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Advancing the multiscale understanding on solid oxide electrolysis cells via modelling approaches: A review

Zheng Li¹, Hao Zhang^{2,*}, Haoran Xu¹, Jin Xuan^{1,*}

¹ Department of Chemical Engineering, Loughborough University, Loughborough, LE11 3TU, UK

² School of Engineering, The University of Edinburgh, Edinburgh, EH9 3FB, UK

* Corresponding authors: Hao.Zhang-1@ed.ac.uk (H. Zhang), j.xuan@lboro.ac.uk (J. Xuan)

Abstract

Solid oxide electrolysis cell (SOEC) is a clean and highly efficient technology that converts electrical energy into chemical energy, which is regarded as a promising approach to enable hydrogen production, carbon dioxide utilization and nitrogen reduction, and more. One of the main challenges faced by SOEC is performance descending. Numerical modelling is expected to provide insights on performance evolution and material degradation. Different assumptions and methodologies are applied to model the physicochemical processes in a length scale from molecule scale to system scale. It is rational and can be brought great convenience into modelling to make assumptions and simplifications when focusing on a single length scale, however, valuable details can be missing. Multiscale modelling is expected to maintain more information and generate a systematic understanding of the working mechanism of SOEC. In this paper, the modelling methods at various scale levels are summarized. Then, the recent advances in numerical studying on SOEC are reviewed with a focus

1 on multiscale modelling works bridging two or more contiguous length scales. The
2 challenges and future research directions are proposed to promote the multiscale
3 modelling.

4

5 **Keywords:** Solid oxide electrolysis cell, multiscale modelling, performance
6 optimization, sustainable fuel

7 **Word Count:** 11606

8

9 **Nomenclature:**

AEC	Alkaline electrolyser cell
BoP	Balance of plant
CFD	Computational fluid dynamics
DEM	Discrete element method
DFT	Density functional theory
DGM	Dusty-Gas model
DME	Dimethyl ether
FM	Fick's model
KMC	Kinetic Monte Carlo
LBM	Lattice Boltzmann Method
LSCF	Lanthanum Strontium Cobalt Ferrite
MC	Monte Carlo
MD	Molecular dynamics
MR	Methanation reaction
PEMEC	Proton exchange membrane electrolyser cell
RWGSR	Reverse water gas shift reaction

SDC	Samarium-doped ceria
SMM	Stefan–Maxwell model
SOEC	Solid oxide electrolysis cell
SOFEC	Fuel-assisted SOEC
TPB	Triple phase boundary

1. Introduction

As fossil fuels is still the dominant energy source for more than a century, the environmental problems caused by the accumulated CO₂ emission have raised global concerns. Many countries and regions have set strict measures to control the CO₂ emission and laid ambitious targets of decarbonization. For example, both the UK government and the EU have set goals to achieve net-zero greenhouse gas emissions by 2050 [1,2]. Additionally, China, as one of the world's largest emitter, raised a binding target to realise carbon neutral by 2060 [3].

Solid oxide electrolysis cell (SOEC) provides a viable option to support the sustainable development of modern society with clean energy. Provided by renewable energies like solar and wind energy, SOEC is capable of producing H₂ and hydrocarbons from H₂O electrolysis and CO₂ reduction, and even producing ammonia from N₂ reduction. As shown in Figure 1 (a), in ion-conducting SOEC, the reactant (H₂O/CO₂) is diffused to the interface area of electrolyte, electrode and gas pores, known as triple phase boundary (TPB), where the electrochemical reaction occurs to produce cathodic product (H₂/CO), oxygen ion (O²⁻) and electrons. Besides, in proton-conducting SOEC (as shown in Figure 1 (b)), at the anode side, the feed gas (H₂O/H₂) provides the protons (H⁺) which are transferred through the electrolyte to generate H₂ directly, or react with other reagents like NO and N₂ to generate N₂/N₂O/NH₃ [4,5].

Figure 1 Schematic diagram of SOEC working principles. (a) ion-conducting SOEC operation; (b) proton-conducting SOEC operation.

As shown in Table 1, although SOEC is yet as mature as other electrolyser configurations like proton exchange membrane electrolyser cell (PEMEC) and alkaline electrolyser cell (AEC), SOEC presents much higher energy conversion efficiency and shows great potential to be deployed in large scale.

Table 1. Characteristics of SOEC, PEMEC and AEC.

Electrolysis technologies	SOEC	PEMEC	AEC
Maturity	not yet widely commercialised	Commercial	Mature
Voltage efficiency (HHV%)	<110 [6]	67-82 [7]	62-82 [7]
Nominal stack efficiency (LHV%)	100 [8]	60–68 [8]	63–71 [8]
Nominal system efficiency (LHV%)	76–81 [8]	46–60 [8]	51–60 [8]
Stack lifetime (h)	<10,000 [9]	20,000-90,000 [10]	60,000-90,000 [10]
Operating temperature (K)	923-1273 [11,12]	323-353 [7]	333-353 [7]
Degradation rate (%/kh)	<1 [13]	<0.78 [7]	<0.17 [7]
Stack electric energy consumption (kWh/m ³ _{H₂})	>3.2 [6]	4.2-5.5 [7]	4.2-5.9 [7]

Due to the high efficiency, SOEC enjoys a much more competitive cost of electricity, especially in high energy price circumstances, according to economic analysis, as shown in Figure 2.

Figure 2 Levelized cost of H₂ versus electricity price, reproduced with permission [14], copyright 2015, Elsevier.

In recent years, SOEC has undergone rapid development with the state-of-art current density up to 1.9×10^4 A/m². However, SOEC is still facing significant challenges in performance degradation and short lifetime, which is closely related to the material properties [15]. The composition and morphology of materials pose a strong effect on the electrochemical/chemical processes and mass/heat/charge transports within the SOEC as well as the operation lifetime of SOEC. Multiscale numerical modelling provides an opportunity to give a mechanistic description of material performance and thus to guide optimization designs of material and structure. It improves the understanding of the SOEC properties and their effects on the behaviour of the SOEC. For example, electrochemical/chemical reaction kinetics are dominated by the fundamental properties of catalytic sites on the surface of materials. Microscale modelling can be used to study and predict the properties of materials to enhance the reaction kinetics. Mass/charge/heat transfer is governed by the microstructural property of materials. Mesoscale models provide insights into transport processes in microstructures [16]. The macroscale modelling generates strategies for the optimal operations of the SOEC unit and system. In addition, multiscale modelling covers a

1 large range of time scale (from femtoseconds to hours) and length scale (from
2 Angstroms to meters). Corresponding to different scale models, a variety of numerical
3 modelling approaches have been developed. Specifically, at a certain modelling scale,
4 several mathematical approaches can be adopted to reveal the properties of SOEC
5 on that scale.

