 for $l = 1, \dots, 40,370$ time steps. The Pt^{2+} concentration $c(t)$ in Figure 4a and PtO coverage ratio $\theta(t)$ in Figure 4c oscillate periodically between zero and some positive value. In contrast, the Pt particle diameter $d(t)$ in Figure 4b demonstrates a steady decrease over time with small oscillations.

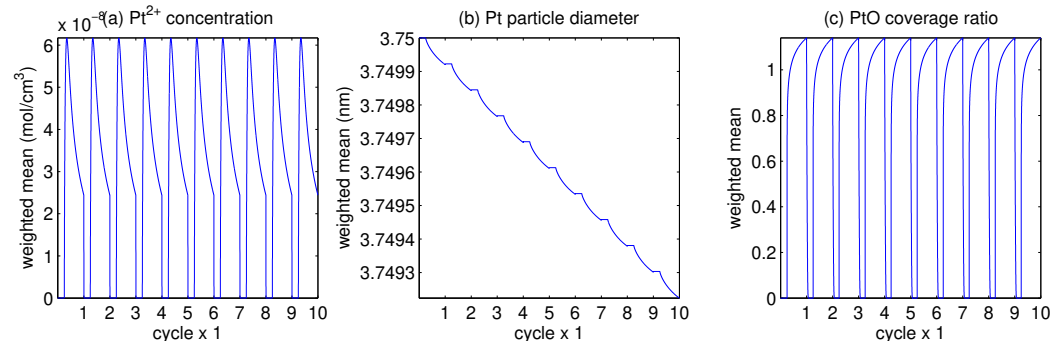


Figure 4. Weighted integral means within 10 cycles: Pt^{2+} concentration c (a), Pt particle diameter d (b), and PtO coverage ratio θ (c) against time $t \in (0, 400)$ (s).

Furthermore, degradation under AST cycling is investigated in terms of the Pt particle diameter d , electrochemical surface area

$$ECSA := 0.63 \frac{\pi N_{\text{Pt}}}{2} d^2,$$

where the rescaling parameter is derived from experimental data to adjust a model geometric surface area, measured by transmission electron microscopy, to experimental ECSA, measured by cyclic voltammetry (see [42]) and Pt mass

$$m := \frac{\pi}{6} d^3.$$

We measure the relative loss ratio with respect to initial value at $t = 0$ using the weighted integral mean defined by the CGL quadrature (18) such that

$$d_{\text{rat}}(t) := \frac{\tilde{d}(t)}{\tilde{d}(0)}, \quad E_{\text{rat}}(t) := \frac{\widetilde{ECSA}(t)}{\widetilde{ECSA}(0)} = d_{\text{rat}}^2(t), \quad m_{\text{rat}}(t) := \frac{\tilde{m}(t)}{\tilde{m}(0)} = d_{\text{rat}}^3(t). \quad (22)$$

For 100 cycles during 1.1 (h), the ratios $(d_{\text{rat}}, E_{\text{rat}}, m_{\text{rat}})$ from (22) are presented in Figure 5a–c for 403,700 time steps. Here, small oscillations for each cycle become invisible along the decaying curves. It is evident that d_{rat} has the lowest loss rate and m_{rat} the highest loss rate over time.

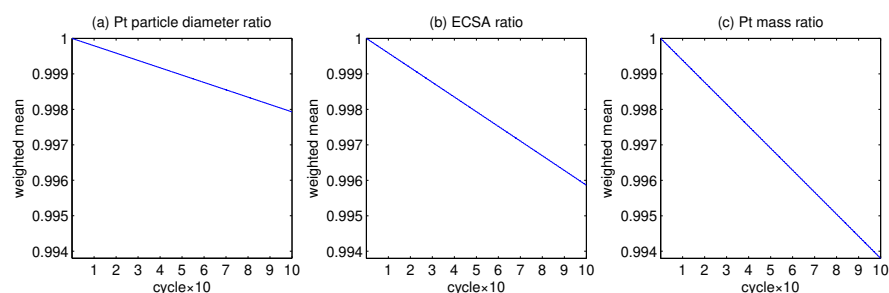


Figure 5. Ratio of weighted integral means within 100 cycles: Pt particle diameter $d_{\text{rat}}(t)$ (a), ECSA $E_{\text{rat}}(t)$ (b), and Pt mass $m_{\text{rat}}(t)$ (c) against time $t \in (0, 4000)$ (s).

