



## Justifying the significance of Knudsen diffusion in solid oxide fuel cells



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### ABSTRACT

Developing an appropriate diffusion mechanism to analyze the gas transport in porous electrodes of SOFCs (solid oxide fuel cells), has been a crucial step towards analyzing accurately the cell performance. In this report, the errors in evaluating the gas diffusivity, limiting current density and concentration polarization, are calculated quantitatively by taking bulk diffusion and the previously-overlooked Knudsen diffusion into account. In particular, this work analyzes the deviation between ignoring and considering the Knudsen diffusion of hydrogen transport in SOFC anodes. The study facilitates the rational pre-evaluation of micro- and nanoscale materials prior to assembly into SOFCs.

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## 1. Introduction

In addition to traditional power resources, renewable energy sources including hydrogen, wind and solar energy, have been the focus of both academic and industrial investigations over the past decades [1–6]. SOFCs (Solid oxide fuel cells), one of the most promising energy conversion devices, have received extensive attention due to the flexibility in assembly [7,8], widespread applicability to a variety of fuels [9,10], high efficiency overcoming the Carnot cycle [11,12], etc. To develop high-performance SOFCs, tremendous efforts have been focused on the evaluation of the important factors such as effective diffusivity ( $D_{H_2}^{eff}$ ) [13], limiting current density ( $i_{qs}$ ) [14] and CP (concentration polarization) [1,15,16]. It is widely accepted that the three pivotal factors are influenced significantly by the electrode parameters in SOFCs, including pore size, porosity, tortuosity and thickness [17,18]. For a feasible performance assessment, the theoretical evaluation of electrode diffusion mechanisms has attracted extensive attention. In particular, for micro- and nanoscale materials, both Knudsen

diffusion and bulk diffusion should be considered simultaneously as the mean free path of gas species becomes close to the size of electrode pores [19,20]. Dreyer et al. simulated gas transport in porous nanostructures with consideration on Knudsen diffusion [21]. Cayan et al. corrected the diffusivity coefficient inside the porous electrode in SOFCs with Knudsen diffusion included [22]. Qu et al. stated that Knudsen diffusion could not be neglected in modeling gas diffusion in an SOFC system [23]. Undoubtedly, neglecting Knudsen diffusion in evaluating micro/nano-scale pores could cause inaccuracy in the evaluation of SOFC performances [24] and, thus, an insightful systematic error analysis on micro/nano-scale porous SOFCs is critically needed. In this article, two diffusion models, the model only based on bulk diffusion and the model combining both Knudsen and bulk diffusions, are analyzed systematically. By employing the model proposed by Zhao et al. [25], and developed by He et al. [1,16,26], the errors at different conditions are evaluated. This work facilitates the assessment on the efficiencies of different diffusion models, as well as the rational design and selection of electrode materials for improving the performance of SOFCs.

## 2. Theoretical analysis

The structure schematic of an SOFC is shown in Fig. 1, with both the anode and cathode supported with porous materials. At the

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cathode, oxygen molecules are converted into oxygen ions and diffuse through the electrolyte to the anode upon employing a concentration gradient. Mixed nickel/yttria-stabilised zirconia cermet is assembled into the anode, where the fuel gas diffuses into anode/electrolyte interface and reacts with oxygen ions under the pressure gradient [27–30].

Within pores in the porous electrode of a typical fuel cell, gas transports in bulk and Knudsen diffusion mechanisms. The collisions of molecules form bulk diffusion while the collisions between molecules and the pore wall result in the Knudsen diffusion [31]. Here, Knudsen number ( $Kn$ ), a key parameter representing the ratio of gas mean free path to average pore diameter, is utilized to distinguish the aforementioned diffusion mechanisms. With a large value of  $Kn$  ( $Kn > 10$ ), bulk diffusion is weak and negligible compared with Knudsen diffusion. On the contrary, as  $Kn < 0.1$ , bulk diffusion dominates the gas transport [16,32]. As for a moderate  $Kn$  ( $0.1 < Kn < 10$ ), both diffusion mechanisms should be taken into consideration. Therefore, underestimating the Knudsen diffusion effect could lead to inaccurate results including imprecise diffusivity measurement and evaluations of limiting current density and concentration polarization.

