Solid oxide fuel cells (SOFCs) with enhanced fast ramping power capability and overload tolerance can find important applications in grid stability management and critical data center overload protection. Recently, we have demonstrated a new SOFC configuration featuring a built-in chemical Fe-bed in the anode chamber of a tubular SOFC with exceptional fast power ramping capability and overload tolerance. In the present study, we showed our theoretical understanding of the enhanced performance through a two-dimensional axial symmetrical numerical model. The model couples the charge and mass transport in the tubular SOFC with chemical reaction kinetics in the Fe-bed, producing longitudinal distributions of Nernst potential, \( \frac{H_2O}{H_2} \) molar ratio, local current density and fuel utilization under various operating conditions. The crucial role of Fe-bed in providing instant \( H_2 \) to support fast ramping and overload currents has been explicitly explained by this computational model.

Solid oxide fuel cell (SOFC) has long been deemed an ideal efficient and clean power generator for uninterrupted steady-state baseload and distributed generation.\(^6–8\) In reality, however, the load is not always constant, fluctuating periodically from peak to valley throughout a day. Typically, SOFC can follow these load variations provided that the interval of load change is long enough to allow SOFC system to adjust fuel flow to meet the power demand.\(^4,5\) However, if the load increase is too sudden that the fuel supply system could not have sufficient time to respond and provide the necessary fuel for the overload, it would result in oxidation of Ni-based anode and cause mechanical failure of SOFC stacks.\(^5–8\)

Recently, we presented a new tubular SOFC concept featuring a chemical Fe-bed loaded in the anode chamber and demonstrated that such Fe-bed loaded SOFC can produce fast ramping power and operate at high overload currents.\(^9\) The built-in Fe-bed reacts with \( H_2O \) in the fuel stream to produce extra \( H_2 \) for supporting fast power and overload operation. The demonstrated new functionalities suggest that the Fe-bed SOFCs are well suited for applications in grid stability management to provide timely fast power for grid power management and critical overload protection for data center. However, the fundamental aspects including distributions of Nernst potential (\( E_N \)) and local current density of the newly configured SOFC are still lacking at this point. It is worth mentioning that the Fe-bed concept presented in this study is fundamentally different from early studies that used Fe to alloy with Ni in the anode to boost its coking resistance so as to operate on methane fuel.\(^10,11\)

In the present study, we report our theoretical analysis of the enhanced dynamic and electrochemical performance of an anode-supported tubular SOFC with a built-in Fe-bed through a two-dimensional axial symmetrical multi-physics numerical model. The physical-chemical processes considered by the model include the charge/mass transport in a tubular SOFC and chemical reaction kinetics in the Fe-bed. For high-fidelity prediction, the model parameters were validated by experimental V-I data obtained from a pilot-scale anode-supported tubular SOFC. Longitudinal distributions of Nernst potential, composition, local current density and fuel utilization are simulated under various load conditions.

The Numerical Model

The numerical model is built from the configuration of a tubular solid oxide fuel cell loaded with a Fe-bed in the anode chamber shown in Fig. 1. The operating temperature for the model is set to 750°C to reflect the practical operating temperature of such SOFC.\(^9\) At this temperature, FeO is the prevalent product of Fe oxidation by \( H_2O \) through the reaction \( Fe + H_2O = FeO + H_2 \). The cell operates at ambient pressure with the cathode constantly open to air.

The physical and chemical processes occurring in the tubular SOFC with a Fe-bed include: electron/oxygen-ion transport in the SOFC, electrochemical reactions at triple phase boundaries of SOFC electrodes, and gas diffusion through the porous electrode, open-space chamber and porous Fe-bed.\(^12–17\) In addition, the kinetics of steam oxidation in the Fe-bed depends on temperature and Fe/FeO molar ratio. The fuel velocity in the chamber’s open space is assumed to be constant, while that in the porous electrode and porous Fe-bed is deemed zero for simplicity. The governing equations and corresponding variables for each domain are given in Table I, while the source terms and associated parameters are listed in Table II.

