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Direct numerical simulation of near-wall turbulent flow and ionic mass transport in electrochemical reactors using a hybrid finite element/spectral method

M. Krivilyov [a,b,*], M. Rasquin [c,d], L. Stappers [b], G. Gordeev [a], J. Fransaer [b], G. Degrez [c]

[a] Udmurt State University, Department of Physics, Universitetskaya str. 1, 426034 Izhevsk, Russia
[b] KU Leuven, Department of Materials Engineering, Kasteelpark Arenberg 44, 3001 Heverlee, Belgium
[c] Université Libre de Bruxelles, Service de Mécanique des Fluides, CP 165/43, Av. F.D. Roosevelt, 50, 1050 Brussels, Belgium
[d] Cenaero Research Center, Rue des Frères Wright 29, Bâtiment Eole, 6041 Gosselies, Belgium

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ABSTRACT

An experimental study and direct numerical simulation of near-wall turbulent flow and ionic mass transport was performed in a cylindrical electrochemical reactor for Reynolds numbers up to 18,000 (friction Reynolds number of 1245). The experimental part involved the determination of velocity gradients close to the wall of a rotating cylinder. These velocity gradients are determined by electrochemical mass transport measurements to a rotating cylinder electrode and to micro-electrodes embedded in a rotating cylinder. Simulation of the fluid flow with passive scalar is accomplished using a hybrid finite element method (FEM) in meridian planes coupled to a Fourier expansion in the azimuthal direction. It was shown that the method reproduces the turbulent flow statistics with high accuracy. Due to its high parallel efficiency and the possibility of stretched meshes in finite element planes near the wall, this hybrid method is suitable to study laboratory electrochemical systems. Coupling with mass and energy transport equations allows prediction of the concentration and temperature fields. This feature makes the model suitable for large-scale design and optimization of different electrochemical processes where accurate prediction of near-wall turbulence and ionic mass transport is required.

1. Introduction

Turbulent flow in combination with mass and heat transfer is encountered in many chemical and electrochemical processes. For example, forced flow is used to enhance mass transport during electrolytic deposition of metal coatings. Fluid flow influences the concentration of ions at the electrode and hence influences the current density. As a result, local variations in flow can result in non-uniform metal deposition. In case of metal alloy plating, local flow variations can also result in non-uniform alloy composition. Temperature variations at electrodes are also important since they can lead to electrical "burning" and bubble formation. Therefore, the study of fluid flow in electrochemical reactors is of practical importance and 3D numerical simulation has become an essential tool for this purpose.

Turbulent flow between rotating co-axial cylinders in a Taylor–Couette (TC) apparatus has been studied intensively for decades since the pioneering works of Couette [1], Mallock [2,3] and Taylor [4]. TC flow exhibits a wide variety of flow regimes which makes it an ideal subject for analysis. Due to curvature of the cylinders, instabilities develop in TC systems. With increasing Reynolds number, these instabilities lead to annular vortices called Taylor vortices (TV) and finally result in fully turbulent flow. Many experimental and theoretical results on TC flow (TCF) were obtained by Swinney and coworkers during last two decades, see [5] and references herein. The most recent numerical simulations of TCF are found in [6,7].

Apart from its fundamental importance, TC flow has a lot of practical applications such as dynamic filtration, viscosimetry and turbulent chemical or electrochemical reactors. However, to use TC flow for electrochemical reactors, it is important to understand mass transport in this geometry. Experimental studies of transport phenomena in electrochemical processes on rotating cylinders were performed by different authors [8–13], but only a few studies are devoted to 3D numerical modeling. A comprehensive study was performed in [14,15] where Large Eddy Simulation (LES) modeling was used to calculate the fluid flow in a reactor

* Corresponding author.
E-mail address: mk@udsu.ru (M. Krivilyov).