6 Many numerical efforts have been devoted to understanding the working mechanism
7 of SOEC from micro to macro scales. It is worth reviewing the researches from the
8 aspect of multiscale modelling to establish a comprehensive understanding of SOEC
9 modelling by introducing various modelling methods suitable for different length scales.

11 **2. Modelling SOEC at different scales**

12 Generally, the modelling of SOEC can be categorized in several ways. In terms of
13 geometry dimension, the models are normally classified into zero-dimension (0D),
14 one-dimension (1D), two-dimension (2D), three-dimension (3D) model. Models can
15 also be categorised as white-box (physical model), black-box (empirical model) and
16 grey-box (semi-empirical model) [17]. The white-box method aims to provide a clear
17 description of physicochemical behaviours in the cell, which is based on objective
18 physical equations and realistic geometric dimensions of cells [18]. Conducting a
19 white-box model requires tremendous work to accomplish the calculations of complex
20 mathematical formulations. In contrast, the black-box method strongly depends on the
21 experimental data [19]. Although the black-box method does not really require a full
22 understanding of the physicochemical processes, large scale of experimental data is
23 required as the input to make sure the model can give reliable predictions [20]. In
24 addition, grey-box, combining the properties of white-box and black-box, requires both
25 physical processes knowledge and experimental data [20,21]. Moreover, SOEC

1 models can be classified into microscale model, mesoscale model, and macroscale
2 model, in terms of length scale. The macroscale model can be subdivided into cell-
3 level model, stack-level model, and system-level model. Table 2 summarises the
4 different scales of length and their corresponding modelling methods.

1 *Table 2 Different modelling scales and the corresponding modelling approaches.*

Modelling scale		Modelling methods		Reference
Microscale		Density functional theory (DFT)		[28,29,31,42,43]
		Molecular dynamics (MD)		[32,37–39]
		Kinetic Monte Carlo (KMC)		[33,42,43]
Mesoscale		Lattice Boltzmann Method (LBM)		—
		Elementary kinetics approach		[45]
		Morphology - reconstruction approach	Stochastic correlation method	[47,48]
			Discrete element method (DEM)	[49,51–54]
			Monte Carlo (MC)	[49,55]

Cell-level		Computational fluid dynamics (CFD)	[61,62,78–80,64,69,70,72–76]
		Continuum approach	
Stack-level		Computational fluid dynamics (CFD)	[81,84–90,92]
System-level		Process simulation	[82,96,109,111,97–101,104,105,108]

1

2 The above five scales and the corresponding modelling approaches are reviewed in
3 the following sections. Microscale models are employed to study the detailed
4 electronic structure of materials as well as the atomic/molecular interactions.
5 Mesoscale models provide valuable insights into the transport phenomena and
6 reactions inside the microstructure of SOEC electrodes. In order to conduct multiscale
7 modelling, the reaction kinetics derived from microscale models could be used as the
8 input of mesoscale ones, while the results of mesoscale models provide key
9 parameters for macroscale modelling. The physicochemical information yielded from
10 cell-level modelling can be delivered to build larger stack-level and system-level
11 modelling, which are used to describe the working conditions and macroscopic
12 properties of SOEC stack and whole SOEC system. In the following section, various
13 scales of SOEC models are introduced via the corresponding modelling approaches.

14 **2.1 Microscale modelling**

15 The microscale model plays a vital role in understanding the elementary reaction

pathways on the surface of materials from an atomic/molecular view [22]. Microscale modelling is regarded as an effective way to reveal the interaction mechanism between reactants and catalytic surfaces. Thus, it provides practical guides for developing and optimizing catalyst material configuration. There are several accessible approaches for microscale modelling: density functional theory (DFT), kinetic monte carlo (KMC) and molecular dynamics (MD), which are reviewed in detail in the following part.

2.1.1 Density functional theory (DFT)

DFT is a computational quantum chemistry modelling method to investigate electronic-structure and complex dynamics of multi-particle involved systems [23]. The Schrödinger equation is the fundamental correlation describing the state function of a quantum-mechanical system.

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \quad (3.1)$$

$$\hat{H} = \hat{T} + \hat{V} + \hat{W} \quad (3.2)$$

where E is the total energy level of the system; Ψ is the wave function; $\hat{H}$ is Hamiltonian, $\hat{T}$ is the kinetic energy operator; $\hat{V}$ is the potential energy operator, $\hat{W}$ is the electron-electron interaction. DFT is an efficient method to solve the Schrödinger equation. The potential energy surface is a useful conceptual tool for analysing atomic configuration or electrochemical/chemical reaction dynamics and can be derived from the DFT computation [24]. An ‘energy landscape’ describing the potential energy of a collection of atoms as a function of atomic positions can be provided by potential energy surface [25]. Several commercial software such as VASP and Gaussian are available for DFT calculation [26].

In the study of SOEC, one of the most prominent concern is the stability of the materials, which is a challenging problem impeding the SOEC development [27]. From

an atomic level of view, the stability of the structure depends on the level of binding energies. DFT has been using to study the evolution of binding energy and the degradation mechanisms of materials. Rashkeev et al. [28] developed a DFT model to investigate the mechanism of oxygen delamination in the SOEC consisting YSZ and LSM. The formation energies and migration barriers for the defects were calculated. The results indicate that the substitutional defects of Sr and La can strongly affect the migration of oxide ions, and may eventually result in delamination process. In addition, several improvement strategies were proposed to mitigate the oxygen delamination accordingly.

Catalysts supported on the electrode strongly affect the electrochemical performance. DFT is used to investigate the role of catalyst atoms on the surface of the support. Cadi-Essadek et al. [29] conducted DFT modelling to assess the stability of various Ni cluster configurations on the ZrO_2 and YSZ using clustering energy as an index. Besides, the cohesive energy and the interaction energy was calculated to understand the interaction among Ni atoms, and the interaction between the electrolyte surface and the Ni clusters, respectively. It was found that the formation of Ni–Ni bond was easier than Ni-electrolyte interaction. As a result, Ni cluster is preferred to form pyramidal shapes rather than flat structures. Under different temperatures, the stability of Ni clusters was affected owing to the aggregation formed by Ni with other atoms or clusters.