Construction of Numerical Model with Boundary/Initial Conditions

According to the schematic shown in Fig. 2a, there are three components considered in the model: SOFC, free space (chamber) filled with \( H_2 \) and \( H_2O \) and Fe-bed. Figure 2b shows a 2D axial symmetric computational domain corresponding to the area highlighted by the dashed line in Fig. 2a. The SOFC is an anode-supported tubular design with a 22 mm OD, 18 mm ID and 323 mm length. The effective surface area is 220 cm\(^2\). The makeup of the cell consists of a \(~2\) mm thick Ni-Zr\( _{0.84} \)Zr\( _{0.16} \)O\( _2 \) (Ni-YSZ) anode substrate, a \(~10\) \( \mu \)m thick YSZ.
Def \[ f \]

**Table II.** Associated parameters used in the model.

| Source terms/Parameters | Mathematical expressions |
|-------------------------|--------------------------|
| **Butler-Volmer equation** | \[ i_{ct.o} = i_0 \left( \exp \left( \frac{\Delta F \eta_2}{RT} \right) - \exp \left( \frac{-\Delta F \eta_2}{RT} \right) \right) \] |
| | \[ i_{ct.h} = i_0 \left( \frac{c_{H_2}}{c_{O_2}} \exp \left( \frac{\Delta F \eta_1}{RT} \right) - \exp \left( \frac{-\Delta F \eta_1}{RT} \right) \right) \] |
| | \[ \eta_{o/h} = \phi_e - \Delta \phi_{eq,o/h}, \Delta \phi_{eq,h} = 0 \] |
| | \[ E_N = \Delta \phi_{eq,o} = E^0 - \frac{RT}{\Delta F} \ln \left( \frac{P_{H_2,o,h}}{P_{O_2,o,h}} \right), E^0 = 0.992V \] |
| **Binary diffusion** | \[ D_{ij} = \frac{k_D}{\rho} \left( 1 + \frac{s_i}{s_j} \right)^{1/2} \] |
| **Knudsen diffusion** | \[ D_{K,i} = \frac{\sqrt{2}}{3} d_{pore} \sqrt{T/M_i}, q_{pore} = \frac{3}{2} \frac{d_{pore}}{T} \] |
| **Average Bosanquet diffusion coefficient** | \[ D_{ij}^{eff} = \frac{1}{2} \left( \frac{1}{1 - \frac{1}{R_{ij,o}}} + \frac{1}{1 - \frac{1}{R_{ij,h}}} \right) \] |
| **Source term** | \[ R_{0,i} = -\frac{i_{ct,o} S_{pore} M_{H_2}}{\Delta F} \] |
| | \[ R_{H_2,H_2} = \frac{-i_{ct,o} S_{pore} M_{H_2}}{\Delta F}, R_{H_2,O,H_2} = \frac{i_{ct,o} S_{pore} M_{H_2}}{\Delta F} \] |
| **Reaction equilibrium constant for Fe-bed** | \[ K = \exp \left( -\frac{\Delta G^0}{RT} \right) = \frac{[H_2]_{eq}}{[O_2]_{eq}}, \frac{K}{RT} = 2.05, \text{ under 750°C} \] |

Numerical Solutions and Model Validation

There are a total of 8 dependent variables in the model, including the electronic potential \( \phi_e \), ionic potential \( \phi_i \), mass fraction of the gas species, \( \omega \) (\( \omega_0, \omega_{H_2}, \omega_{O_2}, \omega_{H_2O} \)) in the porous air electrode, \( \omega_{O_2} \) and \( \omega_{H_2} \) in the fuel electrode, chamber and Fe-bed, the reacted fraction ratio of Fe (or Fe utilization) \( x_{Fe} \). By combining governing equations in Tables I–II with the boundary conditions in Table III and initial conditions,
Since some of Fe-oxidization in the Fe-bed is determined by an early study of solid and fuel utilization of 75% without Fe-bed. The reaction rate constant was a common practice in the SOFC community. Figure 3 shows the best fitting approach is used to extract these parameters, which has been obtained parameters are well within a reasonable range as reported in the open literature. Note that the use of obtained exchange current density for Fe-bed SOFC represents a conservative action since higher 

\[ H_2 + H_2O \rightarrow H_2O + H_2 \]

density of the performance enhancement, the longitudinal distributions of Nernst potential, local current density, fuel utilization and molar ratio of H_2O and H_2 at a predefined stabilizing time step of 180 seconds are computed.

**Results and Discussion**

A focus of the present work is to investigate the dynamic responses of the power generation of a tubular SOFC loaded with and without a Fe-bed. In the following section, the performance improvement of the tubular SOFC by the Fe-bed will be presented under different cell voltages and different Feedings. To understand the mechanism of the performance enhancement, the longitudinal distributions of Nernst potential, local current density, fuel utilization and molar ratio of H_2O and H_2 at a predefined stabilizing time step of 180 seconds are computed.

