2010 Comsol Conference

Presented at the COMSOL Conference 2010 China

COMSOL Multiphysics application in modeling PEMFC transients

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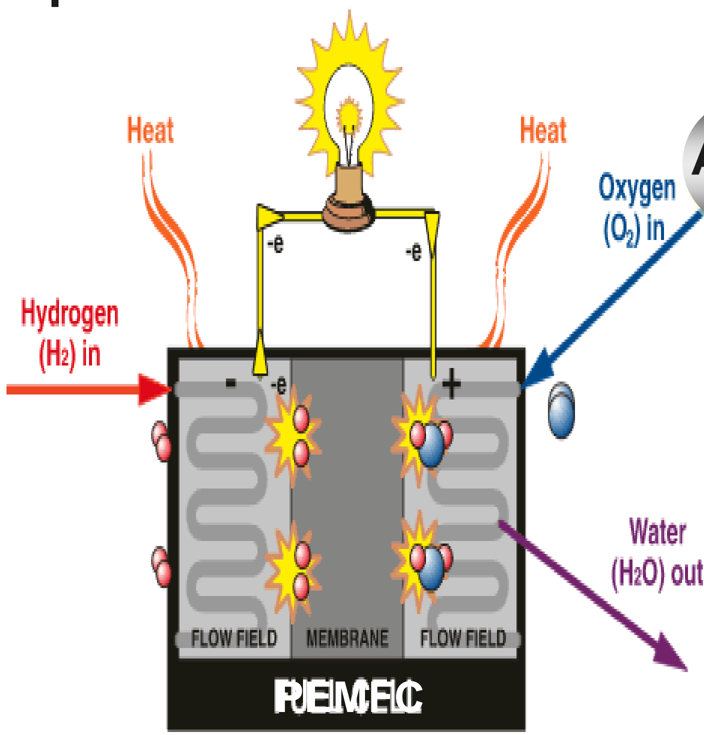
Shanghai 26th, October, 2010

Main content

- Principle of PEMFC and transient characteristics
- Study on PEMFC transient characteristics
  - Develop the PEMFC transient model
  - Air stoichiometry change on PEMFC transient
  - Water transport on PEMFC transient
  - Modeling high temperature PEMFC
- Conclusion

Principle of PEMFC & application



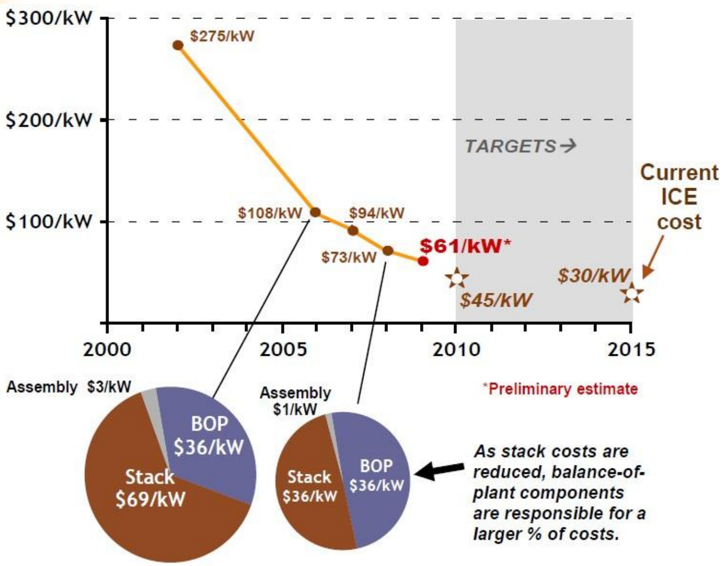
Advantages

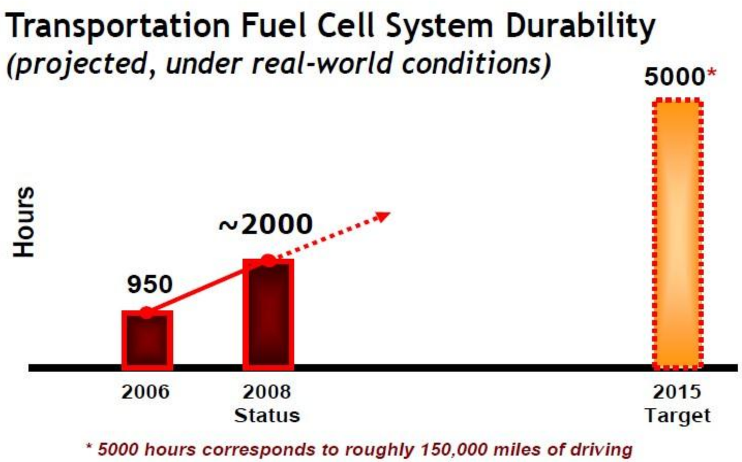
- High efficiency
- Environment friendly
- High power density
- Fast startup

Anode: $H_2 \rightarrow 2H^+ + 2e^-$

Cathode: $1/2\ O_2 + 2H^+ + 2e^- \rightarrow H_2O$

Bottleneck of FC technology





Commercialization

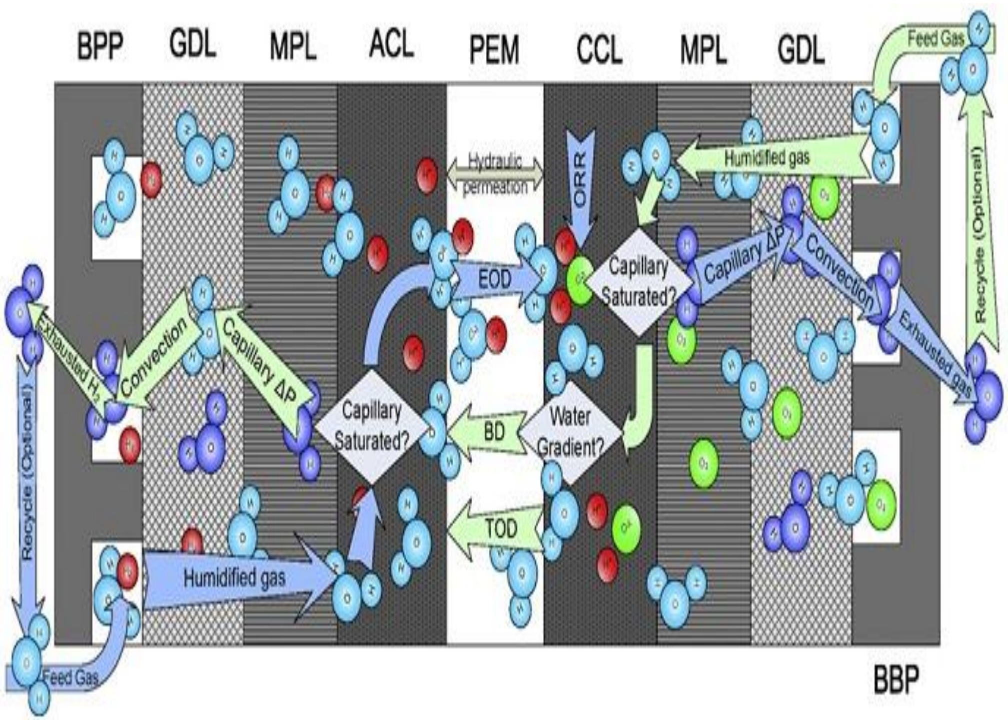
- **System stability & reliability**

Transient characteristics

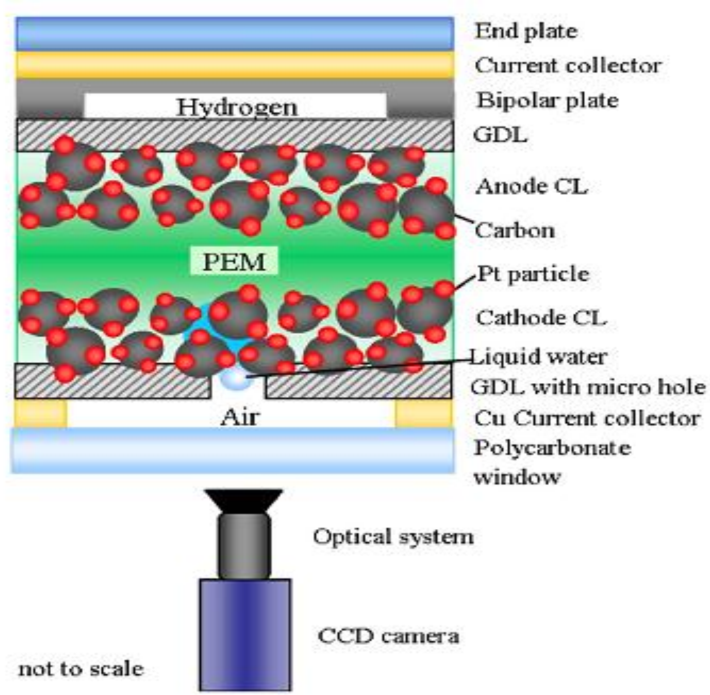
- **System cost**
- **Environment adaptability**

Water transport in FC

FC water transport principle



Experiment observation



Model assumptions

1. The gravity effect is neglected ；
2. The gas mixture is an incompressible ideal gas；
3. The flow in the gas channel is laminar；
4. The diffusion layer, catalyst layer and membrane are isotropic and homogeneous, and the membrane is impermeable to gas species；
5. The contact resistance between any two parts in the fuel cell is neglected；
6. The dissolved reactive gas in electrolyte phase of catalyst layer is neglected;
7. It is considered that water exits in the gas phase at the electrodes as well as in the liquid phase within the membrane. In channels, existence of liquid water is in a small volume fraction and in finely dispersed droplets so that it dose not affect the gas flow.