DFT was also used to evaluate the catalytic/electrocatalytic reactions of gaseous reactants in porous materials [30]. The calculation of interaction site geometries (such as bond lengths and bond angles) can be conducted [30]. Furthermore, in order to understand catalytic reaction kinetics, activation energies through the different reaction pathways can be calculated from DFT. Cadi-Essadek et al. [31] studied the interactions of CO_2 with YSZ and Ni_n/YSZ ($n=1,4-7,10$ and 20) surfaces. The

calculation results suggested that the surface of Ni_n/YSZ performed better than YSZ and Ni_1/YSZ in the aspect of adsorption. The most energetically favourable geometries for CO_2 adsorption were proposed (as shown in Figure 3 (a)). It is also found that the size of Ni clusters exerted no effect on the strength of CO_2 adsorption.

Figure 3 (a) Most stable configurations of CO_2/YSZ and $\text{CO}_2\text{-Ni}_n/\text{YSZ}$ ($n=1, 4-7, 10$ and 20). Ni, Y, Zr, O, oxygen vacancy and C are represented by blue, cyan, grey, red, yellow and black spheres, respectively, reproduced with permission [31], copyright 2018, American Chemical Society; (b) the coexistence of rutile structure and rutile twin structure, reproduced with permission [32], copyright 2013, Elsevier; (c) a cross-section of double-surfaced GDC cell after MC simulation. Ce^{4+} , O^{2-} and Gd^{3+} are represented by blue, red and purple spheres. L1 layer is closest to the surface, then is L2 layers and the bulk. A representative unit cell is shown overlaid on the figure, reproduced with permission [33], copyright 2018, Elsevier.

2.1.2 Molecular dynamics

The molecular dynamics (MD) method, can be broadly defined as a physics-based modelling method to investigate a multi-body system, which consists of many

interacting particles [34]. The classical Newton's laws of motion are employed in the MD modelling to describe the motion of molecules. Consequently, MD is commonly used to calculate the particle trajectories and to simulate the interactions between particles. The interactions can be expressed as forms of interatomic potentials, which can be provided by DFT. In order to resolve atomic vibrations accurately, the time step used in the MD method should be short enough to correspond to the time scale of molecular motion [35]. For example, a typical vibration of C-H bond corresponds to a period of 10^{-14} s [35]. Thus, MD is not suitable to simulate a process occurring on a much larger time scale.

The MD method has been applied to investigate the transfer processes within the material. It was proved a powerful tool to explore the diffusion coefficient (D) which can be yielded from Einstein formula [36].

$$\langle \Delta r(t)^2 \rangle = B + 6Dt \quad (3.3)$$

where $\langle \Delta r(t)^2 \rangle$ is the mean square displacement of oxygen, B is a constant, Δt is the time interval to obtain the mean square displacement of atoms. The diffusivity can convert to conductivity (σ) from Nernst–Einstein relation [36]:

$$\sigma = \frac{DC(q_e)^2}{k_B T} \quad (3.4)$$

where C is the concentration of ionic carriers; q_e is the charge, k_B is the Boltzmann constant. Li et al. [37] proposed a MD model to investigate the mechanism of ion transfer in YSZ. The results demonstrated that the structural environment of Zr^{4+} ions was more ordered than that of the Y^{3+} ions. It was found that the generation of Y^{3+} - Y^{3+} clusters can result in a decrease in conductivity when Y_2O_3 contents in YSZ is higher than 8%. Inaba et al. [38] investigated the oxygen diffusion in GDC using MD modelling. The formation enthalpy and lattice parameter of Gd–Gd pairs and isolated Gd ions

1 were calculated by MD. The results suggested that Gd–Gd pairs were more stable
2 than the isolated Gd ions. Additionally, the results also revealed the dependence of
3 the conductivity of GDC on dopant concentration. In terms of short-range interaction,
4 the formation of Gd^{3+} –vacancy– Gd^{3+} clusters impede the oxygen hopping into the
5 vacancy. On the other hand, in terms of long-range interaction, a shorter vacancy-
6 vacancy distance decreases the possibility of oxygen jumping into a vacancy.

7 MD modelling also shows the ability to investigate the mechanical performance of
8 electrolyte and interfaces, i.e., the mechanism of deformation behaviour of the material.

9 Sun et al. [32] measured the deformation behaviour of GDC under uniaxial tensile.

10 The MD modelling results indicated that the GDC structure experienced a phase
11 transformation to a rutile twin structure from a fluorite structure caused by stress when
12 a tensile load was applied in the [0 1 0] direction. In contrast, when the load was
13 applied in the direction of [0 1 1], the coexistence of both rutile structure and rutile twin
14 structure was detected (shown in Figure 3 (b)).

15 Further, the thermal properties of materials can be explored by the MD method as well.

16 Schelling and Phillpot [39] numerically calculated the thermal conductivity for both
17 ZrO_2 and YSZ. The thermal conductivity was found to behave like amorphous
18 materials when the concentration Y_2O_3 was greater than 12%. In contrast, when Y_2O_3
19 content is less than 12%, the thermal property of the material behaved like a crystalline
20 solid.

22 **2.1.3 Kinetic Monte Carlo (KMC)**

23 Kinetic Monte Carlo (KMC) is a useful tool for simulating the stochastic behaviour of
24 atoms (e.g., diffusion) in the many-particle system and the evolution of the system with
25 time [40]. Different from MD, KMC is a stochastic approach and can generate a series

1 of microscopic states without considering the equations of particles' motions [41].
2 Therefore, a large time-step can be carried out in KMC modelling.
3 Gunn et al. [33] developed a model (as shown in Figure 3 (c)) to study the diffusion of
4 oxygen and cation in a 10 mol% GDC system. In their study, a rigid-ion model with
5 Buckingham potentials was included for simulating the atomic interactions. The
6 composite monte carlo method was applied to yield structures at the condition of
7 thermodynamic equilibrium, while the final output structure from HMC was used as the
8 input structure for adaptive KMC. Then the adaptive KMC was employed to study the
9 diffusion and its mechanism in the GDC. Composite monte carlo results indicated that
10 Gd^{3+} concentration and oxygen vacancies were augmented at the surface of GDC
11 rather than in the bulk area. As a result, the average activation energy for oxygen
12 migrations from the bulk was twice that from the surface layer. Correspondingly, the
13 ionic conductivity of the bulk area was approximately half of the surface layer.
14 Dopants can have a significant impact on the performance of electrolytes. Through
15 KMC, not only the optimal dopant concentration but also the optimal distribution of
16 dopant can be determined. Krishnamurthy et al. [42] investigated the oxygen diffusion
17 in YSZ. In the model, DFT was used to calculate the activation energies used as the
18 input of KMC. The optimum oxygen diffusivity was found can be achieved when the
19 content of Y is in the range of 8-12%. Another study done by Lee et al. [43] investigated
20 the interacting energy barrier based on DFT and a KMC model. The results indicated
21 that the optimal Y distribution was the microstructure in which the Y ions segregate
22 into lines parallel to the conduction direction and arrange into a rectangular
23 superlattice in the perpendicular directions.
24 To sum up, the microscale modelling approaches mainly include DFT, MD and KMC.
25 The output of DFT, such as interatomic potentials and activation energies, can be

