Dear editor Valerie Eveloy:

I have received your letter about the comment for our manuscript “Design of Multi-Sensor Fusion Water State Observer for Proton Exchange Membrane Fuel Cell based on Particle Filter” (ECM-D-24-01719). We quite appreciate your favorite consideration and the reviewer’s insightful comments. We have made some revision to our manuscript accordingly and we hope the revision will make our paper more acceptable. All the revisions have been highlighted in the revised manuscript.

Please let me know if you and reviewer have any other questions. Thanks again for your and reviewer’s patience, help and constant attention to our manuscript.

Sincerely

Yanbo Yang

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**Responses to the reviewers’ comments:**

We highly appreciate the reviewers’ kind consideration of the scientific content of our work. The comments and suggestions made by the reviewers are very helpful for us to revise the manuscript. A detailed reply to the comments and suggestions has been made as follows. (Note: The responses to the reviewers’ comments are highlighted in blue).

Reviewer: 1

Comments 1: At the end of section 2, it is said: "Therefore, based on the understanding of the model and the characteristics of the measured data, manually adjust the parameters to determine the order of magnitude of the parameters, making the trend of the model reasonable. Then the Parameter Estimator function is used in the Simulink Design Optimization toolbox for small-scale parameter optimization."  
The authors should better explain this point. Refering a MATLAB toolbox is not an appropiate justification in a cientific journal.  
What to you exactly tune? How do you do it? which cost function do you optimize?

Reply: Thanks for the reviewer’s suggestion. We adjust the parameters subjected to optimization encompass the critical variables delineated in Table 1, including but not limited to the oxygen and water diffusion coefficients, the water conversion coefficient governing the membrane-cathode interphase, and the charge transfer coefficient at the cathode. Our objective is to calibrate these parameters in a manner that minimizes the discrepancy between the model's predictions and the empirical observations, thereby enhancing the fidelity of our simulations.

To achieve this objective, we employ the recursive least square estimator algorithm, a powerful iterative technique that facilitates the convergence of our model's parameters towards their optimal values. This method, which underpins MATLAB's parameter estimation toolbox, operates by sequentially updating the parameter estimates in a recursive manner, leveraging the incoming stream of data to refine the accuracy of the approximations.

Specifically, the algorithm commences by initializing the parameter estimates to user-supplied values, akin to an educated guess. Subsequently, it evaluates the model's output against the observed data, quantifying the residual error. Through a sophisticated weighing and minimization process, the algorithm then calculates the adjustments required to the parameter estimates, with the objective of minimizing the cumulative sum of squared residuals – a metric that encapsulates the collective deviation between the model's predictions and the empirical observations.

This iterative process is repeated recursively, with each iteration incorporating the latest available data point and refining the parameter estimates accordingly. The algorithm's convergence is governed by a predefined termination criterion, such as a threshold for the maximum permissible error or a stipulated number of iterations.

Ultimately, the recursive least square estimator's prowess lies in its ability to rapidly converge to the optimal parameter values, even in the presence of nonlinear relationships and dynamic systems, thereby minimizing the discrepancy between our model's simulations and the empirical observations, as shown in multiple research paper by Zhang, and Kim. (*X. Zhang, P. Pisu.* *An Unscented Kalman Filter based on-line Diagnostic approach for PEM fuel cell Flooding. Int J Progn Health Manag 2014; 5: 004.* and *J.* *Kim, I. Lee, Y. Tak, B. Cho. State-of-health diagnosis based on hamming neural network using output voltage pattern recognition for a PEM fuel cell. Int J Hydrogen Energy 2012; 37: 4280-9*).

Comments 2: I don't understand section 3. The authors refer to an observer, but what they propose has little to do with what I understand by an observer.