**Transient average current density.—** For a tubular SOFC, the current is typically collected by two bus bars attached longitudinally to the anode and cathode, respectively. Under this circumstance, the electric potential at the electrode/current collector interface along the longitudinal direction is uniform, equalling the potential applied. The overall performance of the tubular SOFC evaluated by the average current density along the longitudinal axis under four operating conditions is shown in Figure 3. Validation of exchange current density from a V-I curve obtained from a tubular SOFC without Fe-bed at 750 °C.

![Figure 3](image-url)
In Table IV, the parameters used in the model are listed. For instance, the atmospheric pressure, $p_0$ (atm), is 1, and the temperature, $T_0$ ($^\circ$C), is 750. The inlet molar fraction of H$_2$, $x_{cell,H2}$, is 0.97, and the inlet molar fraction of O$_2$, $x_{cell,O2}$, is 0.204.

A transient process is observed at the very first few seconds, followed by a stabilized current density. Therefore, in the following, we choose a step of 180 seconds as a stabilization time to study the longitudinal distributions under various operating voltages. A replot of cell voltage ($V_{cell}$) vs stabilized average current density ($J_{avg}$) in Fig. 4a is shown in Fig. 4b. The increase of $J_{avg}$ by 5.6%, 12.5%, 19.3% and 26.4%, respectively, is shown in Fig. 4b. The increase of $J_{avg}$ by Fe-bed SOFC stabilizes at a certain value for each operating voltage, whereas it falls for the baseline cell. Such a "stabilized Nernst potential" ($E_N(z)$) distribution along the longitudinal direction of the cell under operating voltage is shown in Fig. 5, where it is fairly obvious that for the baseline cell, Fig. 5a, the $E_N(z)$ drops rather quickly in the first 50-mm, followed by a slower linear decrease with cell length, especially under high operating voltages. The lower the cell voltage or the higher the cell current, the more pronounced the $E_N$ decrease especially under high operating voltages. The lower the cell voltage, the greater the improvement. Therefore, the Fe-bed is more beneficial to high current density operation.

### Distribution of nernst potential ($E_N(z)$) along the longitudinal direction ($z$).

Different from the button cell previously studied in our lab, the fuel is introduced through a fuel injector to the close-end and then flowed back toward the open-end over the inner surface of the anode for a pilot scale anode supported tubular SOFC, where it meets with air that flows over the outer cathode surface of the cell. As both fuel and air co-flow along the longitudinal direction, the electrochemical cathodic and anodic reactions take place, resulting in a depleted fuel (or increased oxide) distribution along the inner anode surface of the flow direction, thus lowered Nernst potential ($E_N(z)$). In other words, instead of a constant $E_N$ for the button cell, there will be an $E_N(z)$ distribution along the longitudinal direction of the cell during operation.

In this section, we compute the $E_N(z)$ profiles along the longitudinal direction for both the baseline and Fe-bed SOFC under different voltages. The results are shown in Fig. 5, where it is fairly obvious that for the baseline cell, Fig. 5a, the $E_N(z)$ drops rather quickly in the first 50-mm, followed by a slower linear decrease with cell length, especially under high operating voltages. The lower the cell voltage or the higher the cell current, the more pronounced the $E_N$ decrease along the cell length. In comparison, for a tubular Fe-SOFC, the $E_N$ distribution, Fig. 5b, is less sensitive to the cell voltage than that of the baseline cell. It is also noticed that the distribution of Nernst potentials are similar in magnitude for both cases for the first ~100 mm. The major difference is seen toward the open-end of the cell: the $E_N(z)$ of Fe-bed SOFC stabilizes at a certain value for each operating voltage, whereas it falls for the baseline cell. Such a "stabilized Nernst potential" phenomenon toward the open-end region infers that H$_2$ produced from the reaction of Fe-H$_2$O stabilizes the H$_2$/H$_2$O that exclusively from the reaction of Fe-H$_2$O stabilizes the H$_2$/H$_2$O that exclusively determines the $E_N(z)$ at a fixed temperature.