employed as the input parameters of MD and KMC. A series of fundamental physicochemical properties, such as thermodynamics, kinetics, electrical /thermal conductivity, defect formation energies, diffusion coefficient, etc., can be yielded from the calculations. Microscale modelling has been becoming a powerful tool for the researches of developing novel materials and obtaining optimized material structure from the atomic aspect. Nevertheless, microscale modelling is limited by its simulating time and length scale. The larger length scale properties like the porous structure of electrodes and species transport within the electrodes are not suitable to be derived from microscale modelling.

2.2 Mesoscale modelling

Mesoscale models are widely used to describe the species transport phenomena and reactions in the microporous structure of electrodes [22]. Since it could provide significant underlying fundamentals within electrodes, it becomes a more and more important method for the development of advanced electrode structure. Since the length scale and time scale of mesoscale modelling are greater than that of microscale modelling, the detailed information regards to molecule motions are simplified. The elementary kinetic-based electrochemistry approach, morphology-reconstruction approach and Lattice Boltzmann Method (LBM), are the most widely applied approaches to build mesoscale models [40].

2.2.1 Elementary kinetics approach

Elementary kinetics provides an in-depth description of the mechanisms of electrochemical reactions. The electrochemical reaction can be resolved into several steps. The reaction rate constants: k_f (forward) and k_r (backward) describe the kinetic

properties of the reactions [44]:

$$k_f = k_f^0 \exp\left(-\frac{\Delta E_f}{RT}\right) \exp\left(-(1 - \alpha) \frac{zF}{RT} \Delta\Phi\right) \quad (3.6)$$

$$k_r = k_r^0 \exp\left(-\frac{\Delta E_r}{RT}\right) \exp\left(\alpha \frac{zF}{RT} \Delta\Phi\right) \quad (3.7)$$

where k_f^0 and k_r^0 are the pre-exponential factors (can obtained from DFT); ΔE_f and ΔE_r are activation energies (can obtained from DFT); α is the symmetry factor F is the Faraday's constant; $\Delta\Phi$ is the potential difference [44]:

$$\Delta\Phi = \phi_{electrode} - \phi_{electrolyte} \quad (3.8)$$

The current density is derived from the generalized Arrhenius-type expression of rate constants [44].

$$i = zFL_{TPB} \left[k_f \prod_j^{R_f} \theta_j^{v_j^f} - k_r \prod_j^{R_r} \theta_j^{v_j^r} \right] \quad (3.9)$$

where L_{TPB} is the TPB length; z is the number of charges transferred; θ_j is the surface coverages of species j ; v_j is the stoichiometric coefficients.

Ren et al. [45] has developed a microkinetic model to investigate the mechanism of CO_2 reduction at the TPB of Ni/samarium-doped ceria (SDC). At first, DFT was employed to calculate the total energies of elementary reaction steps (shown in Figure 4). DFT results discovered that interface oxygen vacancy was capable of enhancing CO_2 adsorption and subsequent reduction by lowering its energy barrier. Two different surface models were built: model 1 was the Ni/SDC with noninterface oxygen vacancy; model 2 was the Ni/SDC with interface oxygen vacancy. It was found that the rate-controlling step (model 1) would change from the oxygen spill-over step to the CO desorption step when the overpotential at cathode experienced an increase. However, it was suggested that the rate-controlling step (model 2) was the CO desorption and independent of the overpotential.

Figure 4 Elementary reaction steps for CO_2 reduction on Ni-SDC: (a) model 1; (b) model 2. Dashed circle represents the oxygen vacancy; R represents the reaction; IM represents intermediate species, reproduced by permission [45], copyright 2018, American Chemical Society.

2.2.2 Morphology-reconstruction approach

Morphology-reconstruction requires detailed morphology of porous electrodes as the physical boundary of the model. Generally, two steps are required in the morphology-reconstruction approach: 1. generate a microstructure; 2. simulate the transfer processes within the microstructure [40]. The structure of electrodes can be reconstructed by either experimental or numerical methods. The experimental reconstruction base on a series of images of the microstructure. Alternatively, the numerical methods include stochastic correlation reconstruction, discrete element method (DEM), and Monte Carlo (MC) method.

Stochastic correlation reconstruction, based on the analyses of statistical spatial correlations, can be used to reproduce the 3D microstructures [46]. Moussaoui et al. [47] presented a 3D model to simulate the microstructure of Lanthanum Strontium Cobalt Ferrite (LSCF) and Ni-YSZ. The real microstructure morphology was accomplished by using X-ray nano-tomography, while the synthetic microstructure

1 was developed by using a 3D Gaussian 'Random Field Model'. The microstructural
2 parameters, such as tortuosity and TPB length density, were used as the target
3 indexes to govern the reconstruction process. It is found that the two-phase LSCF
4 model was able to predict the electrode microstructural architecture precisely.
5 Furthermore, the model was extended to three-phase for Ni-YSZ. Moreover,
6 stochastic modelling is capable of studying the quantitative relationship between the
7 manufacturing process and the microstructural architectures. Based on stochastic
8 modelling, Gaiselmann and co-workers [48] proposed a quantitative relationship
9 between the Lanthanum Strontium Cobaltite production processes (different sinter
10 temperatures and different pore former contents) and the corresponding final
11 microstructures.

12 DEM has been commonly applied to reconstruct the electrodes as random structures
13 consisting of ionic and electronic conductive particles [49]. DEM is an effective
14 approach to optimize the morphology of electrodes and to bridge the gap between the
15 microstructure at a particle scale and macroscopic electrode performances. The main
16 feature of DEM is to treat each particle as a discrete object and deal with the sum of
17 the contact force, which determines the motion of individual particles [50]. DEM was
18 also used to generate the microstructure of electrodes with consideration of the
19 realistic sintering process of powder packings [51]. Besides, DEM is capable of
20 investigating the mechanical properties of electrodes. Liu et al. [52] conducted a study
21 to simulate the mechanical behaviour of LSM/YSZ and NiO/YSZ under mechanical
22 loadings. The elastic properties of the electrodes were evaluated. Moreover, DEM has
23 been used to calculate the resistance and the effective conductivity of the electrodes
24 [53,54].