Reply: Thanks for the reviewer’s suggestion. An observer is a computational construct designed to reconstruct the internal states of a dynamic system based on available measurements and a mathematical model of the system's behavior. In our work, the term "observer" refers to the estimation function that assimilates the sensor data acquired from various sources and produces estimates of the internal states or parameters of interest, and the same description is used in existing research by Yuan. (*H. Yuan, H. Dai, X. Wei, P. Ming. Model-based observers for internal states estimation and control of proton exchange membrane fuel cell system: A review. J Power Sources 2020; 468: 228376)*

Comments 3: The authors assume one state is known to estimate the next? How do you know that the initial state is correct?

Reply: Thanks for the reviewer’s comment. For first question, a previous state is required to estimate the current state. Our methodology uses the estimated state from the previous time step as a foundation for inferring the current state. This recursive approach is a hallmark of numerous state estimation techniques, wherein the temporal evolution of the system's internal dynamics is captured through an iterative process of sequential updates.

For the second question, we conducted an extensive exploration of the parameter space, systematically evaluating various sets of initial values. Using heuristic optimization process, we identified the set of values that exhibited the closest alignment with the observations, thereby minimizing the discrepancy between our model's predictions and the actual system behavior.

Furthermore, to increase the credibility of our initial state estimates, we leveraged the comprehensive studies conducted by previous researchers such as Wu & He (*H. Wu, X. Li, P. Berg. On the modeling of water transport in polymer electrolyte membrane fuel cells. Electrochim Acta 2009; 54: 6913-27*. and *W. He, J.S. Yi, T. Van Nguyen. Two‐phase flow model of the cathode of PEM fuel cells using interdigitated flow fields.* *AIChE Journal 2000; 46: 2053-64*.)

Comments 4: What sensory information do the authors use?

Reply: Thanks for the reviewer’s comment. In our research, we employed a multifaceted array of sensory data to ensure a thorough analysis of the system dynamics and performance. Specifically, we utilized the following sensory inputs:

1. Pressure on hydrogen/air side, including input & output pressure.
2. Temperatures of hydrogen, air and coolant on input and output sides.
3. The system’s power output, and average voltage/current of each cell unit.
4. The system’s impedance measurement in real time.

The integration of sensory inputs above provides comprehensive observation information of the system’s operational state from multiple perspectives.

Comments 5: Authors should make an effort to properly position their work in the literature. There are various works in the literature that use observers to estimate the state of fuel cells and, from them, the humidity of the membranes. But they are not cited in the references nor are the results compared with theirs.

Reply: Thanks for the reviewer’s comment. We have added the comparation in the introduction, and the revisions had been highlighted in the revised manuscript.

**Reviewer: 2**

Water management is one of the key approaches to enhance the durability of PEMFC. Therefore, it is necessary to identify the internal water state of the PEMFC accurately and quickly and control it within a reasonable range. The current paper verifies simulation, experiment and the simplified mechanism model of PEM containing water in ionomer, liquid water and water vapor. Based on the simulation, the internal water state trend of the PEMFC was analyzed and can accurately estimate the water state inside PEMFC, contributing to the advancement of PEMFC technology and its wide application in the automotive field. Thus, the work can be considered relevant to the area, so, I recommend the publication to the Energy Conversion and Management after minor revision:  
Comments 1: Page 5, Information about reason of choosing certain measurement noise and process noise are missing and needs corresponding literature.

Reply: Thanks for the reviewer’s comment. As for the selection of specific measurement noise and process noise parameters, we have referenced the work of Xu et al. (*.* and *L. Xu, Z. Hu, C. Fang, J. Li, P. Hong, H. Jiang, et al. Anode state observation of polymer electrolyte membrane fuel cell based on unscented Kalman filter and relative humidity sensor before flooding. Renewable Energy 2021;168:1294–307.* and *H. Yuan, H. Dai, X. Wei, P. Ming. A novel model-based internal state observer of a fuel cell system for electric vehicles using improved Kalman filter approach. Appl Energy 2020;268:115009. https://doi.org/10.1016/j.apenergy.2020.115009.*). Xu and Yuan’s research provides a comprehensive analysis of noise characteristics in similar experimental setups and offers empirical data, in “*Anode state observation of polymer ”, the author introduces variance of impedance to better simulate the real environment, in “A novel model-based internal state observer”, the author uses another variance on processing to simulate the natural process noise in real systems. We consider these two methods are critical to our research and use them in our research.*

Comments 2: Page 5, description, and physical explanation of Figure 1 are needed.