### Distribution of H$_2$O/H$_2$ molar fraction ratio along the longitudinal direction ($z$).

From the Nernst potential $E_N$ equation in Table II, $E_N$ can be directly related to the molar fraction ratio of H$_2$O and H$_2$ ($r(z) = x_{H2O}(z)/x_{H2}(z)$). The computed $r(z)$ distributions along the cell length are shown in Figs. 6a and 6b, for both baseline and Fe-bed SOFC. It is evident that the longitudinal variation of $r(z)$ is significant for the baseline cell. With an operating voltage of 0.755 V, $r(z)$ could reach 20 at the open-end of the cell, whereas it is only 1.2 for the Fe-bed SOFC. Such a low $r(z)$ for the Fe-bed SOFC is the fundamental reason for the flatter and higher $E_N(z)$ distribution than

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**Table IV. Parameters used in the model.**

| Parameters                          | Values       |
|-------------------------------------|--------------|
| Atmospheric pressure, $p_0$ (atm)   | 1            |
| Temperature, $T_0$ ($^\circ$C)      | 750          |
| Inlet molar fraction of H$_2$, $x_{cell,H2}$ | 0.97        |
| Inlet molar fraction of O$_2$, $x_{cell,O2}$ | 0.204       |
| Porosity, Anode/Cathode $\varepsilon$ | 0.404        |
| Electronic conductivity, $\sigma_e$ (S m$^{-1}$) | $5 \times 10^6$ |
| Ionic conductivity, $\sigma_i$ (S m$^{-1}$) | 1.2          |
| Exchange current density for SOFC, $J_{avg}$ | 1064/3192 |
| Anode/Cathode $i_0^*$ (A m$^{-2}$) | $1 - e_{(a/c)} \times 1.43 \times 10^5$ |
| Specific surface area, Anode/Cathode $S_s^*$ (m$^{-2}$) | 0.5          |
| Transfer coefficient, $\alpha_1/\alpha_2$ | 0.5/0.5      |
| Number of electrons, $n$            | 2            |
| Reference diffusivity, $k_B$ (m$^2$ s$^{-1}$) | $3.16 \times 10^{-6}$ |
| Kinetic volume of H$_2$, $v_{h2}$    | $6 \times 10^{-6}$ |
| Kinetic volume of O$_2$, $v_{o2}$    | $16.6 \times 10^{-6}$ |
| Kinetic volume of N$_2$, $v_{n2}$    | $17.9 \times 10^{-6}$ |
| Kinetic volume of H$_2$O, $v_{h2o}$  | $12.7 \times 10^{-6}$ |
| Diameter of spherical particle, $d_p$ (μm) | 34.16        |
| Loading of Iron, $m_{Fe}$ (g)       | 34.16        |
| Initial reacted Fe ratio, $x_{Fe,0}$ | $10^{-4}$   |
| Initial porosity of RCU, $\varepsilon$ | 0.7          |
| Reaction rate constant of JMAK, $k_{2}/k_{0}$ (s$^{-1}$) | $9.4 \times 10^{-4}/4.585 \times 10^{-4}$ |
| Avrami exponent of JMAK, $N$         | 0.8          |
| Flow velocity in the Chamber, $u_0$ (m s$^{-1}$) | 0.0839 |

Note: The parameters with * are adjusted in order to validate the model with the experimental results.
the baseline cell observed in Fig. 5. It is also worth mentioning that the nature of nonlinear $i$-$\eta$ relationship (Butler-Volmer equation in Table II) and the logarithm relationship between $E_N(z)$ and $r(z)$ can yield a more pronounced variation of $E_N(z)$ along the cell length in a regular baseline cell under a load condition. However, if an extra $H_2$-source such as Fe-bed is present very next to the anode, the $E_N(z)$ variation can be effectively mitigated. This is extremely important to applications such as fast ramping power and overload protection since conventional SOFCs may suffer Ni-oxidation due to slow response to fuel demand, ultimately threatening the lifetime of stack.

**Distribution of local current density ($J_{loc}(z)$) along the longitudinal direction $z$.**—In Distribution of nernst potential ($E_N(z)$) along the longitudinal direction ($z$) section, we show that $E_N$ varies along the length of the tubular SOFC. Since the operating cell voltage is fixed along the length by the bus bars, the local current density will vary along the cell. In this section, we here compute the local current density ($J_{loc}(z)$) profiles along the cell length under different cell voltages for both baseline and Fe-bed SOFC.