25 MC method is an alternative numerical option to generate the microstructure. Tabei et

al. [55] applied a modified MC to yield the 3D microstructure of Ni/YSZ. The computational microstructure showed a good agreement with the real ones. The finite element method was applied to characterize the mechanical and thermal properties of the reconstructed electrode. Yan et al. [49] proposed a model to study the role of powder morphology in affecting the final microstructure of LSCF. DEM was used to simulate the powder packing, while the output of the DEM (numerical structural samples with different particle morphologies) can be obtained, which acted as inputs of KMC to simulate the powder sintering (shown in Figure 5).

Figure 5 A morphology-reconstruction model, reproduced by permission [49], copyright 2017, Elsevier.

2.2.3 Lattice Boltzmann Method (LBM)

LBM is a promising computational fluid dynamics (CFD) approach that is capable of simulating mass transport over a wide range of Knudsen numbers in the porous electrodes through considering the non-continuum effects, complex geometries and multiple species [56].

1 The simulation region in LBM is regarded as a lattice system, where the particle moves
2 from site to site. The most significant difference between LBM and MD is that LBM
3 calculates the particle velocities distribution function (PDF) other than the positions
4 and velocities of the particles [41]. The PDF f_{α}^i at any lattice point x and time t is
5 proportional to the moles of each species i ($= 1, 2, 3, \dots$) presented at x with a velocity
6 e_{α}^i along a specific direction α [56]. An LBM process includes two basic steps:
7 streaming and collision. In streaming, the particles of i with e_{α}^i at x stream to
8 neighbouring points, and the collision represents the interactions between particles
9 arriving at that the lattice point from neighbouring points (of the same or different
10 species) [56]. The lattice Boltzmann equation is given by combining the streaming and
11 collision steps:

$$12 \quad f_{\alpha}^i(x + e_{\alpha}^i, t + 1) = f_{\alpha}^i(x, t) + \Omega_{\alpha}^i \quad (3.10)$$

13 where Ω_{α}^i is the collision term. Therefore, some macroscopic properties such as
14 velocities, densities can be calculated from resolving the moments of f_{α}^i over velocity
15 space [41,57]. The complex microstructure provided by morphology-reconstruction
16 models could be employed as the physical boundaries of LBM model (shown in Figure
17 6).

Figure 6 Schematic of the simulation domain and physical boundaries of LBM model, reproduced by permission [58], copyright 2016, Elsevier.

2.3 Macroscale modelling

2.3.1 Cell-level modelling

The principal objectives of cell-level modelling are the transfer processes, including mass, heat and charge transfer, and chemical/electrochemical reactions in the SOEC [22]. CFD is a powerful research tool to resolve the distribution of physicochemical processes based on conservation equations of mass, energy and momentum, and reaction kinetics. Commercial software such as COMSOL and FLUENT and open-source platforms like OpenFOAM are available to resolve the governing equations.

In cell-level modelling, the continuum approach is often applied, which treats the porous materials and medium filling in the pores as a homogenized continuum [40].

Continuum approach gives a complete description of transfer processes in the electrodes. The modelling based on the continuum approach strongly relies on the effective microstructure parameters such as porosity and permeability. Besides, the electrochemistry in the SOEC is also investigated at a continuum-level. It is based on

1 the Nernst equation and the polarizations of the SOEC.

$$2 \quad E = E_0 + \frac{RT}{nF} \ln \left(\frac{\prod a_{products}^{v_i}}{\prod a_{reactants}^{v_i}} \right) \quad (3.11)$$

$$3 \quad V = E + \eta_{act} + \eta_{conc} + \eta_{ohmic} \quad (3.12)$$

4 where E is the equilibrium voltage; E_0 is the standard potential; R is the universal gas
 5 constant; n is number of electrons transferred; a is the activity of the species; η is the
 6 polarization (activation, concentration and ohmic) of the cell; V is the external voltage.
 7 Generally, the activation overpotential is usually determined by the Butler-Volmer
 8 equation [59,60]:

$$9 \quad i = i_0 \left[\exp \left(\frac{\alpha n F \eta_{act}}{RT} \right) - \exp \left(- \frac{(1 - \alpha) n F \eta_{act}}{RT} \right) \right] \quad (3.13)$$

10 Where i is the current density; i_0 is the exchange current density; α is the charge
 11 transfer coefficients. However, it is worth mentioning that the Butler-Volmer equation
 12 may not be the most suitable equation to describe the activation overpotential. In some
 13 studies, a modified Butler-Volmer equation was applied [61,62]. The concentration
 14 overpotential is caused by the diffusion losses in the SOEC. The mass transport
 15 through porous media can be explained by the multi-component gas transport models.
 16 For example, Fick's model (FM) is the simplest model, whereas, FM cannot be used
 17 when the molecular weights of gas species vary significantly [63]. It was found that
 18 cathode is more susceptible to concentration overpotential. Stefan–Maxwell model
 19 (SMM) accounts for the molecular weights, however, the effects of Knudsen diffusion
 20 is ignored [63]. Dusty-Gas model (DGM) can be considered as an extension of SMM
 21 that takes into account Knudsen diffusion:

$$22 \quad \sum_{j=1, j \neq i}^n \frac{y_j \mathbf{N}_i - y_i \mathbf{N}_j}{D_{ij,B}^{eff}} + \frac{\mathbf{N}_i}{D_{i,k}^{eff}} = - \frac{1}{RT} \left(P \frac{dy_i}{dz} + y_i \frac{dP}{dz} \left(1 + \frac{K_0 P}{D_{i,k}^{eff} \mu} \right) \right) \quad (3.14)$$

23 Where $\mathbf{N}_i$ is the molar diffusion flux of species i; y_i represents the molar fraction of

species i ; $D_{ij,B}^{\text{eff}}$ is the effective binary diffusion coefficient, $D_{i,k}^{\text{eff}}$ is the effective Knudsen diffusion coefficient; P is the pressure. Considering the simplicity and computational cost, FM and SMM are usually applied in the literature [64,65]. On the other hand, in order to realize a more precise description of mass transfer in porous electrodes, DGM has been used by many groups in the modelling studies as well [66,67]. The ohmic overpotential is typically described by Ohm's law [68].