Similarly, for 1000 cycles during 11.1̄ (h) of AST, time-dependent values of $(d_{\text{rat}}, E_{\text{rat}}, m_{\text{rat}})$ are shown in Figure 6a–c for 4,037,000 steps. Both Figures 5 and 6 illustrate a linear degradation for all the physical quantities starting at a value of one as $t = 0$. Thus, electrochemical degradation in the early stage is dominated by dissolution of small platinum particles. If it continued in this way, then the Pt mass ratio would reach zero in about 15.5 thousand potential cycles.

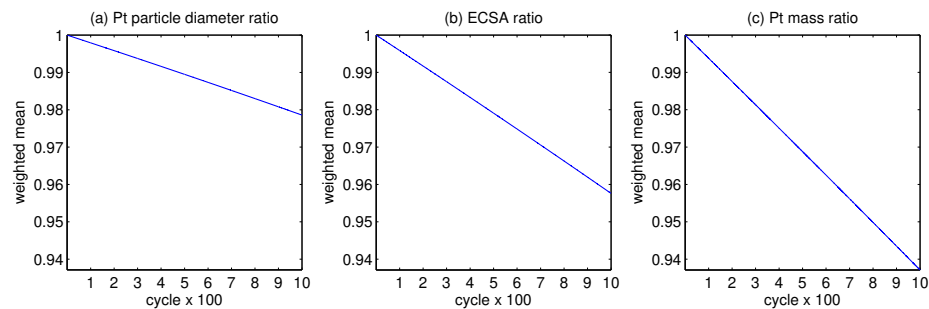


Figure 6. Ratio of weighted integral means within 1000 cycles: Pt particle diameter $d_{\text{rat}}(t)$ (a), ECSA $E_{\text{rat}}(t)$ (b), and Pt mass $m_{\text{rat}}(t)$ (c) against time $t \in (0, 40,000)$ (s).

The above behaviour changes dramatically to a nonlinear degradation when AST testing is continued for 10,000 cycles during 111.1̄ (h), that is, $l = 1, \dots, 40,370,000$ time steps. Transition toward the nonlinear phase is likely governed by coarsening of platinum nano-particles due to Ostwald ripening and coalescence mechanisms. In Table 5, we collect selected values of losses $(d_{\text{rat}}, E_{\text{rat}}, m_{\text{rat}})$ together with the loss rates $(d'_{\text{rat}}, E'_{\text{rat}}, m'_{\text{rat}})$ given per ten thousand cycles (that is, times 10^{-4} per cycle).

Table 5. Losses of physical quantities and loss rates over ten thousand cycles.

#Cycles	d_{rat}	d'_{rat}	E_{rat}	E'_{rat}	m_{rat}	m'_{rat}
1000	0.98	0.22	0.96	0.43	0.94	0.64
2000	0.95	0.24	0.91	0.46	0.87	0.66
3000	0.93	0.26	0.86	0.49	0.80	0.69
4000	0.90	0.29	0.81	0.54	0.73	0.73
5000	0.87	0.34	0.75	0.59	0.66	0.78
6000	0.83	0.40	0.69	0.68	0.57	0.85
7000	0.78	0.52	0.61	0.82	0.48	0.97
8000	0.72	0.75	0.52	1.10	0.37	1.20
9000	0.60	2.04	0.36	2.50	0.51	2.30