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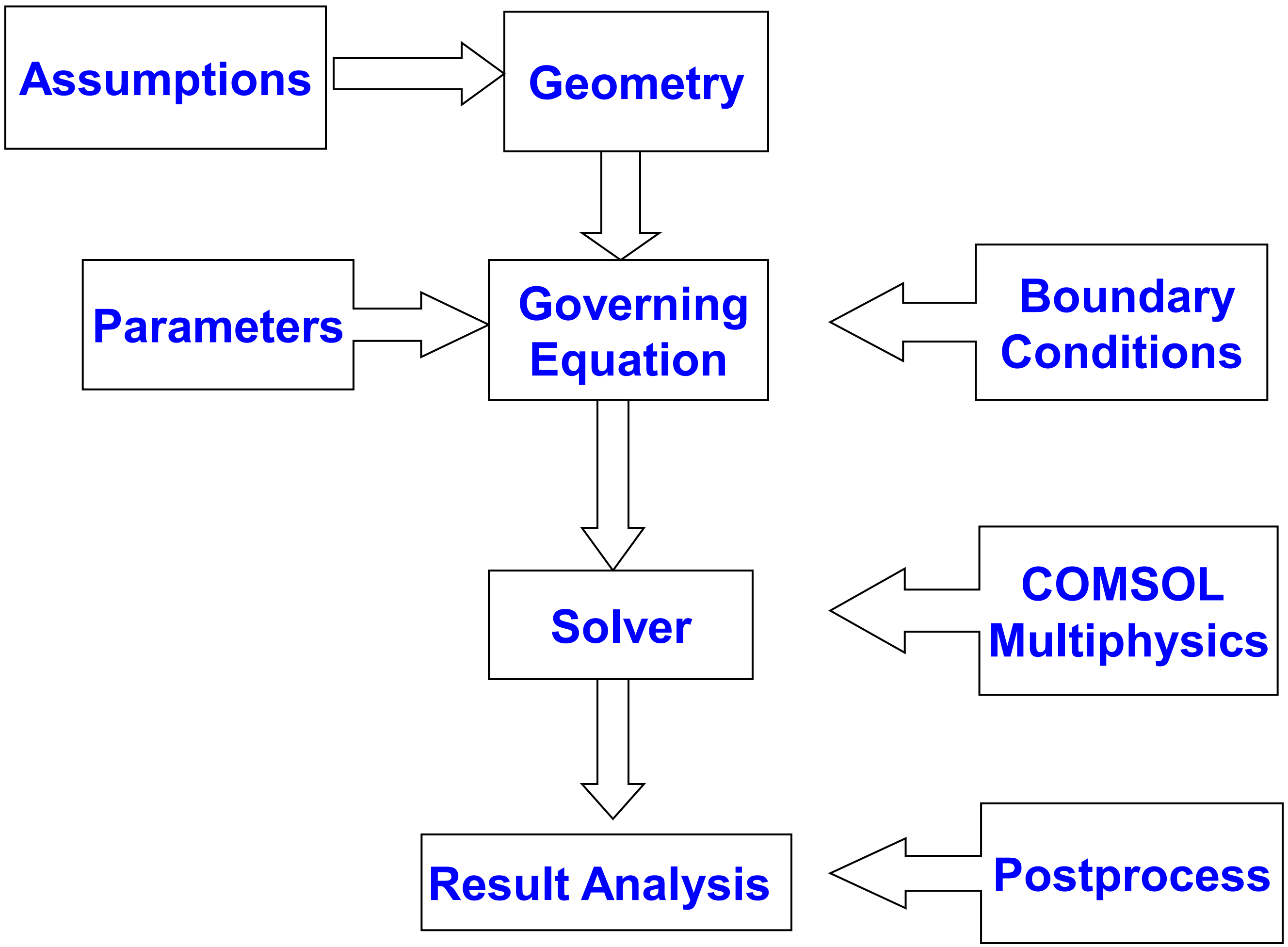
Procedures


Assumptions
Geometry
Parameters
Governing Equation
Boundary Conditions
Solver
COMSOL Multiphysics
Result Analysis
Postprocess

Model equations

Continuity: $\nabla \cdot (\rho u) = S_m$

Momentum: $\frac{1}{\varepsilon^2} \nabla \cdot \left(\rho \vec{u}\vec{u} \right) = -\nabla p + \nabla \cdot \tau + S_u$

Species: $\nabla \cdot \left(-D_i^{eff} \nabla C_v \right) + \nabla \cdot \left(u_g C_i \right) = S_i$

Water in membrane: $\nabla \cdot (\frac{n_d I}{F} - D_w \nabla c_w) = 0$

Energy: $\rho c_p u \cdot \nabla T + \nabla \cdot (-k_f \nabla T) = \mathrm{S_T}$

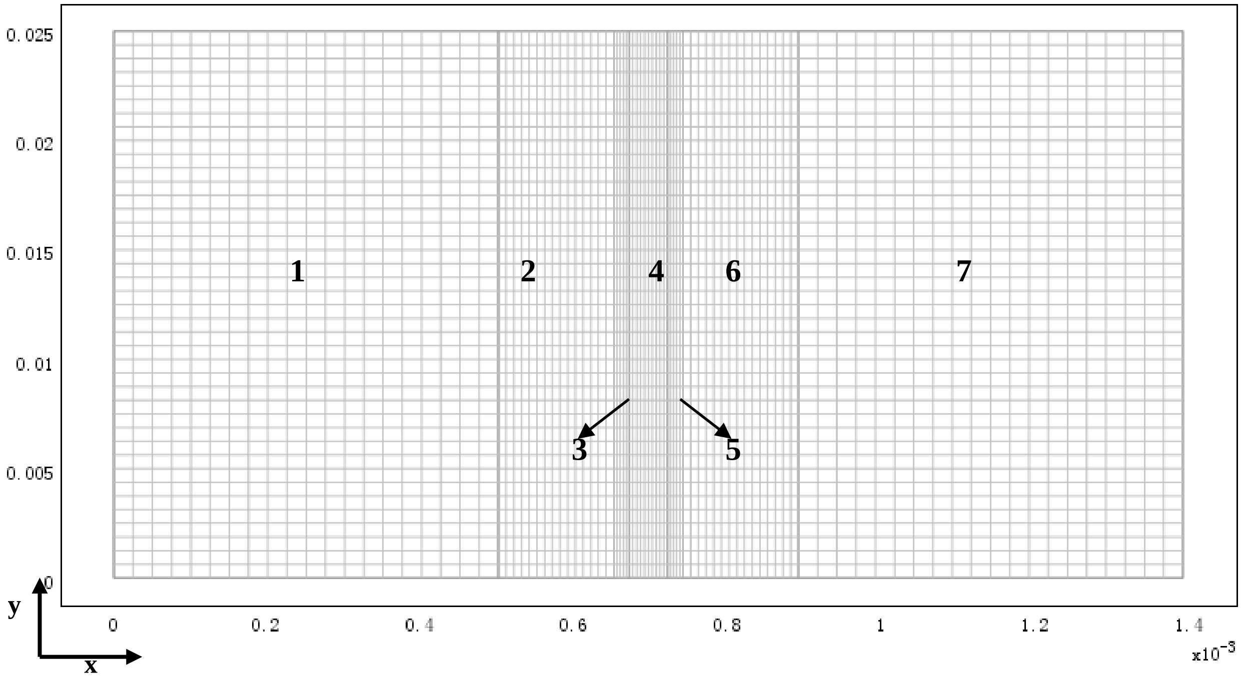
Electron: $\nabla \cdot \left(-\sigma_e^{eff} \nabla \Phi_e \right) = S_e$