Reply: Thanks for the reviewer’s comment. We have added the description in the Figure 1, and the revisions had been highlighted in the revised manuscript.

**Reviewer: 3**  
In order to quickly identify the water state in PEMFC, a simplified model of the mechanism of proton exchange membrane containing water in ionomers, liquid water and water vapor is established. The simplified mechanism model is verified by simulation and experiment. Then, the influence of measurement noise and process noise setting values on the performance of the observer is analyzed. The article has the following features:  
1. A simplified mechanism model of PEM containing water in ions, liquid water and water vapor is established.  
2. Influence of measurement noise and process noise setpoints on observer performance.  
3, noise variance 10-4, process noise 10-8.  
4. Internal state observer based on membrane model and particle filter algorithm.  
5, the change trend of the internal water state is simulated.  
6. The performance of the state observer based on voltage, high frequency resistance and sensor fusion is compared.  
To sum up, the research work presented in this paper is relatively complete, the model verification is highly accurate, and the innovation is strong, which is worthy of publication in Energy Conversion and Management. However, before this, some questions need to be explained:

Comments 1: What does the simplified model do? What is the most prominent role of this simplified model in monitoring internal water status compared to existing studies? Can it be put into practical production applications?

Reply: Thanks for the reviewer’s comment. The simplified model proposed in our study serves as an efficient computational framework for estimating the intricate internal water status in the MEA. Its paramount contribution lies in the incorporation of distinct modeling constructs for the cathode's flow channel and diffusion layer. Moreover, our model introduces a series of equations defining the interfacial interactions between the various layers and components, a critical aspect that has been largely overlooked in prior investigations. This comprehensive characterization of the boundaries and interfaces enables our model to calculate water status in fuel cell with a high degree of fidelity, ultimately yielding more accurate and reliable predictions of the internal water status.

Our model enhances its predictive capabilities, it requires more computational resources for its practical implementation than previous models. Which could be challenging to deploy on resource-constrained embedded controllers or microprocessors with limited computational capacities.

Comments 2: What are the meanings of online and offline? What is the difference in the measurement process?

Reply: Thanks for the reviewer’s comment. The online estimation approach entails a dynamic process, wherein new data is continuously generated from fuel cell, and real-time estimations are generated concurrently with the fuel cell's operation. Conversely, the offline estimation technique is a retrospective endeavor, undertaken upon the completion of the fuel cell's execution phase. In this mode, the water status calculations are performed retrospectively, leveraging the collected data corpus from the concluded operational cycle.

Comments 3: The existing measurement method does not distinguish the flow channel, GDL, CL, how did the existing research measure?

Reply: Thanks for the reviewer’s comment. At present, the X-ray imaging techniques (*Lee SJ, Lim N-Y, Kim S, Park G-G, Kim C-S. X-ray imaging of water distribution in a polymer electrolyte fuel cell. Journal of Power Sources 2008;185:867–70.* and *Aroge FA, Parimalam BS, MacDonald JA, Orfino FP, Dutta M, Kjeang E. Analysing operando 2D X-ray transmission images for liquid water distribution in polymer electrolyte fuel cells. Journal of Power Sources 2023;564:232820.*) and neutron imaging techniques (*Pang Y, Wang Y. Water spatial distribution in polymer electrolyte membrane fuel cell: Convolutional neural network analysis of neutron radiography. Energy and AI* and *Satija R, Jacobson DL, Arif M, Werner SA. In situ neutron imaging technique for evaluation of water management systems in operating PEM fuel cells. Journal of Power Sources 2004;129:238–45.*) are used to distinguish the flow channel, GDL, CL. However, these methods need to use more sophisticated measuring equipment, and the measuring time is longer, which cannot be detected online real-time.

