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Technical Communication

# On the source terms of species equations in fuel cell modeling

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ABSTRACT

By checking the unit of the source terms, it is found that the source terms used in some fuel cell modeling studies are incorrect. The correct source terms of species equations are proposed in this communication.



The fundamental fuel cell model consists of conservation principles for mass, momentum, species, charge, and energy. These governing equations are coupled with chemical/electrochemical reactions through sources terms, which can be described in the general form as [1],

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla(\rho\mathbf{V}\phi) = \nabla(\Gamma\nabla\phi) + S \tag{1}$$

where $\phi$ is a general variable to be solved, t is time, $\rho$ is density, **V** is the velocity vector, $\Gamma$ is the general diffusion coefficient, and S is the general source term including all terms that cannot be included in other terms. By setting $\phi = Y_j$, mass fraction of species j, the general transport equation becomes the species equations. In the species equations, the source terms represent the species' **volumetric consumption/generation** rate through chemical/electrochemical reactions. Therefore, in 3D modeling of fuel cells, the unit of source terms must be volumetric-based, for example, the unit for source term of species equations must be kg/(m$^3$ s), or mol/(m$^3$ s). Similarly, the unit for source term of energy equation must be W/m$^3$.

For fuel cells running on hydrogen and oxygen, the source terms of species equations are usually calculated as

$$S_{O_2} = -\frac{M_{O_2}}{4F} i_c \tag{2}$$

$$S_{H_2} = -\frac{M_{H_2}}{2F} i_a \tag{3}$$

$$S_{H_2O} = \frac{M_{H_2O}}{2F} i_a \tag{4}$$

where M is the molecular weight (kg/mol), F is the Faraday constant; $i_c$ and $i_a$ are local current density, which are **volumetric-based** (A/m$^3$).

Through a short literature survey, it is found that in some 3D fuel cell modeling studies, for example [2,3], kg/(m$^2$ s) and W/m$^2$ are used for source terms of species equations and energy equation, respectively. In these studies the authors assume that the electrochemical reaction only takes place at the electrode–membrane interface, thus the unit of A/m$^2$ is used for $i_c$ and $i_a$ in Eqs. (2)–(4). However, kg/(m$^2$ s) and W/m$^2$ are not consistent with other terms of the species equations and energy equation (Eq. (1)) for a 3D modeling study, thus the source terms are incorrect. If the electrochemical reaction only takes place at the electrode–membrane interface, the $H_2$ mass change should be $-(M_{H_2}/2F)i_a\Delta x\Delta y$ for a finite volume (grid cell) at the electrode–membrane interface (at the electrode side), since the local current density is area-based (A/m$^2$). Here $\Delta x\Delta y$ is the area of a unit grid cell (for electrochemical reaction) at the electrode-membrane interface. Thus, the **volumetric** $H_2$ mass change (that is, the source term for species equation) should be,

$$S_{H_2} = -\frac{\frac{M_{H_2}}{2F} i_a \Delta x\Delta y}{\Delta x\Delta y\Delta z} = -\frac{M_{H_2}}{2F\Delta z} i_a \tag{5}$$

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where $\Delta x\Delta y\Delta z$ is the size of the finite volume (grid cell) and $\Delta z$ is the height of the finite volume (grid cell) considered above (at the electrode-electrolyte interface). Similarly, the source terms for $H_2O$ and $O_2$ should be,

$$S_{H_2O} = \frac{M_{H_2O}}{2F\Delta z} i_a \tag{6}$$

$$S_{O_2} = -\frac{M_{O_2}}{4F\Delta z} i_c \tag{7}$$

Eqs. (5)–(7) are the correct source terms for species equations in 3D fuel cell modeling when electrochemical reactions are assumed to occur only at the electrode–electrolyte interface (the unit of $i_c$ and $i_a$ is $A/m^2$ in this case). If the local current densities are volumetric-based, then Eqs. (2)–(4) can be used for calculating the source terms of species equations.

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