Proton: $\nabla \cdot \left(-\sigma_m^{eff} \nabla \Phi_m \right) = -S_m$

Source term for model equations

	GDL	CL, a	CL, c	Membrane
Mass	/	$S_m = M_{H_2} S_{H_2} + M_{H_2O} S_W^a$	$S_m = M_{H_2O} S_{O_2} + M_{H_2O} S_w^c$	/
Momentum	$S_u = -\frac{\mu}{k_p} u$	$S_u = -\frac{\mu}{k_p} u$	$S_u = -\frac{\mu}{k_p} u$	/
Species	/	$S_{H_2} = -\frac{i_a}{2F}$	/	/
	/	/	$S_{O_2} = -\frac{i_c}{4F}$	/
	/	$S_w^a = -\frac{n_d}{F} i_a$	$S_w^c = \frac{n_d}{F} i_c + \frac{i_c}{2F}$	/
Electron	/	$S_s = -i_a$	$S_s = i_c$	/
Proton	/	$S_e = i_a$	$S_e = -i_c$	/
Energy	$S_T = \frac{i^2}{\sigma_s}$	/	$S_{rn} = -j(\Phi_e - \Phi_s - \frac{T\Delta S}{nF})$	$S_T = \frac{i^2}{\sigma_m}$

Model geometry & mesh



Model geometry：1anode flow channel, 2anode gas diffusion layer, 3anode catalyst layer, 4membrane, 5 Cathode catalyst layer, 6 Cathode gas diffusion layer, 7 Cathode flow channel

Comsol Multiphysics 3.5

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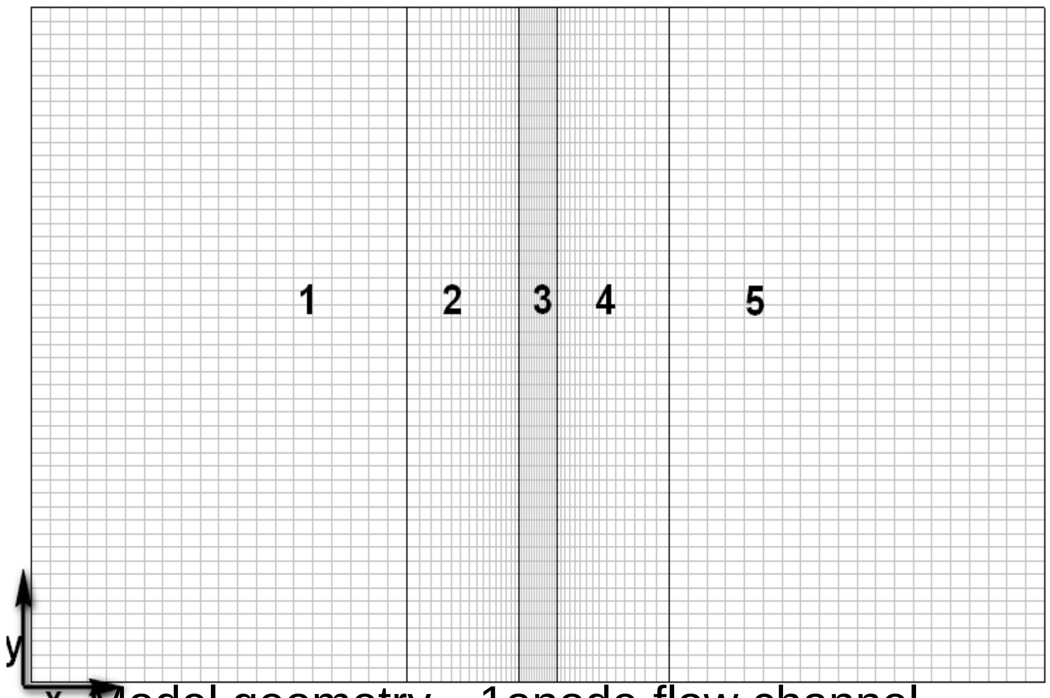
PEMFC transient model



Model geometry：1anode flow channel, 2anode gas diffusion layer, 3membrane, 4Cathode gas diffusion layer, 5 Cathode flow channel

Mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = S_m$$

Momentum conservation

$$\frac{1}{\varepsilon}\left[\frac{\partial \rho \vec{u}}{\partial t} + \frac{1}{\varepsilon}\nabla \cdot (\rho \vec{u}\vec{u})\right] = -\nabla p + \nabla \cdot \tau + S_u$$

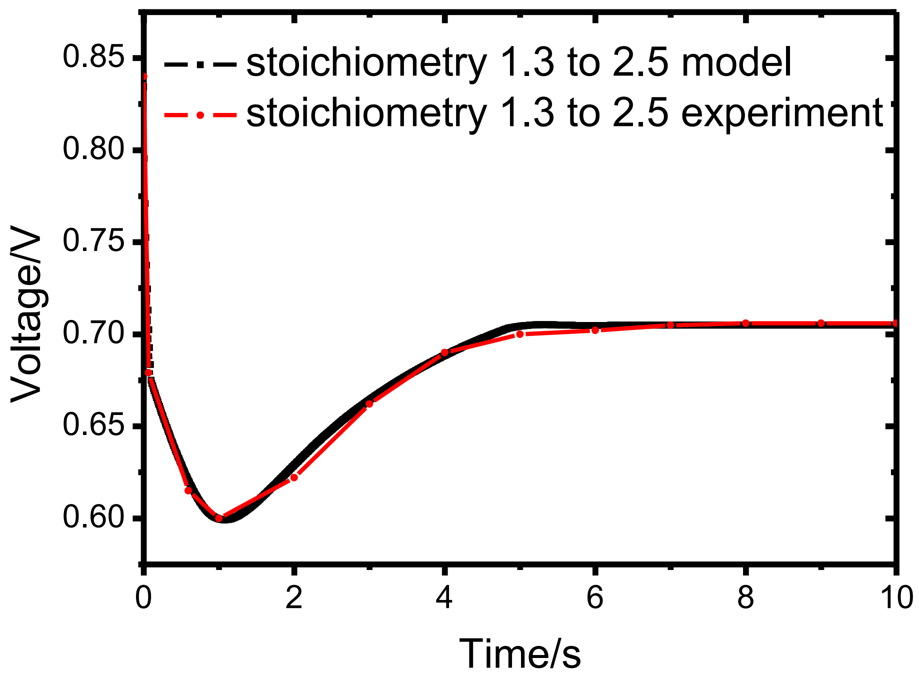
Species conservation

$$\frac{\partial c_k}{\partial t} + \nabla \cdot (\vec{u} c_k) = \nabla \cdot (D_k^{eff} \nabla c_k) + S_k$$

Cell potential:

$$V_{cell} = E - \eta_{act} - \eta_{ohm} - \eta_{conc}$$

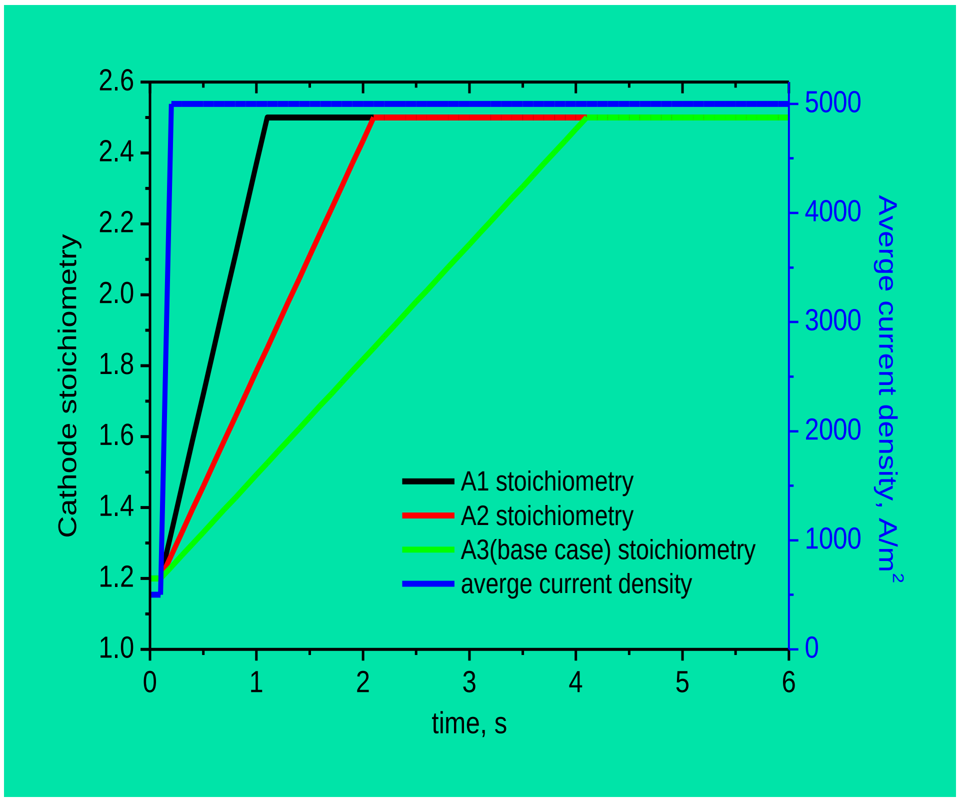
Model validation

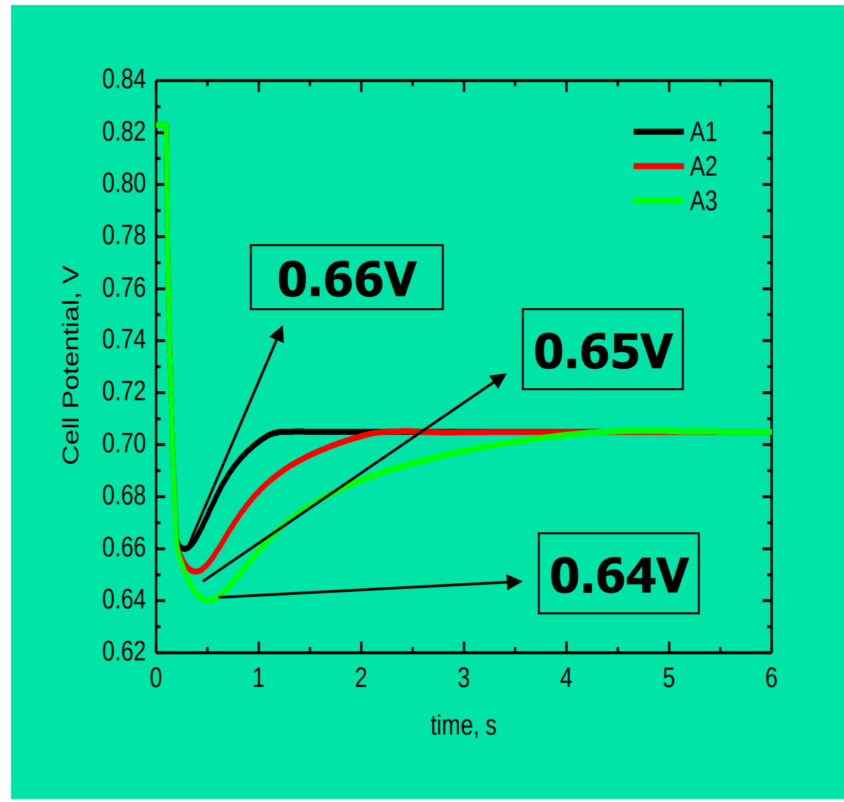


Comparison between model and experimental cell voltage evolution

Q. Shen, M. Hou, et. al J. Power Sources. 2008, 179: 292–296

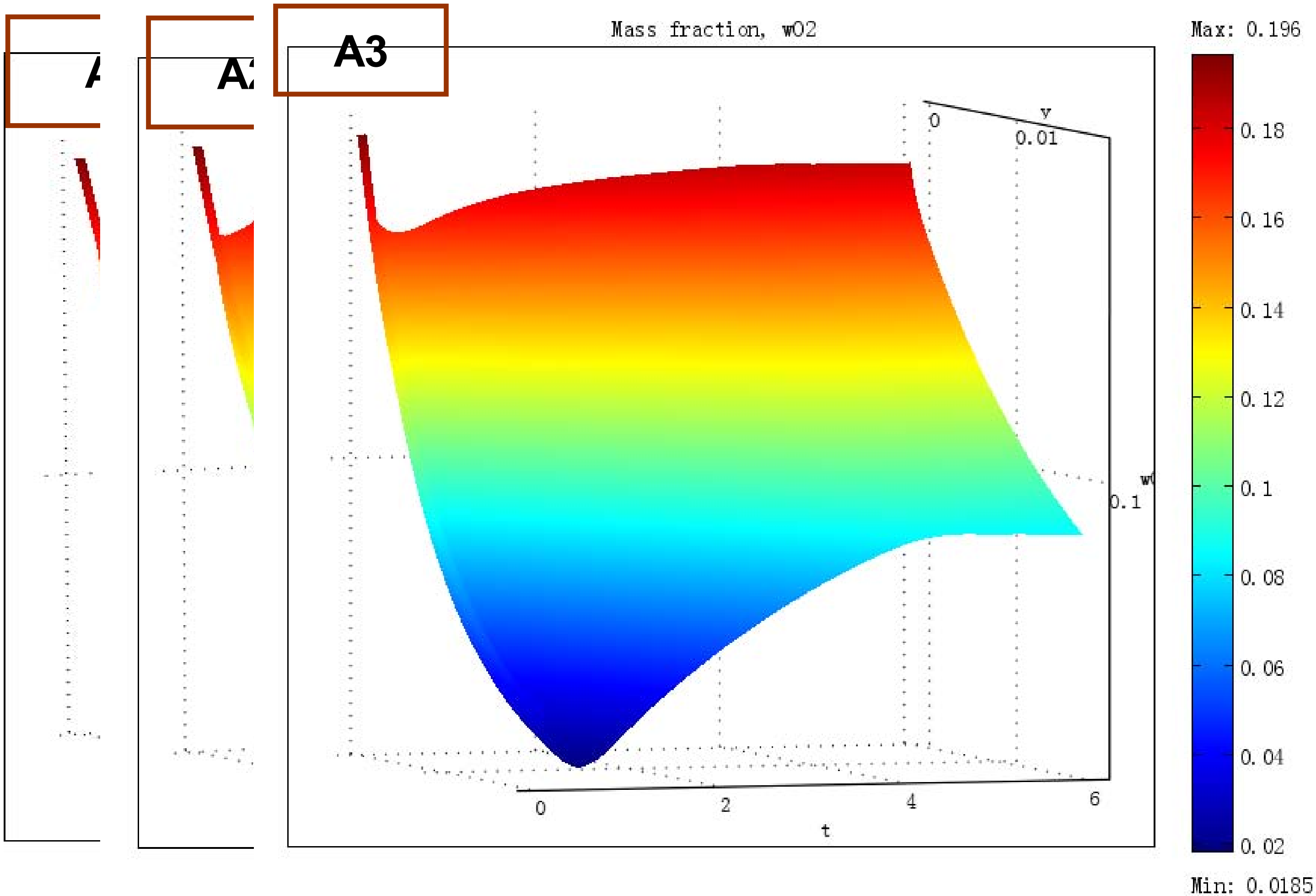
Air stoichiometry change on PEMFC transient





Qu Shuguo, Li Xiaojin, etc., J Power Sources 185 (2008), 302-310

Reactant starvation under different conditions



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Experiment study on water dynamic transport

Aim： Study water transport in fuel cell under different humidity on cell potential and as model validation