Cell-level models can combine the continuum approach with the elementary kinetics approach to simulate the mass/charge transports coupling with a more precise electrochemistry. Grondin et al. [61] developed a 1D model to simulate the cathodic behaviour of Ni-YSZ. This model offered a description of mass and charge transports in the cathode. The elementary kinetics approach was used to investigate two different electrochemical reaction mechanisms of H_2O electrolysis, which concluded that the adsorption process of H_2O has a significant effect on modelling results. An elementary reaction-based model was proposed to predict the SOEC behaviour for CO_2 reduction by Shi and co-workers [69]. An elementary reaction model, which adopted a heterogeneous mechanism, was established to understand adsorption/desorption reaction kinetics on the catalytic surface. It also took into account the carbon decomposition, which can damage the cell structure and reduce the performance of SOEC. The modelling results showed that the major elemental species were (Ni) and CO(Ni). Operating SOEC at a high temperature condition can be favourable for CO_2 (Ni) consumption and CO production. It also indicated that the possibility of carbon decomposition could be mitigated at a low CO level. Menon et al. [62] developed a model to simulate the SOEC operation during co-electrolysis. The impacts of microstructural properties (such as porosity and tortuosity) and operating conditions (such as temperature and inlet gas velocity) on the syngas (H_2 and CO) production

1 were explored by this model. By using the elementary kinetics approach, a detailed
2 reaction mechanism on Ni catalyst, which took into account the reverse water gas shift
3 reaction (RWGSR) and methanation reaction (MR), was applied to conduct a
4 parametric analysis. It was found that increasing the input of CO₂ cannot enhance the
5 MR, whereas the increase in the H₂O hindered the MR. Additionally, a most likely
6 reaction pathway of MR was determined in their study.

7 Cell-level models provide a good comprehension of the performance of the cell at
8 various operation conditions, which can be used to provide guidelines for optimization
9 design. Ni [70] proposed 1D and 2D models for CO₂ electrolysis to study the
10 comprehensive reaction-transfer phenomena. Li et al. [64] developed SOEC models
11 for co-electrolysis to study the competitive effect between electrochemical and
12 chemical reactions. The modelling results suggested that the rate of heterogeneous
13 chemical reactions was faster than that of electrochemical reactions. Moreover, it was
14 found that the cathode thickness posed a significant influence on the active sites for
15 reactions. CFD model was also used to optimize the gas distribution in solid oxide
16 devices [71]. A further study [72] suggested that the structure parameters, material
17 performance, and gas composition could remarkably influence the zone sizes of
18 heterogeneous reaction electrochemical reactions. Du et al. [73] developed a 3D
19 model of SOEC to study the effect of operation pressure on co-electrolysis of water
20 and carbon dioxide. Optimal operation conditions were proposed and counter-flow
21 arrangement is found a better configuration than co-flow.

22 The degradation of electrodes caused by thermal stress and strains is a challenging
23 problem that the SOEC is facing. Jin and Xue [74] presented a 2D CFD model to study
24 the delamination phenomenon at the anode-electrolyte interface. It is found that the
25 delamination of the electrode and electrolyte significantly impacts the distribution of

current density. Moreover, the SOEC performance was more sensitive to the delamination occurred at the central area of the cell than at the edges. Nerat et al. [75] proposed another model to study the delamination of SOEC in long-term operation. The anode delamination was modelled by modifying the geometry of the cell (shown in Figure 7 (a)). It was concluded that the increase of the delaminated area at anode could be the main reason causing the efficiency drop of SOEC in the long term. A 3D model was proposed by Navasa et al. [76] to investigate local conditions (i.e., gas composition, potentials and temperature) that can result in cell degradation. In particular, the authors simulated the conditions in the electrodes, and generated an accurate description of the spatial variations of these factors through the electrodes. Moreover, the impacts of thermal boundary conditions on cell performances were also explored aiming at extending the lifetime of SOEC.

A recent study shows that the use of low-cost fuels reacting with O_2 at the anode can reduce the operating potential of SOEC as well as the electricity demand [77]. This type of SOEC is also known as 'fuel-assisted SOEC (SOFEC)'. Luo et al. [78] developed a 1D SOFEC model. This model contained a mesoscale sub-model to simulate the elementary reactions on the catalyst surface. The elementary reactions modelling results revealed the reason why CH_4 -assisted SOFEC performed better than the CO-assisted SOFEC. The results indicated that carbon deposition was a critical problem in CH_4 -assisted SOFEC. Xu et al. [79] developed a 2D CH_4 -assisted SOFEC model, including an electrochemical module (describing overpotentials), a CFD module (simulating mass/heat transfer) and a chemical module (studying the RWGS and steam methane reforming reaction). The results suggested that the effect of the anode gas flow rate on cell performance was significant, which was quite different from the behaviour of conventional SOEC.

2.3.2 Stack-level modelling

Stack-level models simulate the behaviour of the SOEC stack, which consists of multiple cells, interconnects, manifolds, seals, and cell frames [22]. Stack-level models provide a comprehensive description of stack operations and give valuable insights into how to optimize the stack performance by changing the operating strategy or the stack design. Additionally, it can serve as design guidelines to eliminate the uneven distribution of species and temperature within the stack and maximize the power of the SOEC stack. CFD can also be a computational tool to explore the transport processes within the stack. The electrochemistry of the SOEC stack is developed at a continuum-level. Since the geometry of the SOEC stack is far more complicated than that of a single SOEC, the resolution of stack-level modelling often relies on the simplification assumption [40], which sacrifices some information in the cell-level. Therefore, a concept of single repeat unit (SRU), i.e., a cell coupled with other auxiliary components, is introduced [83]. First, the transport and electrochemistry properties of SRU are described at the cell-level. Then, a SOEC stack with a large number of equivalent SRUs is simulated to build the stack-level model. Such a method illustrates the relationship between cell-level and stack-level with the computational cost for stack-level modelling can be dramatically reduced.

Hawkes et al. [84] proposed a 3D model of a SOEC stack to investigate the effect of operating conditions on the stack performance. The effects of different operating voltages on the temperature, operating potential, current density, anode/cathode side gas composition were evaluated. Laurencin and co-workers [85] proposed a 2D model, including both electrochemical (studying overpotential and local current density) and thermal modules (simulating the thermo fluid and temperature field) of SOEC. The simulation suggested that the thermal equilibrium was intensively dependent on the

radiative heat losses.