Comments 4: FIG. 5, What was the cause of the sudden change in the average voltage in the 80s?

Reply: Thanks for the reviewer’s comment. The initial phase manifests as an abrupt ascension in the voltage profile. This aberration can be attributed to increase of compressor speed, whose augmented operational capacity precipitated an overall increase of the system's air flow on the inlet. Consequently, the average voltage exhibited an upward inflection.

Upon the attainment of a steady-state equilibrium by the air compressor, the subsequent phase was initiated through an augmentation of the current load imposed upon the fuel cell stack, which caused a drop in the average voltage.

Comments 5: Please explain why Observer-HFR and Observer-Fusion observations of membrane water content and CL liquid water volume fraction are close.

Reply: Thanks for the reviewer’s comment. The similarity observed between the Observer-HFR and Observer-Fusion estimations of the membrane water content and catalyst layer liquid water volume fraction can be attributed to the intrinsic relationship between high-frequency resistance (HFR) and the fuel cell's water status. Extensive research has reported a robust correlation between HFR measurements and the water status within the fuel cell system, as the high-frequency impedance is primarily affected by the water content inside the proton exchange membrane.

The Observer-HFR method uses HFR information to calculate the water status accurately. The Observer-Fusion method takes a broader perspective, integrating multiple type of sensors to capture different aspects of the system's behavior. By fusing data streams from voltage and HFR data, the Observer-Fusion model effectively incorporates complementary information that is intimately coupled with the fuel cell's water status. *(M. Zhu, X. Xie, K. Wu, A-U-H. Najmi, K. Jiao. Experimental investigation of the effect of membrane water content on PEM fuel cell cold start. Energy Procedia 2019;158:1724–9.* and *B. Zhou, W. Huang, Y. Zong, A. Sobiesiak. Water and pressure effects on a single PEM fuel cell. Journal of Power Sources 2006;155:190–202.* and *H. Görgün, M. Arcak, F. Barbir. An algorithm for estimation of membrane water content in PEM fuel cells. Journal of Power Sources 2006;157:389–94.).*

Despite the disparate approaches employed by these two observer methods, their similar estimations of membrane water content can be attributed to the importance of HFR information to water status calculations. Though extra voltage information could enhance the accuracy of calculation in various state parameters, the HFR information constitutes the major component of the computational process.

**Reviewer: 4**

The long, detailed manuscript presents the development of a sensor for PEM fuel cell based on particle filter. The overall investigation comprises an effective model for the fuel cell, a few dedicated experiments, the methodology used for the state observer, and the results, namely the efficiency of observers relying on different statistical criteria, on some variables (or states) of the fuel cell. The paper seems of high relevance in the domain, the structure of the paper appears appropriate, as well as the illustrations. The language is in overall OK to me, but should nevertheless be improved : (i) some words used in the MS sound not suitable for the targeted meaning ; (ii) the position of adverbs has to be checked and corrected in some places ; (iii) tense of verbs as in section 5. More detailed questions/comments/suggestions are listed below.   
Comments 1: Abstract : a couple of concepts mentioned is not straightforward for any reader e.g. « The state online indirect method .. », « sensor fusion ». Besides, is the abstract not somewhat too long ?

Reply: Thanks for the reviewer’s comment. We have revised the abstract, and the revisions had been highlighted in the revised manuscript.

Comments 2: The list of symbols is of real use in the paper, but a few are missing such as « omega », or « MAPE ».

Reply: Thanks for the reviewer’s advice, and we have revised the mistakes in the manuscript. The revisions had been highlighted in the revised manuscript. Besides, the Ω symbol is only a base unit for resistance.