Conditions：

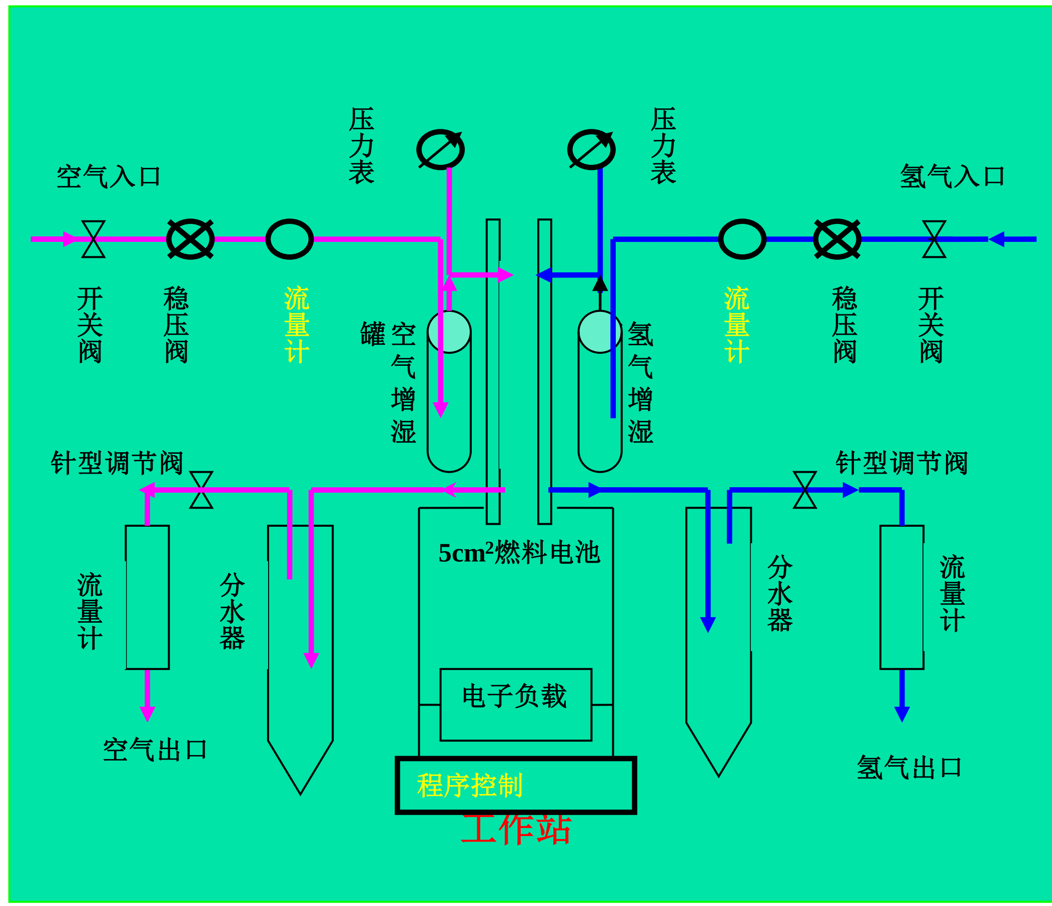
Current：step from 0.05 to 2.5A

Air flow：parabolic pattern 22-110ml/min

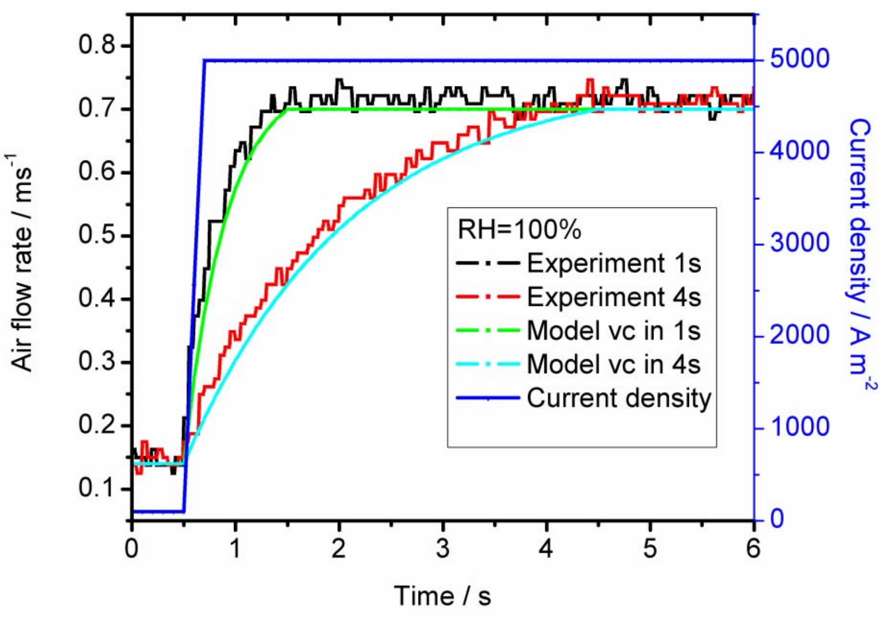
Hydrogen flow：fixed

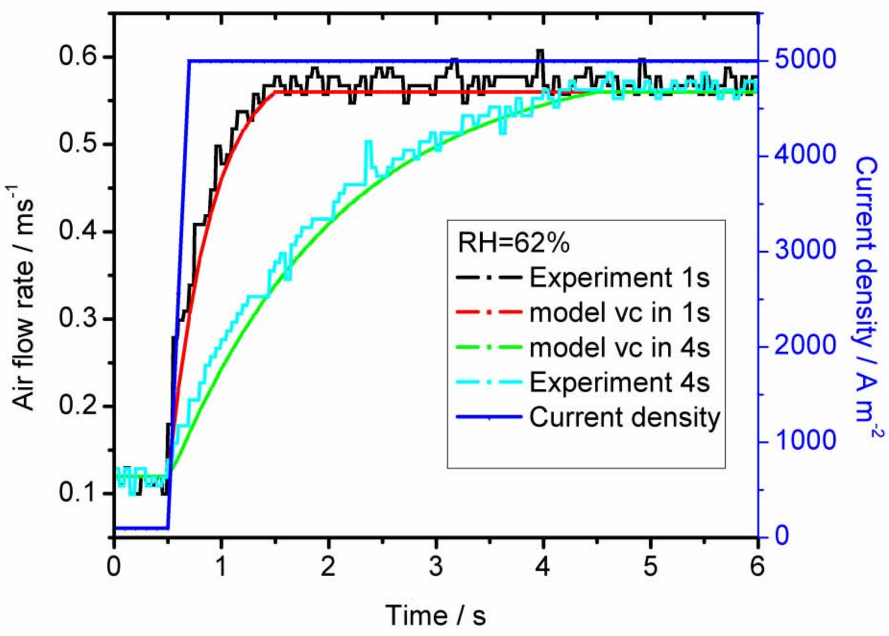
Humidity：100%

62%

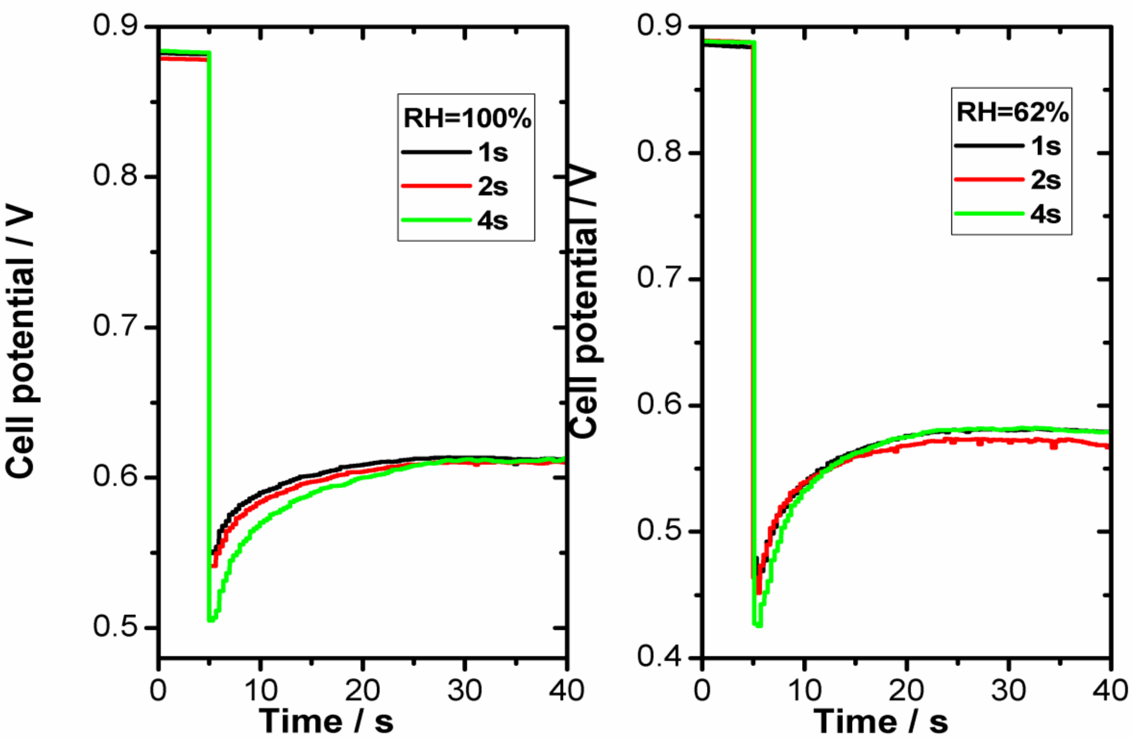


Average current density & cathode inlet velocity change



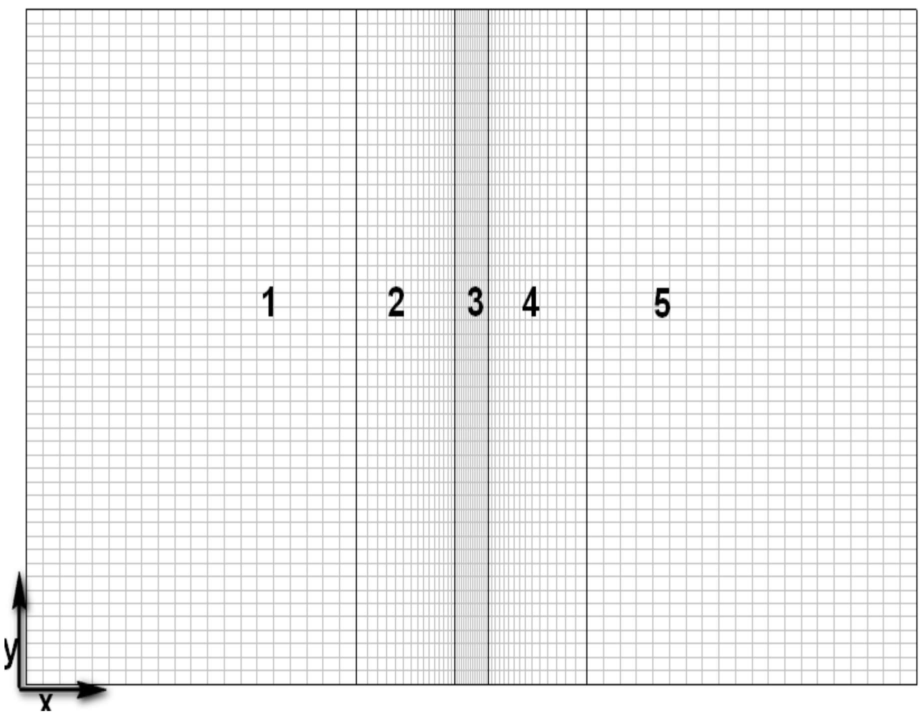


Experiment results



- For same relative humidity, the lower the change rate, the greater the cell potential undershoots.
- For different relative humidity, the magnitude of cell potential undershoots increased as the relative humidity decreased
- The steady state cell potential also decreased as the relative humidity was decreasing

Model geometry