Keeping the mechanical integrity is a tough task in stack operation. In the long-term operation, deformation and material failure caused by the thermo stresses can result in hot spots, accelerating thermal mismatch and eventually cause leak problem and performance decline. Therefore, it is essential to achieving a uniform temperature distribution within the stack. Udagawa et al. developed a 1D model for a SOEC stack operating at a steady/dynamic state [86–88]. The influences of temperature and current densities under exothermic/endothermic operations were investigated. The impacts of airflow rates on temperature were investigated. A potential temperature control strategy was proposed to prevent the fracture of cell components. Xu et al. [81] developed a 3D model to simulate the influence of operating mass flow rates on the behaviour of a SOEC stack (shown in Figure 7 (b)). The performances of cells in different layers of the stack were investigated. The authors discussed the distribution of pressure, temperature, and fluid flow under different operating gas flow rates. Stack-level models have been used to study the degradation issues as well as determine the operating strategy for mitigating the degradation. Molla et al. [89] developed a model to study the stresses in different design configurations and the effects of temperature distribution. It was found that delamination can be caused by stress reversal in over rigid stack design. Furthermore, it was indicated that much lower stress and temperature gradients can be achieved through convection cooling than conduction.

In order to increase the computational speed of the stack-level model, Navasa et al. [90] proposed an original stack model with a low computational cost. Such advantages are attributed to so-called homogenization, which substitutes the repeating unit with an equivalent homogeneous medium. The authors took a further step to increase the computational efficiency by applying the homogenization to the whole repeating unit.

Hereby, compared with conventional models, the simulating time of this model can be mitigated by two orders of magnitude. Additionally, the researchers pointed out that further modelling studies can focus on explicitly representing the local details and maintaining the high computation efficiency at the same time.

In practice, the stack is an essential element in a solid oxide plant which can work in electrolysis mode to store the electrical energy into hydrogen or in a fuel cell model to generate electricity [91]. The behaviour of the stack in real practice can be investigated by modelling, subsequently generating the optimal stack design and operation strategies. Wang et al. [92] introduced a novel dynamic stack-level model which extensively studied the various designing and operating factors (temperature, pressure, heat capacity, current density, fuel fraction and mode switching frequency) on the performance of the stack during switching processes. According to their modelling results, to extend the lifetime of the stack, it is advisable to increase the heat capacity of the stack and inlet hydrogen molar fraction. Additionally, increasing the operating pressure and decreasing the current density is favourable to improve the reversible efficiency.

2.3.3 System modelling

System-level modelling takes the entire SOEC system into account. SOEC system consists of SOEC stacks and the balance of plant (BoP) components like pumps and ac/dc converter [22,93]. The primary purpose of system-level modelling is to maximize the overall efficiency of the system by optimizing the system design and operating strategies. The system-level model is not intended to understand the detailed stack behaviour, but to use the output of stack-level sub-model to investigate the interaction between stack and BoP. However, the interactions between the cells within the stack,

1 and between the stack and BoP are complex. Thus, the in-situ system-level modelling
2 to simulate the real-time operation is costly. To address this issue, the simplification
3 of the geometry of sub-models, such as BoP models, is often applied in system-level
4 modelling [22]. The process simulator, also known as flowsheeting software, can be
5 employed to construct a system-level model. Flowsheeting can be broadly defined as
6 a systemic description of material and energy streams in a system with the aid of
7 computer simulation [94]. Several commercial process simulators are available for
8 system-level modelling, such as ASPEN and SIMULINK [95].

9 System-level modelling is an economical approach to find the optimal operating
10 schemes to maximize overall efficiency. This is often accomplished by analysing the
11 thermodynamic of the system, with the aid of first/second laws of thermodynamics.
12 Both energy and exergy analyses can be included in the thermodynamic modelling of
13 the SOEC system. Ni et al. [96] developed a system-level model to conduct the
14 energy/exergy analyses and corresponding efficiency calculations. The effects of
15 operating conditions on the efficiency were investigated as well. It was found that
16 energy/exergy efficiency can be maximized through adapting the current density, the
17 gas velocity, and operating temperature. Mingyi et al. [97] proposed a thermodynamic
18 model concerning the efficiencies of the SOEC system. The model explored the
19 impacts of three essential parameters (electrical efficiency, thermal efficiency, and
20 electrolysis efficiency) on the overall energy efficiency. Stempien et al. [98] carried out
21 a thermodynamic model to simulate the effects of operating parameters on system
22 performance. With the aid of energy and exergy analysis, the optimal operating voltage
23 of the system was determined.

24 In order to develop an economical SOEC for commercial promotion, it is essential to
25 carry out a techno-economical assessment to assess the economic performance of

the system. Such an assessment is useful to evaluate the economic feasibility and future commercialization potential of the system. In addition, the techno-economical assessment can be used as a guide tool to optimize the operating strategies for minimizing the operating/capital cost. Samavati et al. [99] presented a system-level model for syngas production. A thermodynamic sub-model, including energy and exergy analyses, was developed. The economic analyses indicated that the electricity price showed the largest contribution to the final cost of reduction products. Rivera-Tinoco et al. [100] assessed a system coupling water electrolyser (either PEMEC or SOEC) with a CO₂ reactor to produce methanol. The H₂ produced from water electrolysis was transferred to a CO₂ reactor to generate methanol. The techno-economic assessment demonstrated that the SOEC approach was more capital-consuming, whereas the PEMEC option expensed more on operation cost. Buttler et al. [101] performed a techno-economical assessment of a SOEC system with heat integration on the basis of a high temperature electrolysis plant. The results illustrated that the high temperature electrolysis plant with heat integration was economically feasible. Furthermore, an extensive sensitivity analysis demonstrated the positive/negative influential factors of the application of heat integration.

System-level models have been used to evaluate the feasibility of a novel system design. For a given design problem, a new proposed system configuration can be assessed through simulating and integrating the individual units of the system. Pozzo et al. [82] presented a novel system design to enhance the dimethyl ether (DME) production. The system, combining a woody biomass gasifier and a SOEC unit, was modelled by ASPEN (shown in Figure 7 (c)). Pinch analysis was performed for the whole system. Furthermore, it was found that the overall efficiency and specific productivity of the novel plant were much higher than that of the conventional design.