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Nomenclature

Greek symbols

α	velocity gradient [s^{-1}]
γ	scaling coefficient [–]
Γ	aspect ratio [–]
η	radius ratio [–]
θ	tangential coordinate [rad]
λ_z	periodicity in the axial direction [m]
μ	dynamic viscosity [Pa s]
ν	kinematic viscosity [$m^2\ s^{-1}$]
ρ	density [$kg\ m^{-3}$]
ω	rotation speed [$rad\ s^{-1}$]

Latin symbols

A	shape factor [–]
C	concentration [$mol\ m^{-3}$]
D	diffusion coefficient [$m^2\ s^{-1}$]
G	torque [N m]
H	transfer function [–]
I	limiting current [$A\ m^{-2}$]
T	period [s]
W	power spectral density [$A^2\ Hz^{-1}$]
d	micro-electrode diameter [m]
f	frequency [Hz]
h	height of the reactor [m]
n	valence [–]
p	kinematic pressure [$m^2\ s^{-2}$]
r	radial coordinate [m]
s	gap width [m]
t	time [s]
z	axial coordinate [m]
$\mathbf{u}$	velocity vector [$m\ s^{-1}$]

Subscripts

i,j	index of r, θ or z

Other

C_M	torque coefficient [–]
Pe	Péclet number [–]
Re	Reynolds number [–]
Re_τ	friction Reynolds number [–]
Sc	Schmidt number [–]
Ta	Taylor number [–]
r_i	inner radius [m]
r_o	outer radius [m]
NSE	Navier–Stokes equations
TC	Taylor–Couette
TCF	Taylor–Couette flow
TV	Taylor vortices
RCE	rotating cylindrical electrode
DNS	direct numerical simulation
LES	Large Eddy Simulation
RANS	Reynolds-Average Navier–Stokes
FFT	Fast Fourier Transform
FEM	finite-element method

with a planar geometry. Nevertheless, comprehensive analysis of electrochemical systems using combined modeling of the Navier–Stokes equations (NSE) and heat and mass transport equations is still lacking. Some studies related to turbulent flow and passive scalars are available in the literature (see [16] and references herein).

In principle, three different approaches of theoretical description of turbulent flow are possible. The first approach is based on the Reynolds-Average Navier–Stokes (RANS) method [17] where the effect of turbulence is introduced into the model by filtering (averaging) of NSE in time. The second approach is based on direct numerical simulation (DNS) of NSE with spatial and time resolution fine enough to capture all scales present in the flow. Although this is the most accurate method, its drawback is a steep growth of the number of degrees of freedom as the Reynolds number increases. The third approach is the LES method where small-scale turbulence is modeled via a subgrid model [18]. Although some subgrid models are well established and confirmed by numerous experiments [19], selection of the case-specific submodel is always based on a preliminary analysis of experimental data. In case of electrochemical systems, correct statistics of turbulence and power spectral density of the velocity gradient, concentration and temperature fluctuations are especially important for adequate evaluation of the local current density. Therefore imposing an inappropriate subgrid model may lead to wrong statistics which are not physical.

So both DNS and LES provide the accurate solution of the flow field in a fully turbulent regime if meshing is fine enough in the computational domain, especially in the near-wall regions. However there is a shortcoming which becomes a serious obstacle if real electrochemical reactors are analyzed. The Schmidt number for the majority of practical applications is about 10^3. At such Schmidt numbers, the boundary layer relevant to the ionic mass transport near the electrode is much thinner than the hydrodynamic boundary layer. So two different scales are observed in the system: the larger scale defined by the fluid flow and the smaller scale controlled by the ionic diffusion. Therefore even if the hydrodynamic boundary layer is properly resolved, the diffusion boundary layer requires a much finer mesh. Consequently simulation of ionic transport in electrochemical systems is a challenging problem due to different time and spatial scales of all relevant processes.

The goal of this research was twofold. The first objective was the development of a numerical tool for the analysis of mass transfer in purely turbulent regimes. In this paper a hybrid finite element method in meridian planes combined with a Fourier expansion in the azimuthal direction for the Navier–Stokes equations coupled with ionic and energy transport equations is first described. Similar hybrid FE/spectral discretization have already been proposed for the Navier–Stokes equation and magnetohydrodynamics equations. See e.g. [20–23] and references therein. Therefore, the first originality of this paper lies in the addition of passive scalar transport to a hybrid FE/spectral discretization.

The second contribution of this paper is the application of this hybrid method to DNS of turbulent flows and ion transport in an electrochemical cell with validation with respect to experiments. As a result, the numerical tool presented in this work can assist or even replace experimental studies where data on mass transfer are difficult to determine by classical electrochemical methods.

This paper is organized as follows. Section 2 contains the description of the experimental setup and the characteristic numbers for the experimental geometry. It also describes the measurements of near wall turbulence and local current density. Section 3 provides the governing equations of the model and explains the details of the numerical implementation. Coupling between momentum, mass transport and energy transport equations is also