Model geometry：1anode flow channel, 2anode gas diffusion layer, 3membrane, 4Cathode gas diffusion layer, 5 Cathode flow channel

Continuity $$\frac{\partial}{\partial t}\left(\varepsilon\rho_g\right)+\nabla\cdot\left(\rho_g u_g\right)=S_m$$

Momentum $$\frac{1}{\varepsilon}\left[\frac{\partial\rho\vec{u}}{\partial t}+\frac{1}{\varepsilon}\nabla\cdot\left(\rho\vec{u}\vec{u}\right)\right]=-\nabla p+\nabla\cdot\tau+S_u$$

Species $$\frac{\partial}{\partial t}\left(\varepsilon^{eff}C_i\right)+\nabla\cdot\left(-D_i^{eff}\nabla C_v\right)+\nabla\cdot\left(u_g C_i\right)=S_i$$

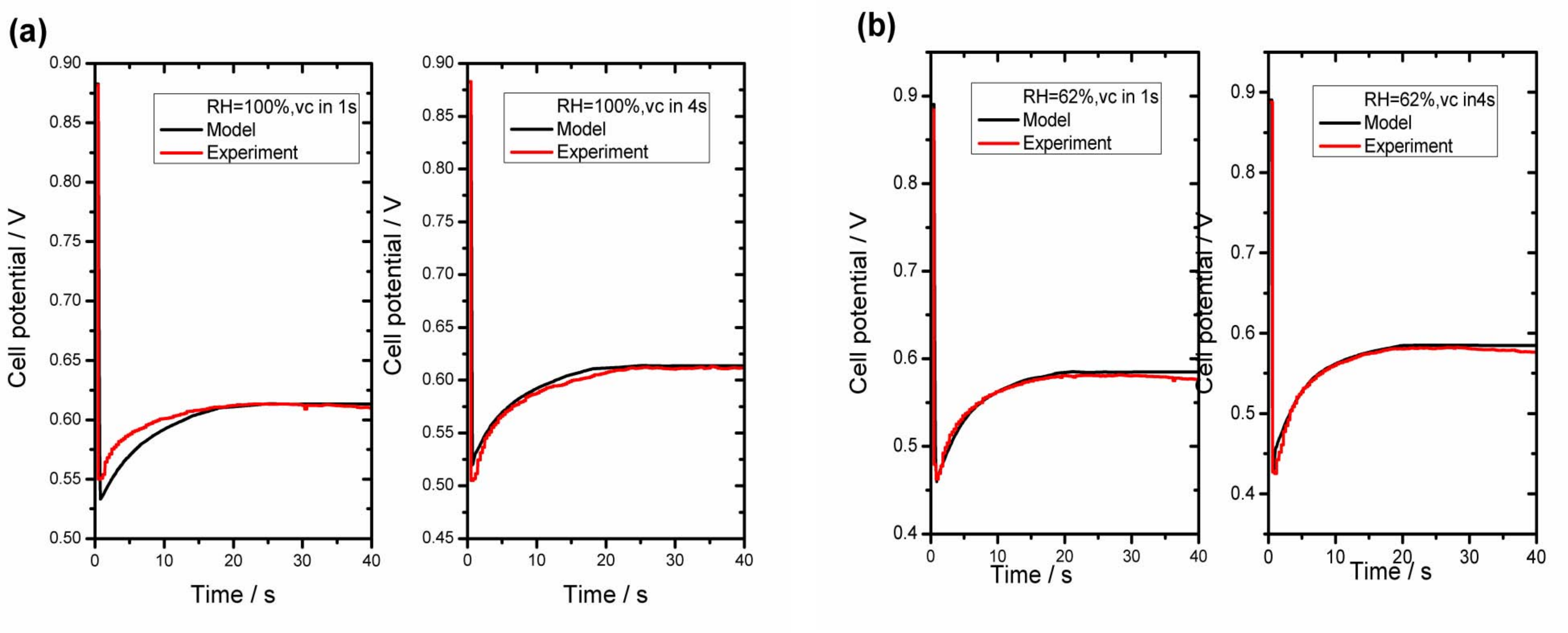
Water in membrane $$\varepsilon_m\frac{\partial c_w}{\partial t}+\nabla\cdot\left(\frac{n_d I}{F}-D_w\nabla c_w\right)=0$$