The corresponding curves $(d_{\text{rat}}, E_{\text{rat}}, m_{\text{rat}})$ depicted in Figure 7a–c start to fall sharply after about 90,000 voltage cycles (that is, 100 h). At this moment, Pt diameter has decreased by 40%, ECSA by 64%, and Pt mass by 49% from the initial values. In this respect, it is worth remembering the quadratic relationship from (22) for the surface area E_{rat} in plot (b) and the cubic relationship for the mass m_{rat} in plot (c) with respect to the particle size d_{rat} given in plot (a). The 1D model assumes spatially homogeneous electrokinetic rates such that all quantities of interest change along one dimension across the catalyst only and remain unchangeable in other directions. Across the CL's thickness, the degradation is stronger at the right surface $x = L$, where the catalyst matches the membrane due to hydrogen and oxygen crossover. At this end the boundary condition $c = 0$ is imposed, and we observe first that $d = 0$ after 92,000 cycles. Then the quantities continue to fall toward the CL left surface $x = 0$ matching gas diffusion layer such that its weighted integral means are zero. Approximately at 96,000 cycles the weighted integral mean of Pt²⁺ concentration

$\tilde{c}$ becomes close to zero, thereafter the weighted integral mean of Pt particle diameter $\tilde{d}$ falls zero at about 98,000 cycles. To this end CL fully loses its operating capability.

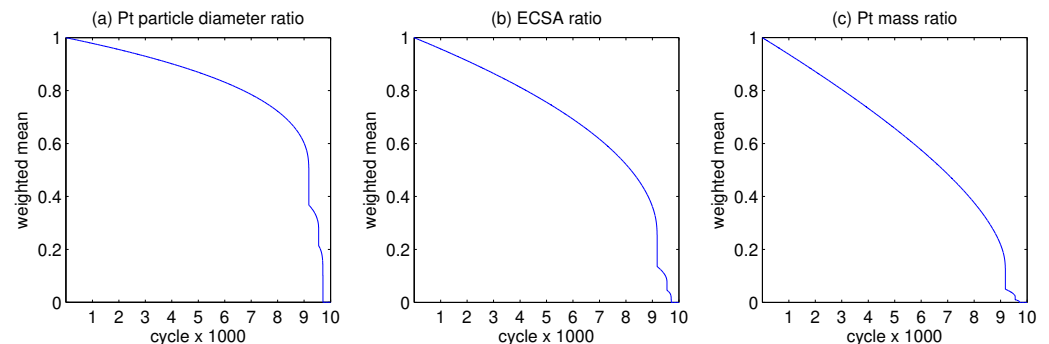


Figure 7. Ratio of weighted integral means within 10,000 cycles: Pt particle diameter $d_{\text{rat}}(t)$ (a), ECSA $E_{\text{rat}}(t)$ (b), and Pt mass $m_{\text{rat}}(t)$ (c) against time $t \in (0, 400,000)$ (s).

5. Discussion

Degradation processes in fuel cells can be studied using both experiments and simulations. Computer models are cost-effective, with simplified 0D or 1D models often being used, and they involve theoretical hypotheses regarding degradation mechanisms.

Numerical simulation of catalysts is particularly beneficial, owing to their small thickness and complex assembly processes for experimental monitoring of internal electrochemical phenomena. Agravante and Gostick [57] developed a novel approach to platinum degradation using a pore network generating a 2D artificial image of the cathode CL. To predict spatially distributed cell states with high computational efficiency, Altmann et al. [58] presented a quasi-2D time-dependent multi-phase model. Through laboratory experiments, Raga et al. [59] validated a 3D numerical model that characterizes the degradation mechanisms of carbon support corrosion, platinum and carbon oxidation, as well as proton conductivity loss due to acid washout in the membrane of a high-temperature PEMFC. Aiming at further reduction of testing duration regardless of the application case, Thiele et al. [60] proposed an optimization method to generate optimal parameters for realistic testing based on automotive driving cycles.