For the baseline cell, Fig. 7a, the highest $J_{loc}(z)$ is located at the close-end ($z=0$ mm), where fresh fuel is introduced. This is understandable in that $E_N$ is the highest at the closed-end. Above the close-end, $J_{loc}(z)$ monotonically decreases with cell length $z$. It is also noticed that the distribution of $J_{loc}(z)$ is deeper at lower cell voltage than at higher voltage. In comparison, for the Fe-bed SOFC, Fig. 7b, $J_{loc}(z)$ also decreases with cell length $z$, but exhibits a much flatter profile than the baseline cell. It appears that the lower the cell voltage, the lower the $z$-value at which the local current density is stabilized. For example, for $V_{cell} = 0.904$ V, the stabilizing $J_{loc}(z)$ occurs at $z = 200$ mm; however, it is 150 mm for $V_{cell} = 0.755$ V. This observation implies that there are more Fe taking part in the reaction due to higher concentration of $H_2O$ at lower cell voltage (or higher current density).

**Distribution of fuel utilization ($U_f(z)$) along the longitudinal direction $z$.**—The fuel utilization $U_f(z)$ is calculated by the ratio of hydrogen molar fraction $x_{H_2}(z)$ at a certain $z$ location vs $x_{H_2}(0)$ at the close-end of the cell, i.e. $U_f(z) = x_{H_2}(z)/x_{H_2}(0)$. Therefore, it is a direct indication of the $H_2$ fuel molar fraction in the anode stream. Because of the 2D axial symmetric configuration, we used the radial integration to calculate the average fuel molar fraction $x_{H_2}(z)$ at each $z$. The results are shown in Fig. 8 for both baseline and Fe-bed SOFCs.

For the baseline cell, Fig. 8a, the local $U_f(z)$ increases monotonously with the cell length $z$. The lower the operating voltage, the steeper the profile. As the fuel approaches the open-end of the cell, the slope of the fuel utilization tends to be smaller than that at the close-end. Overall, $U_f(z)$ at the open-end can be very high, e.g. $U_f(z=324$ mm)$=95$% at 0.755 V. This is a dangerous gas composition since excessive $H_2O$ could potentially oxidize the Ni-anode. In
comparison, the Fe-bed SOFC, Fig. 8b, shows a much flatter profile than the baseline cell at all operating voltage simulated. The highest $U_f(z=324 \text{ mm})$ is 55% at 0.755 V. The additional $H_2$ produced in situ by the Fe-bed is clearly the fundamental reason for the low local $U_f(z)$, demonstrating the tolerance of Fe-bed SOFC to overload operation.

**Longitudinal distribution of Fe-utilization in the chemical bed.**— One observation from the above simulation is that the lower the cell voltage or the higher the cell current, the closer the active Fe-bed to the close-end, inferring that more Fe are involved in the $H_2O$-Fe reaction. To confirm this prediction, we also computed the Fe utilization ($x_{Fe}(z)$) profiles (integration along the radial direction at each z location) under different cell voltages; the results are shown in Fig. 9. It is evident that the Fe-bed begins to be oxidized at different locations for different cell voltages, i.e. $z=180, 124, 91.5$ and 75.4 mm for $V_{cell}=0.904, 0.858, 0.805$ and 0.755 V, respectively. The lower the operating voltage the closer to the close-end the Fe-bed to produce $H_2$. More Fe is consumed at lower cell voltage due to higher concentration of $H_2O$ resulted from higher cell current.

**The effect of Fe-loading on cell performance.**—The effect of Fe-loading on cell performance is also investigated. Figure 10 summarizes the results, which compares the performance of the baseline cell with 34 g Fe-loading with that of a cell with half of the loading, i.e. 17 g. Clearly, there is more impact from Fe-loading at a lower operating voltage, 0.755 V. The average current density $J_{avg}$ is increased by 170 A/m$^2$ by doubling Fe-loading, see Fig. 10a. In comparison, at higher operating voltage, 0.904 V, the average current density $J_{avg}$ is only increased by 10 A/m$^2$ by doubling Fe-loading.