Electrons $$\nabla\cdot\left(-\sigma_e^{eff}\nabla\Phi_e\right)=S_e$$

Protons $$\nabla\cdot\left(-\sigma_m^{eff}\nabla\Phi_m\right)=-S_m$$

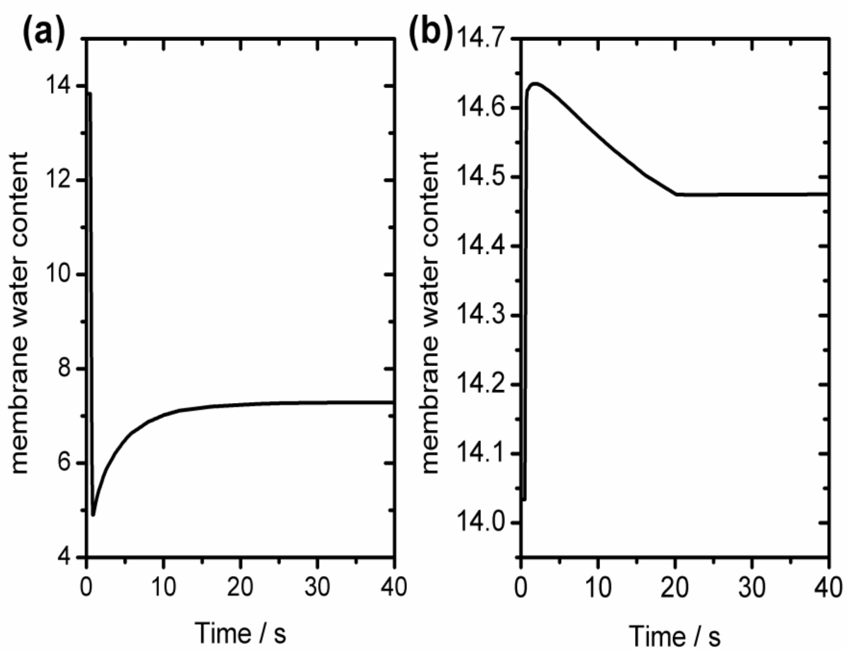
Comsol Multiphysics 3.5求解

Model validation

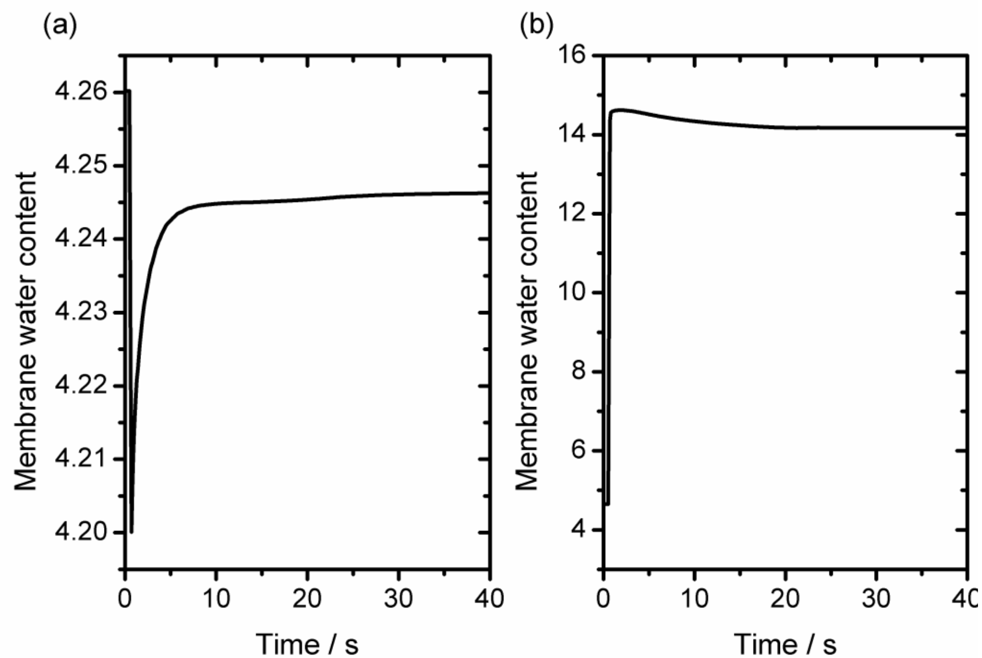


Water content change at membrane/electrode interface

RH=100% water content at membrane/electrode interface



RH=62%water content at membrane/electrode interface



Qu Shuguo, Li Xiaojin, etc.，J Power Sources 195 (2010), 6629-6636

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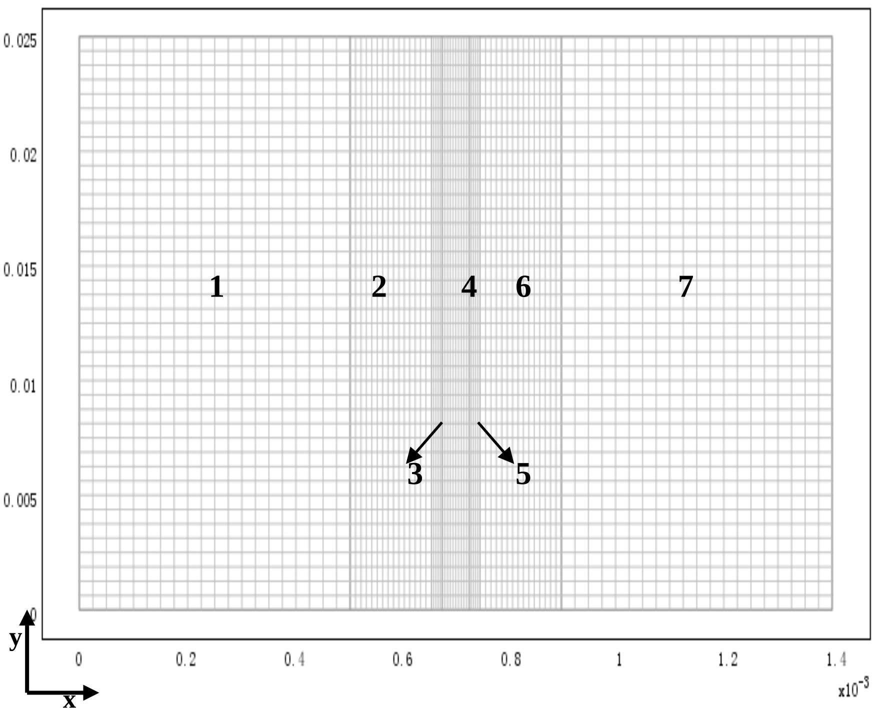
2-D nonisothermal HT-PEMFC model