Comments 3: Numerical modelling, page 5. The assumptions are given. Does assumption 7 means that the various cells in the stack behave the same, i.e. with the same voltage, the same relative humidity and water pressures at various locations?

Reply: Thanks for the reviewer’s comment. In our work, we assume that all cells in the stack have the same voltage, relative humidity, and water pressure at different locations to simplify the model.

Comments 4: Section 2.1.2 what does « .. where the size of the surface tangential force is … » mean ?

Reply: Thanks for the reviewer’s comment. We have excised the phrase "the size of" from the manuscript, as it may have engendered unnecessary obfuscation. And the revisions had been highlighted in the revised manuscript.

Comments 5: Besides, the authors mention vlig in m/s as the liquid flow rate. Why not speak on liquid velocity ?

Reply: Thanks for the reviewer’s comment. We have revised the inappropriate expression in the manuscript and the revisions had been highlighted in the revised manuscript.

Comments 6: Rel (13): Could the exponent 4 for variable s be justified ?

Reply: Thanks for the reviewer’s comment. The equation is an empirical equation referenced from Hu’s research (*M. Hu, X.-J. Zhu, M. Wang, A. Gu, L. Yu. Three dimensional, two phase flow mathematical model for PEM fuel cell: Part II. Analysis and discussion of the internal transport mechanisms. Energy Convers Manag 2004; 45: 1883-916*).

Comments 7: Below rel. (15), the viscosity has to be « µ ».

Reply: Thanks for the reviewer’s comment. We have revised the mistake and the revisions had been highlighted in the revised manuscript.

Comments 8: Section 2.1.6. « The mutual conversion » : is not it actually a phase conversion rate ?

Reply: Thanks for the reviewer’s comment. It’s a phase conversion state, the article used mutual conversion to better demonstrate the focus on liquid and gas. We have revised the manuscript, replace all mutual conversion with phase conversion to rectify the identified inaccuracies. And the revisions had been highlighted in the revised manuscript.

Comments 9: The description of Schroeder's paradox is interesting, but the explanation sentence should be rephrased.

Reply: Thanks for the reviewer’s advice. We have reorganized the order of explanation for Schroeder’s paradox, and the revisions had been highlighted in the revised manuscript.

Comments 10: Rel. (35) : could the factor 2 for variable s be explained ?

Reply: Thanks for the reviewer’s advice. Relation (35) is an empirical equation derived from the work of Dullien (*F.A.* *Dullien.* *Porous media: fluid transport and pore structure. 2nd ed. Academic Press; 1992.*). The presence of the factor 2 is a consequence of the specific formulation proposed by Dullien and the underlying assumptions in his theoretical framework.

Comments 11: General comment for a recurrent point : in many places in the paper, the expression of a variable is introduced in an sentence, the expression is given, and followed by « where X is the variable … ». The lengthy, repetive structure could be easily replaced by introducing the expression of variable X (here give its name !) before this expression. Besides, the recurrent expression « is represented as follows » could be (i) improved, and sometimes be rewritten with alternative words.

Reply: Thanks for the reviewer’s comment. We have revised the expression and the revisions had been highlighted in the revised manuscript.   
Comments 12: Does rel. (55) apply for any polysulfonated membrane, in particular for the membrane used in this work ?

Reply: Thanks for the reviewer’s comment. This equation is an empirical equation referenced from Jiao’s work (*K. Jiao, X. Li. Water transport in polymer electrolyte membrane fuel cells. Prog Energy Combust Sci 2011; 37: 221-291*). And the parameter of this equation is applied to all PEMs.  
Comments 13: Table 1 : could it be specified that the temperature was at 65°C (338.15 K) ?

Reply: Thanks for the reviewer’s comment. We have added the temperature in Table 1, and the revisions had been highlighted in the revised manuscript.

Comments 14: Rel. (62) : what does represent ?

Reply: Thanks for the reviewer’s comment. The is used to represent the state of particle in step k, the state is determined by the previous state .