Correspondingly, at lower operating voltage of 0.755 V, by doubling Fe loading $E_N$ at the open-end is increased by 0.03 V.
Figure 10. A tubular SOFC operated with different Fe-loading. (a) Average current density $J_{\text{avg}}$ vs time; (b) Distributions of $E_s(z)$ along the length ($z$); (c) Distributions of $\gamma(z)=\gamma_{H_2O}(z)/\gamma_{H_2}(z)$ along the length ($z$); (d) Distributions of $J_{\text{loc}}(z)$ along the length ($z$); (e) Distributions of $U_f(z)$ along the length ($z$); (f) Distributions of $x_{Fe}(z)$ along the length ($z$).

(see Fig. 10b), while the $H_2O/H_2$ molar fraction ratio at the open-end is decreased by 1.5 times (see Fig. 10c). Such an enhancement can also be seen from the local current density ($J_{\text{loc}}$) and fuel utilization ($U_f$) profiles shown in Figs. 10d and 10e, where $J_{\text{loc}}$ increases and $U_f$ decreases from $z=100$ mm to the open-end, respectively. To achieve such performance improvement, the Fe is utilized to generate extra $H_2$ to reach a new dynamic equilibrium in the anode chamber. With higher Fe-loading, i.e. 34 g, the Fe utilization is relatively small, which results in a higher Fe-bed reaction rate according to the last rate equation listed in Table I. Therefore, the $H_2O/H_2$ molar fraction ratio is only slightly deviated from its equilibrium, which means more hydrogen exists in the anode chamber and is beneficial to achieve a higher cell performance.

The average current density $J_{\text{avg}} @ 180$ s as a function of Fe-loading is shown in Fig. 11. From the slope change of the curve with Fe-loading, it is inferred that the improvement resulted from Fe-loading is more significant at low Fe-loading than at high Fe-loading. In other words, as Fe loading increases the corresponding increase of $J_{\text{avg}}$ becomes gradually limited. On the other hand, more Fe-loading occupies more space of the anode chamber, resulting in an increased
pressure drop. Overall, the amount of Fe-loading is determined by the volume available and time for overload operation.

**General comments on Fe-bed tubular SOFC.**—Based on the above simulation results, one can conclude that the inclusion of a Fe-bed in the anode chamber of a tubular SOFC is beneficial when the cell is operated under overload or fast ramping conditions. The mechanism leading to the cell performance enhancement is due to the extra $H_2$ generated by the Fe-bed, which increases the local $E_{N}$ and the current density. The minimum Fe-loading depends on the operating current density and operation duration. There is a trade-off between the Fe-loading and fuel flow pressure drop in the anode chamber, since the increased amount of Fe occupies more space in the anode chamber and leads to an increased pumping power. In addition, beyond the minimum Fe-loading content, the improvement of cell performance becomes less significant.

**Conclusions**

In summary, a 2D axial symmetrical multi-physics model has been constructed for an anode-supported tubular solid oxide fuel cell loaded with and without a Fe-bed. The model parameters are validated by experimental data to ensure a high-fidelity computation. The model features the coupling of charge and mass transport in a tubular SOFC with chemical reaction kinetics in the Fe-bed, producing longitudinal distributions of Nernst potential, $H_2O/H_2$ molar ratio, local current density, fuel utilization and Fe-utilization under different load conditions. The simulations explicitly show that the Fe-bed loaded SOFC exhibit a higher and flatter distribution of $E_{N}(z)$, $xH_2/\alpha H_2O(\alpha z)$, local $J_{loc}(z)$ and local fuel utilization along the cell length $z$. The lower the cell voltage (or higher cell current) the more Fe is used. The fundamental reason for the enhanced performance is the production of $H_2$ through in situ $H_2O$-Fe reaction. The ability of Fe-SOFC to produce extra $H_2$ next to the Ni-anode enables the cell to tolerate fast transient overload and provide fast ramping power for practical power generations.

**Acknowledgments**

The information, data or work presented herein was funded in part by the Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy, under Award number DE-AR0000492.