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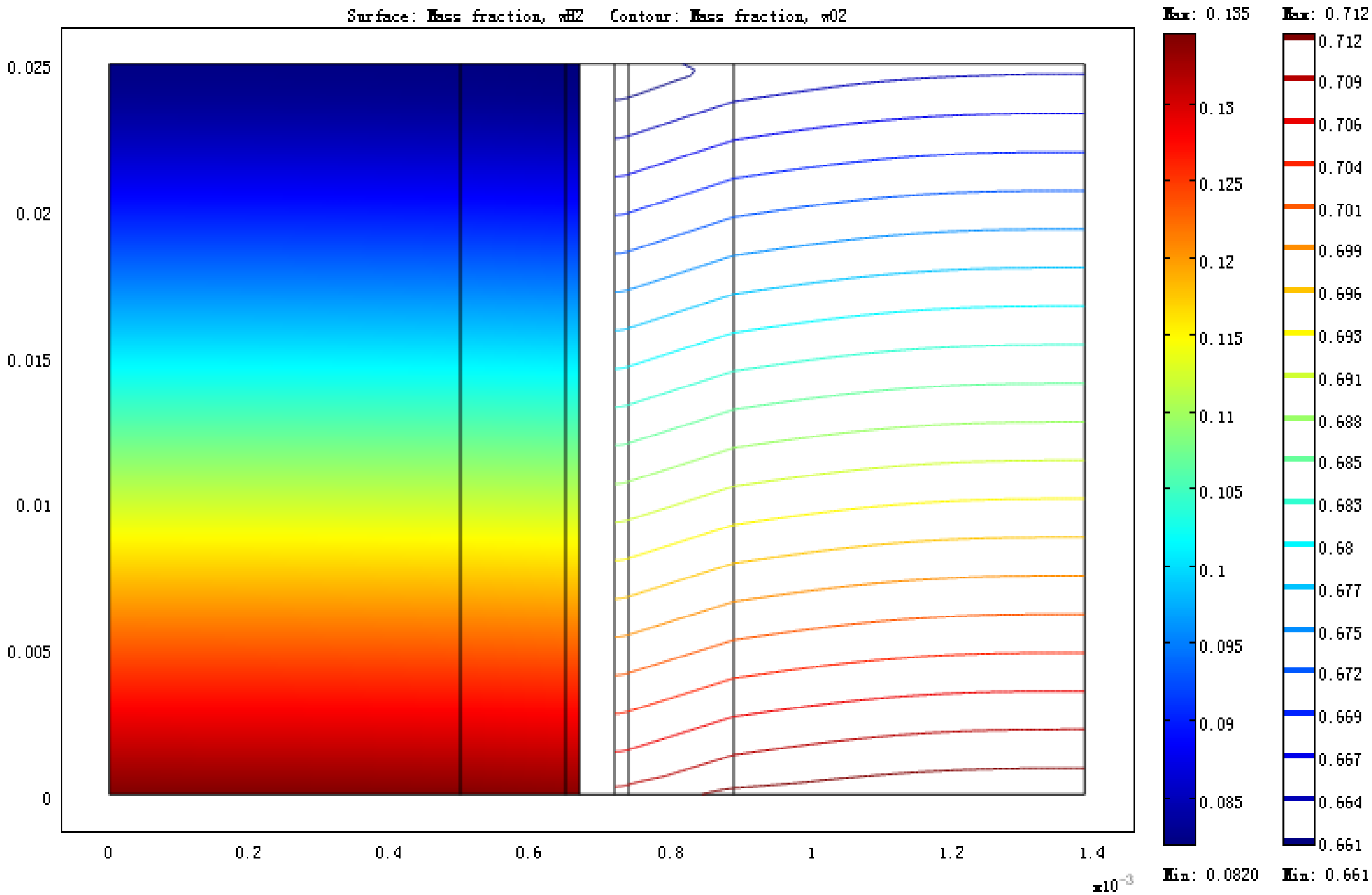
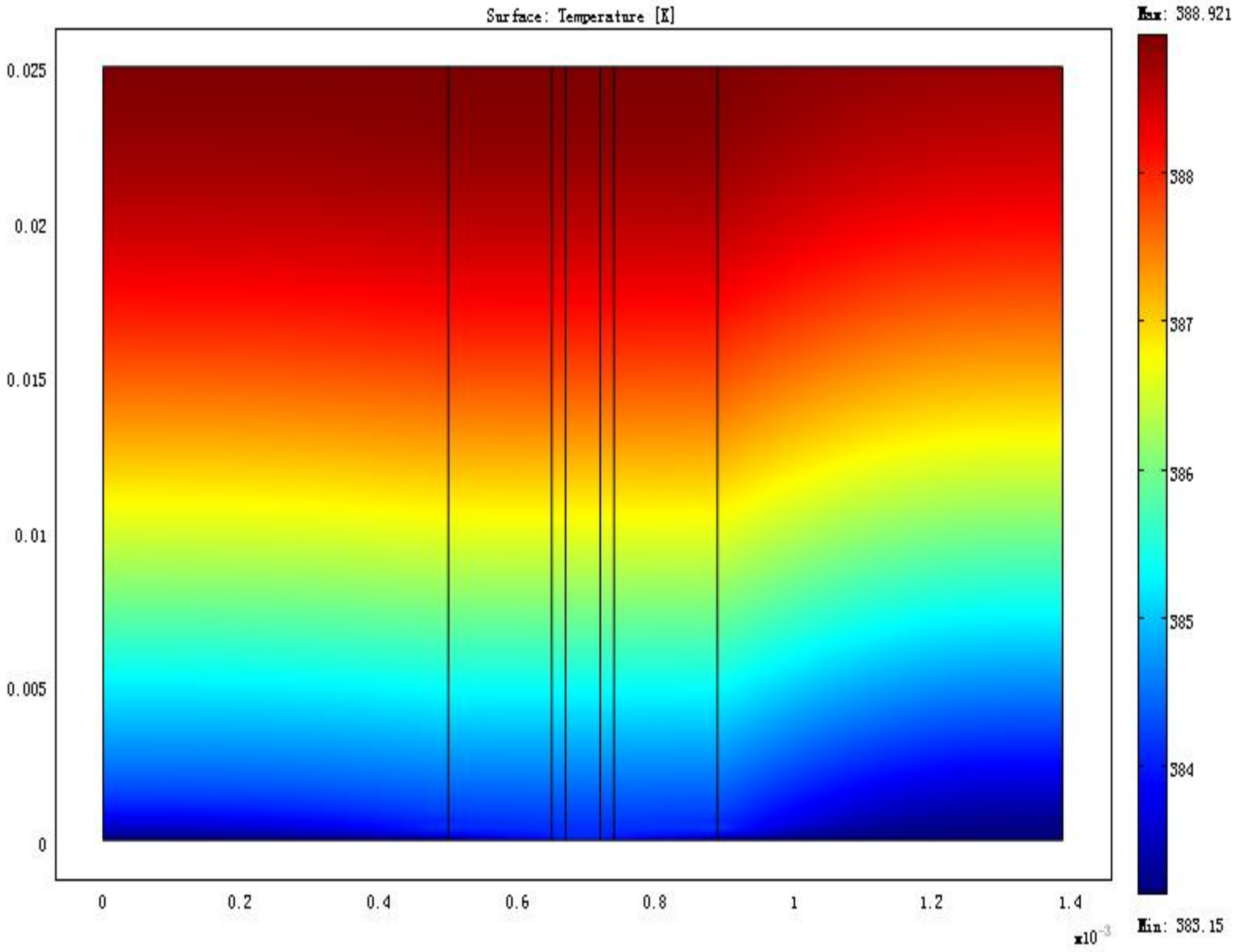
Electron: $\nabla\cdot\left(-\sigma_e^{eff}\nabla\Phi_e\right)=S_e$

Proton: $\nabla\cdot\left(-\sigma_m^{eff}\nabla\Phi_m\right)=-S_m$

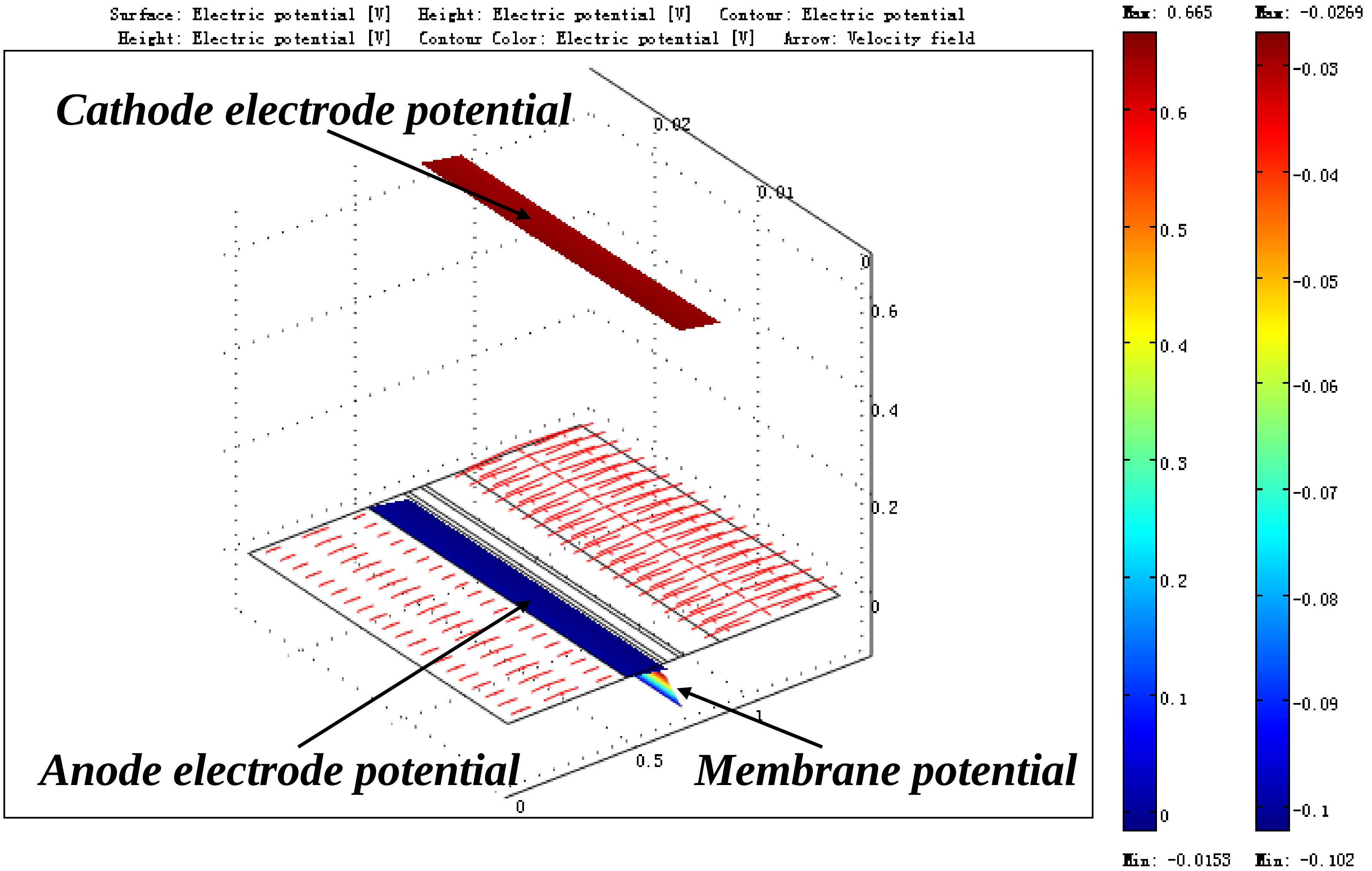
Species distribution in HT-PEMFC



Temperature distribution in HT-PEMFC



Potential distribution in electrode and membrane



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Conclusion

- ✓Modeled fuel cell transient characteristics using COMSOL Multiphysics and the model result validated by experiment；
- ✓Carried out fuel cell dynamic simulation using Comsol and closer to real operation conditions；
- ✓Studied the effect of reactant transport and membrane water transport on the PEMFC cell potential under transient air flow and load change using COMSOL Multiphysics；
- ✓Modeled the high temperature PEMFC based on Nafion/SiO_2 composite membrane using COMSOL Multiphysics .

Thank You !