In the manuscript, we have added the explanation, and the revisions had been highlighted in the revised manuscript.

Comments 15: Page (19) « measurement noise and process noise ». How are they defined? How are they generated?

Reply: Thanks for the reviewer’s comment. Frist we should introduce the system’s state transition function and measurement function for better explanation. The functions can be denoted as:

In which the being the state value at step k, being the observer’s value at step k. and are process and measurement noise at step k. In the context of the formula, Q represents the process noise, which is the deviation between the true state value at time k, denoted as , and the predicted state, denoted as . Given the true state at the last step, could calculate the current state using model (*Bulut Y, Vines-Cavanaugh D, Bernal D. Process and Measurement Noise Estimation for Kalman Filtering. In: Proulx T, editor. Structural Dynamics, Volume 3, New York, NY: Springer New York; 2011, p. 375–86.*). The difference between the calculated state and the actual state represents the process noise, which serves as a measure of the inaccuracy of the state transition equation. This inaccuracy comes from two primary sources: first is the inherent simplifications within the model itself. Second, the real system is subject to unpredictable disturbances. These factors collectively signify that the model fails to fully capture the true dynamics of state changes.

Similarly, the measurement noise R quantifies the deviation between the sensor-observed value and the estimated observation calculated from the true state at time k. This discrepancy is influenced by two key aspects: the precision limitations of the sensors, and the accuracy of the measurement equation ‘h()’.

Both measurement and process noise were adding certain variance to existing values. By adding the variance, we can provide an environment closer to real world environment. We referenced Bao’s research (*C. Bao, M. Ouyang, B. Yi. Modeling and control of air stream and hydrogen flow with recirculation in a PEM fuel cell system — I. Control-oriented modeling. Int J Hydrogen Energy 2006; 31: 1879-96,* and *L. Xu, Z. Hu, C. Fang, J. Li, P. Hong, H. Jiang, et al. Anode state observation of polymer electrolyte membrane fuel cell based on unscented Kalman filter and relative humidity sensor before flooding. Renewable Energy 2021;168:1294–307.* and *H. Yuan, H. Dai, X. Wei, P. Ming. A novel model-based internal state observer of a fuel cell system for electric vehicles using improved Kalman filter approach. Appl Energy 2020;268:115009.*) to determine the value of variance, and apply the variance on observer’s measurement to create noise. External disturbances and state transfer equation errors could cause the process noise. Sensor inaccuracies and measurement equation errors could cause measurement noise.  
Comments 16: Section 4. Tests consisted in a sudden change in air flow rate (or more precisely in rotation speed of something) and at measuring the cell current and the high frequency impedance. OK, but was it done at a fixed, specified voltage ?

Reply: Thanks for the reviewer’s comment. The voltage is not at a fixed specified level. The initial phase manifests as an abrupt ascension in the voltage profile. This aberration can be attributed to increase of compressor speed, whose augmented operational capacity precipitated an overall increase of the system's air flow on the inlet. Consequently, the average voltage exhibited an upward inflection.

Upon the attainment of a steady-state equilibrium by the air compressor, the subsequent phase was initiated through an augmentation of the current load imposed upon the fuel cell stack, which caused a drop in the average voltage.

Comments 17: Table 4 : What does « CMP speed » mean ?

Reply: Thanks for the reviewer’s comment. We have revised the inappropriate expression in the manuscript and the revisions had been highlighted in the revised manuscript.  
Comments 18: The presentation of section 5 is not straightforward for a non-specialist of observers, with a couple of not fully clear concepts e.g. « observer fusion », however, it sounds really interesting since based on a solid methodology (just a comment).

Reply: Thanks for the reviewer’s comment. To make it easier for readers to understand, we changed sensor fusion to sensor signal fusion to interpret observer fusion. And the revisions had been highlighted in the revised manuscript.  
  
To conclude, the paper could be published after minor revision, most of them for the sake of an easier reading by non-specialists of the topic.