**List of Symbols**

- $c$, (mol · m$^{-3}$) Molar concentration
- $d_{por}$, (m) Diameter of spherical particle of the porous medium
- $d_{p}$, (m) Pore radius of the porous medium
- $D_{ij}$, (m$^2$ · s$^{-1}$) Binary diffusion coefficient for a pair of species $i$ and $j$
- $D_{Kn,i}$, (m$^2$ · s$^{-1}$) Knudsen diffusion coefficient of species $i$
- $E_N$, (V) Nernst potential
- $F(C·mol^{-1})$ Faraday’s constant, 96485
- $G$, (J · mol$^{-1}$) Gibbs free energy
- $i_{st}$, (A · m$^{-2}$) Local charge transfer current density
- $J_{loc}$, (A · m$^{-2}$) Local current density along the longitudinal direction of the tubular cell
- $J_{avg}$, (A · m$^{-2}$) Average current density of the tubular cell
- $K$ Equilibrium constant
- $k_D$, (m$^2$ · s$^{-1}$) Reference diffusivity
- $k_{fR}$, (s$^{-1}$) Forward reaction constant in JMAK model
- $k_{bR}$, (s$^{-1}$) Backward reaction constant in JMAK model
- $M_i$, (kg · mol$^{-1}$) Molar weight of species $i$
- $M$, (kg · mol$^{-1}$) Average molar weight of gas mixture
- $N$ Avrami exponent
- $p$, (Pa) Pressure
- $p_r(z)$ Molar fraction ratio of $H_2O$ and $H_2$ at $z$
- $Q_{f}$ (s$^{-1}$) Gas constant, 8,314
- $R$, (kg · m$^{-3}$ · s$^{-1}$) Reaction source term for species $i$
- $R_{a}$, (m$^{-1}$) Electrochemical reaction active area per unit volume
- $r(z)$ Time
- $T$, (K) Temperature
- $U$, (s) Fuel Utilization
- $x_{H_2O}$ Molar fraction of water vapor
- $x_{H_2}$ Molar fraction of hydrogen
- $x_{Fe}$ Reacted Fe ratio/Fe Utilization
- $\alpha$ Transfer coefficient in Butler-Volmer equation
- $\sigma$ Conductivity, (S · m$^{-1}$)
- $\phi$, (V) Potential
- $\phi_{eq}$, (V) Equilibrium potential
- $\eta$, (V) Overpotential
- $\rho$, (kg · m$^{-3}$) Density
- $\omega_{ij}$ Mass fraction of species $i/j$
- $\omega_i$, (m$^{-3}$) Kinetic volume of species $i$
- $\varepsilon$, (m$^{-1}$) Porosity
- $\tau$, (s) Tortuosity
- $\tau_s$, (s) Tortuosity
- $\phi_{eq}$, (V) Equilibrium potential
- $\eta$, (V) Overpotential
- $\rho$, (kg · m$^{-3}$) Density
- $\omega_{ij}$ Mass fraction of species $i/j$
- $\omega_i$, (m$^{-3}$) Kinetic volume of species $i$
- $\varepsilon$, (m$^{-1}$) Porosity
- $\tau$, (s) Tortuosity

**Greek**

- $\alpha$ Transfer coefficient in Butler-Volmer equation
- $\sigma$ Conductivity, (S · m$^{-1}$)
- $\phi$, (V) Potential
- $\phi_{eq}$, (V) Equilibrium potential
- $\eta$, (V) Overpotential
- $\rho$, (kg · m$^{-3}$) Density
- $\omega_{ij}$ Mass fraction of species $i/j$
- $\omega_i$, (m$^{-3}$) Kinetic volume of species $i$
- $\varepsilon$, (m$^{-1}$) Porosity
- $\tau$, (s) Tortuosity

**Subscripts**

- $e$ Electronic
- $el$ Electrolyte
- $i$ Ionic
- $o$ Oxygen electrode
- $h$ Hydrogen electrode

**Superscripts**

- $eff$ Effective
- $0$ Ideal/Initial

**References**

1. K. Huang and J.B. Goodenough, Solid Oxide Fuel Cell Technology: Principles, Performance and Operations. 2009: Woodhead Publishing. 340.
2. Y. Kobayashi et al., Extremely High-efficiency Thermal Power System-Solid Oxide Fuel Cell (SOFC) Triple Combined-cycle System, *Mitsubishi Heavy Industries Technical Review*, 48(3), 9 (2011).

3. A. B. Stamhosili and E. Traverse, Solid oxide fuel cells (SOFCs): a review of an environmentally clean and efficient source of energy, *Renewable & Sustainable Energy Reviews*, 6(5), 433 (2002).

4. F. Gonzalez-Longatt et al., Load Following Function of Fuel Cell Plant in Distributed Environment *Renewable Energies and Power Quality Journal*, 1(3), 285 (2005).