Inhomogeneous catalytic systems stem from a wide range of chemical synthesis coupling surface kinetics with mass transport, which may occur at different time and length scales. Mathematically, this implies systems of PDE with highly nonlinear reactions or boundary conditions imposed by the surface chemistry. Solving numerically stiff problems by the conventional Computational Fluid Dynamic (CFD) methods involves huge computational costs. Qureshi et al. [61] presented a reduced approach achieved by a low-order asymptotic expansion with respect to the catalyst characteristic size and demonstrated it for a 2D channel flow. The idea behind the order reduction is relevant to minimizing the error of basis functions for solutions.

Spectral methods, finite difference methods, and finite element methods are the main discretization techniques suitable for simulation of stationary and evolutionary differential equations on computers. The reader can find key ideas regarding spectral methods and their programming in MATLAB version 5.3 in the handbook by Trefethen [62]. For spectral points, the roots or extrema of Chebyshev polynomials are commonly used (see Tch bychew [63]). The pseudo-spectral collocation method typically approximates a solution expressed in terms of Lagrange basis polynomials. Schillinger et al. [64] demonstrated that collocation is significantly less expensive than standard Galerkin finite element methods.

Aghdam et al. [65] developed a numerical scheme for discretization of the diffusion equation of fractional order. After time stepping by compact finite differences, the spatial

fractional derivative is approximated by the collocation method using Chebyshev polynomials of the fourth kind as test and trial function basis. To demonstrate the performance of different spectral collocation schemes, Nova et al. [66] considered collocation points generated from Gauss–Lobatto nodes; roots of Chebyshev polynomials of the first kind; roots of Legendre polynomials; and equally spaced nodes over the space domain. Supported by time-discrete stability and convergence analysis, numerical examples illustrate the high performance and accuracy of the Chebyshev pseudo-spectral collocation method for representation of integer- and fractional-order diffusion.

6. Conclusions

This study investigated the one-dimensional Holby–Morgan model of electrochemical degradation of platinum in a carbon cathodic catalyst in a proton exchange membrane fuel cell with respect to its lifetime.

A harmonized testing protocol with an asymmetric square-wave potential profile, which is recommended by the European Union, was applied for durability test under accelerated stress cycling. Ion diffusion drives platinum degradation by re-deposition of nano-particles dissolved from the cathode onto larger particles (commonly called Ostwald ripening) and by platinum band formation. This paper aimed to achieve a good approximation of spatial distribution for all physical quantities that change across the catalyst thickness due to diffusion phenomena. Diffusivity is involved in the model directly through platinum ion concentration as well as indirectly through dissolution reaction.

To simulate numerically the long-term behaviour of the platinum catalyst, this study introduced into consideration a highly accurate Chebyshev–Gauss–Lobatto method, which is of the pseudo-spectral collocation type. The spatial approximation attained an error threshold of about 5% by the use of only three Lagrange polynomials on three Chebyshev collocation points. For time stepping, this study employed an advanced implicit–explicit discretization with intermediate time steps incorporated into the standard fourth-order Runge–Kutta method. The efficient discretization makes it possible to overcome the linear degradation within 1,000 voltage cycles obtained in previous works, as well as to achieve nonlinear degradation in 10,000 cycles over more than 100 h. In fact, the degradation curve of platinum particle diameter and, consequently, electrochemical surface area over time falls sharply against zero until operating capability is lost.

Funding: This research received no external funding.

Data Availability Statement: The research data are available upon reasonable request.

Conflicts of Interest: The author declares no conflicts of interest.

Abbreviations

AST	Accelerated Stress Test
CL	Catalyst Layer
CGL	Chebyshev–Gauss–Lobatto
CFD	Computational Fluid Dynamic
ECSA	Electrochemical Surface Area
FCH JU	Fuel Cell and Hydrogen Joint Undertaking
IMEX	Implicit–Explicit
PDE	Partial Differential Equation
PV	Photovoltaic
Pt	Platinum
Pt ²⁺	Platinum (II) Ion
PtO	Platinum Oxide

PNP	Poisson–Nernst–Planck
PEM	Polymer Electrolyte Membrane
RK4	4th-Order Runge–Kutta Method

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