Correlation between bulk diffusion and Knudsen diffusion is shown in Eqs. (1) and (2) [2],

$$\frac{1}{D_{H_2}^{eff}} = \frac{1}{D_{H_2,K}^{eff}} + \frac{1}{D_{H_2-H_2O}^{eff}} \quad (1)$$

$$\frac{1}{D_{H_2O}^{eff}} = \frac{1}{D_{H_2O,K}^{eff}} + \frac{1}{D_{H_2-H_2O}^{eff}} \quad (2)$$

where  $D_{H_2}^{eff}$  and  $D_{H_2O}^{eff}$  are effective diffusivities of  $H_2$  and  $H_2O$ , respectively,  $D_{H_2,K}^{eff}$  and  $D_{H_2O,K}^{eff}$  are Knudsen diffusivities of  $H_2$  and  $H_2O$ , respectively, and  $D_{H_2-H_2O}^{eff}$  is the effective bulk diffusivity of  $H_2$  and  $H_2O$ . The effective diffusivity taking bulk diffusion into account can be described in Eq. (3) [26],

$$D_{H_2,B}^{eff} = D_{H_2O,B}^{eff} = D_{H_2-H_2O}^{eff} \quad (3)$$

where  $D_{H_2,B}^{eff}$  and  $D_{H_2O,B}^{eff}$  are the effective diffusivities neglecting Knudsen diffusion of  $H_2$  and  $H_2O$ . The effective Knudsen diffusion of  $H_2$  and  $H_2O$  can be revealed by Eq. (5) and Eq. (6) [25], and the bulk diffusivity can be calculated by the Chapman–Enskog relation as given in Eq. (6) [33],

$$D_{H_2,K}^{eff} = \frac{1}{3} \lambda d \sqrt{\frac{8RT}{\pi M_{H_2}}} \quad (4)$$

$$D_{H_2O,K}^{eff} = \frac{1}{3} \lambda d \sqrt{\frac{8RT}{\pi M_{H_2O}}} \quad (5)$$

$$D_{H_2-H_2O}^{eff} = \frac{0.00186 \lambda T^{3/2}}{p_t \sigma_{1-2}^2 \Omega} (1/M_{H_2} + 1/M_{H_2O})^{1/2} \quad (6)$$

where  $\lambda$  is the ratio of porosity ( $V_v$ ) to tortuosity ( $\tau$ ),  $d$  is the average diameter of electrode pores,  $R$  is the gas constant,  $T$  is the operation temperature,  $M_{H_2}$  and  $M_{H_2O}$  are the molecular weights of  $H_2$  and  $H_2O$ ,  $\Omega$  is the collision integral,  $\sigma_{1-2}$  is the average collision diameter, and  $p_t$  is the total pressure set as 1 bar. In this article,  $\Omega$  (2.734 Å) and  $\sigma_{1-2}$  (0.8998 m) are fixed. The error in effective diffusion is described in Eq. (7),

$$\varepsilon_D = D_{H_2,B}^{eff} - D_{H_2}^{eff} \quad (7)$$

where  $\varepsilon_D$  is the error of effective diffusion. Eqs. (8) and (9) can be obtained by combining the flux of  $H_2$  ( $J_{H_2}$ ), the effective diffusivity and one-dimensional partial pressure gradient of  $H_2$  [17,26],

$$i_{as} = \frac{2FD_{H_2}^{eff} p_{H_2}^0}{RTL} \quad (8)$$

$$i_{as,B} = \frac{2FD_{H_2,B}^{eff} p_{H_2}^0}{RTL} \quad (9)$$

where  $F$  is the Faraday constant,  $p_{H_2}^0$  set as a fixed value of 0.97 bar is the partial pressure of  $H_2$  outside the anode,  $L$  is the thickness of the anode, and  $i_{as}$  and  $i_{as,B}$  are the limiting current densities with and without Knudsen diffusion, respectively. The error of the limiting current density ( $\varepsilon_I$ ) can be described in Eq. (10).

$$\varepsilon_I = i_{as,B} - i_{as} \quad (10)$$

The concentration polarization of the anode, determined by fixed effective diffusivities, has expressions in Eqs. (11) and (12),

$$CP = -\frac{RT}{2F} \ln\left(1 - \frac{i}{i_{as}}\right) + \frac{RT}{2F} \ln\left(1 + \frac{ip_{H_2}^0}{i_{as} p_{H_2O}^0}\right) \quad (11)$$

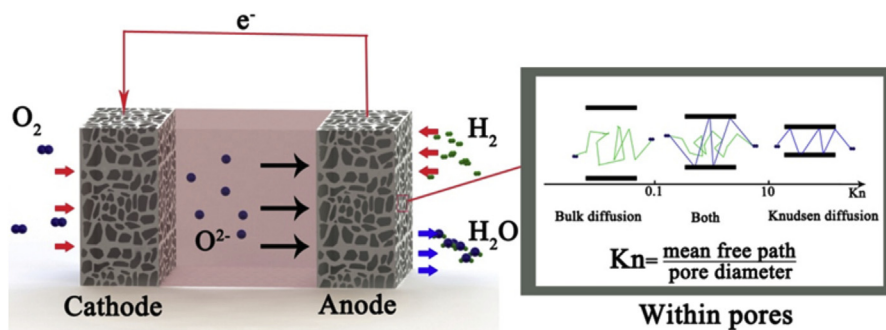


Fig. 1. Schematic demonstrations of SOFC structure, bulk diffusion and Knudsen diffusion within pores.

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