5. O. So-ryeok et al., Dynamic characteristics and fast load following of 5-kW class tubular solid oxide fuel cell/micro-gas turbine hybrid systems, *International Journal of Energy Research*, 37(10), 1242 (2013).

6. F. Abdeljawad et al., Redox instability, mechanical deformation, and heterogeneous damage accumulation in solid oxide fuel cell anodes, *Journal of Applied Physics*, 112(3), (2012).

7. A. Faes et al., A Review of RedOx Cycling of Solid Oxide Fuel Cells Anode, *Membranes (Basel)*, 2(3), 585 (2012).

8. D. Sarantaridis and A. Atkinson, Redox cycling of Ni-based solid oxide fuel cell anodes: A review, *Fuel Cells*, 7(3), 246 (2007).

9. C. Zhang et al., Dynamic solid oxide fuel cell empowered by the built-in iron-bed solid fuel, *Energy & Environmental Science*, 9(12), 3746 (2016).

10. H.C. Park and A.V. Virkar, Bimetallic (Ni-Fe) anode-supported solid oxide fuel cells with gadolinia-doped ceria electrolyte, *Journal of Power Sources*, 186(1), 133 (2009).

11. J. Yan et al., Nanoporous Ni-Fe Bimetallic Plates for Nonfragile, Reliable SOFCs, *Electrochemical and Solid-State Letters*, 10(9), B139 (2007).

12. X. Jin, X. Zhao, and K. Huang, A Computational study of the effects of charging parameters on the performance and reversibility of a new type SOFC storage battery, in MRS proceedings, 2015. Cambridge University Press.

13. X. Jin et al., Analysis of Performance Limiting Factors in Solid-Oxide-Iron-Air Redox Battery Operated with Different Redox Couples, *ECS Transactions*, 68(1), 251 (2015).

14. X.F. Jin and K.V. Huang, Multiphysics modeling of solid-oxide iron-air redox battery: analysis and optimization of operation and performance parameters, *Science Bulletin*, 61(17), 1345 (2016).

15. X.F. Jin, X. Zhao, and K. Huang, A high-fidelity multiphysics model for the new solid oxide iron-air redox battery part I: Bridging mass transport and charge transfer with redox cycle kinetics, *Journal of Power Sources*, 280, 195 (2015).

16. X.Y. Jin et al., Heat Balance in a Planar Solid Oxide Iron-Air Redox Battery: A Computational Analysis, *Journal of the Electrochemical Society*, 162(8), F821 (2015).

17. X.F. Jin et al., Computational Analysis of Performance Limiting Factors for the New Solid Oxide Iron-air Redox Battery Operated at 550 degrees C, *Electrochimica Acta*, 178, 190 (2015).

18. Advances in Crystallization Processes, *Crystallization Kinetics of Metallic Glasses*, ed. A. Pratap and A.T. Patel. 2012: InTech.

19. E.R. Fotsing, Phase Transformation Kinetics and Microstructure of Carbide and Diboride Based Ceramics, *Fakultát für Bergbau, Hüttenwesen und Maschinenwesen of the Technische Universität Clausthal*, (2005).

20. E. Lorente, J.A. Pena, and J. Herguido, Kinetic study of the redox process for separating and storing hydrogen: Oxidation stage and ageing of solid, *International Journal of Hydrogen Energy*, 33(2), 615 (2008).

21. J. Torrens-Serra et al., Non-Isothermal Kinetic Analysis of the Crystallization of Metallic Glasses Using the Master Curve Method, *Materials*, 4(12), 2231 (2011).

22. Y.X. Shi, N.S. Cai, and C. Li, Numerical modeling of an anode-supported SOFC button cell considering anodic surface diffusion, *Journal of Power Sources*, 164(2), 639 (2007).

23. M. Ni, M.K.H. Leung, and D.Y.C. Leung, Parametric study of solid oxide fuel cell performance, *Energy Conversion and Management*, 48(5), 1525 (2007).

24. X. Zhao et al., Exploring Metal-Air Chemistries with a New Solid Oxide Metal-Air Redox Battery, *ECS Transactions*, 58(12), 67 (2014).

25. X. Zhao et al., Solid Oxide Iron-Air Rechargeable Battery - A New Energy Storage Mechanism, *ECS Transactions*, 50(45), 115 (2013).

26. X. Zhao et al., Energy storage characteristics of a new rechargeable solid oxide iron-air battery, *Rsc Advances*, 2(27), 10163 (2012).