SOEC is a pivotal component in Power-to-Gas systems. Such systems have a great potential in storing excess electrical energy into energy carriers such as H_2 (via H_2O electrolysis/co-electrolysis) and CO (via co-electrolysis) [102,103]. By further processing, the produced gases can be easily converted into methane, methanol, DME and gasoline [102]. Techno-economic viability and lifespan are two main challenges to such system operation. System-level models can simulate the system operation and provide an optimal system design as well as a long-term operating strategy. Wang et al. [104] established a model to investigate several essential designing issues, including system-level heat integration, the effects of operating conditions and the avoidance of electrical heating. Based on the modelling results, for both H_2O electrolysis and co-electrolysis, it was found that high system efficiency and high methane production cannot be achieved at the same time. Besides, the SOEC was found to be more favourable operating at exothermic mode other than thermoneutral mode, as that operation improves the flexibility and reliability of the system. Another model proposed by Wang et al. [105] aims to assist the design of a co-electrolysis-based power-to-methane system. In the study, the requirements for maximizing the methane production and the impacts of pressurized operation and internal methanation were investigated. It was found that the dominating reaction of co-electrolysis was H_2O splitting while CO_2 was reacted via RWGSR. The internal methanation can be used as an effective internal heat source to sustain the temperature, which allows the co-electrolysis-based system to obtain a higher efficiency than the H_2O electrolysis-based system.

Moreover, hybrid energy hub, a promising concept for integrated management of energy systems, can be broadly defined as a framework where various energy carriers can be produced, converted, stored and consumed in order to satisfy energy demands

1 [106,107]. Energy hub can be divided into different microgrids regarding its
2 consumption region (such as commercial and residential). It can not only offer low-
3 cost sustainable and clean energy but also enhance the resiliency and stability of local
4 grid [107]. Nevertheless, due to the complexity of both information exchange within
5 the energy hub and the relationships between different units, system-level modelling
6 is required to provide a more accurate description of energy hub behaviours and
7 optimize its operations. Parisio et al. [108] used a robust optimization approach to
8 develop a system model of an energy hub. The aim of this model is to satisfy the time-
9 varying energy output demands while minimise energy costs. Their work obtained a
10 robust operation schedule for the energy hub. Huty et al. [109] introduced a system
11 model to simulate the operation of a microgrid composing of houses coupling with the
12 solar photovoltaic unit and SOEC/battery. The model was used to optimize the size of
13 units of the microgrid and quantify the self-sufficiency ratio. They also did the case
14 studies for UK and Texas, and found that the hybrid energy storage system (SOEC
15 with battery) is superior to the battery-only system when the self-sufficiency ratio of
16 the system was given at a high level. Colombo and co-workers developed a system
17 model of the campus microgrid to simulate existing power plant behaviours and
18 investigate the response of a microgrid to additional renewable installed capacity [110].
19 In this model, a SOEC system was included and showed a good performance in
20 storing the excess renewable capacities of the microgrid. Rispoli et al. [111] proposed
21 another system model of SOEC-based microgrid to optimize the microgrid sizing as
22 well as the year-around energy management. A techno-economic study was
23 conducted to determine the optimal grid configuration by applying a constrained
24 design method. It was found that the payback period for this SOEC-based microgrid
25 was reasonable. This model can serve as a basis for the optimal design of microgrids

as well as the operation strategies.

3. Perspectives

Lots of research efforts have been paid on the multiscale numerical study of SOEC from microscale to system level. However, most of these studies perform different length scales separately, which is known as the hierarchical method [112]. While the modelling approach of performing concurrent multiple scale modelling methods is still lack of investigation. In the concurrent modelling approach, detailed information in multiple length scales is included in a single model, and the calculation should only be carried out once [112]. However, it could require much more computation power than the hierarchical method. Therefore, the priority is to balance the computation ability and calculation accuracy. One of the challenges is how to apply the numerical results from the bottom scale into the upper scale to achieve multiscale modelling. The shorter length scale brings in higher information density. As a result, due to the limitation of calculation capability, it is costly and even impossible to retain detailed information from the bottom level. Strategies are needed to extract and keep the most valuable results with reasonable tolerance. As reviewed in the paper, homogenization is a commonly used strategy to represent the calculated value with an average value. However, this approach is not suitable for the data with a large gradient, which could lose valuable details. One practical solution to bridge CFD modelling and system simulation is provided in a commercial software package, gProms [113]. The ‘multizonal modelling’ strategy can be employed to divide CFD calculation domain into several zones within which the characteristics and distributions are similar. Therefore, parameters within the individual zones can be treated as constant. The concept is

1 similar to discretisation, and is expected to balance the need of accuracy and
2 calculation cost.

3 Algorithms should be developed to treat and simplify the calculation results generated
4 from bottom scale models, which will be provided as inputs to the upper scale model.
5 During this process, the decision-making strategy is crucial to balance detailed
6 information and numerical efficiency. Data-driven artificial intelligence could be a
7 powerful tool assisting us in establishing such strategies.

8 In addition to the multi-length scale modelling, another challenge is multi-time scale
9 modelling. Compared with multi-length scale modelling, multi-time scale modelling has
10 long been overlooked and is more challenging. Modelling in multiple time scales
11 presents dynamic behaviours of transport processes and the transient response
12 corresponding performance of SOEC, which provides guidelines for system control
13 under start-up and fluctuant conditions. Multi-time scale modelling has been applied
14 in Solid Oxide Fuel Cell (SOFC), which can definitely be extended to SOEC [114,115].
15 Moreover, multi-time scale modelling is expected to provide critical information for
16 understanding the micromorphology change and material degradation, and their long-
17 term effects on the SOEC performance evolution. At the same time, a large scale of
18 long-term experimental data is needed to establish reliable correlations of material
19 components and micromorphology.

20 In recent years, the Jiao Group has developed novel '3D+1D' or '2D+1D' multiscale
21 modelling frameworks to integrate sub-models with different dimensions for the
22 purpose of fast and economical large-scale simulation of electrochemical systems
23 [116,117]. In these frameworks, the 3D/2D sub-models are used to describe the
24 computational domains in which the parameters distribute with a large gradient in the
25 volume, while the 1D sub-models are applied in other domains. Different from the

previous multiscale modelling methods focusing on the coordination of length, this strategy brought a new perspective emphasizing dimension combination which can also be used in the study of SOEC to achieve time and cost effective modelling.

4. Conclusion

The working principles of SOEC for various electrolysis modes are introduced in this review. The numerical modelling approaches focus on different length scales are summarized accompanying recent numerical SOEC researches from microscale modelling to system simulation for understanding the reaction kinetics, mass and charge transfer phenomena, and obtaining optimal system operation. The attempts to perform multiscale modelling of SOEC were reviewed, indicating the current development of multiscale modelling is still dominated by the hierarchical method. Concurrent multiscale modelling is lack of investigation. Limitations and the future perspectives of multiscale modelling of SOEC are also discussed. The challenges lie in bridging sperate length scale models and establishing multi-time scale modelling methods. The development of modelling methodologies will continuously support the advance of SOEC.

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