NEURO-FUZZY MEASUREMENT MODELS FOR THE METROLOGICAL ASSURANCE OF COMPLEX MOISTURE–TEMPERATURE–PRESSURE MONITORING IN ANAEROBIC DIGESTION

Abdullayev Husniddin

Associate Professor, Doctor of Philosophy (PhD) in Engineering, Renaissance University, Uzbekistan

Aziza Navruzova

Doctoral student, Bukhara State Technical University, Bukhara, Uzbekistan

e-mail: husniddin.abdullayev9395@gmail.com

Abstract. Reliable monitoring of anaerobic digestion requires simultaneous measurement of moisture W, temperature T and pressure P of a heterogeneous biomass, yet the three channels interact and no certified reference materials exist for the matrix. We formulate this as a multivariate measurement problem, $\mathbf{y} = F(\mathbf{x}, \theta)$, in which an ANFIS/ANN model compensates cross-influences and the uncertainty is propagated through the model (JCGM 101/102). Using a preliminary laboratory data set, we show that (i) a linear dielectric calibration is physically inconsistent and yields $U_{95}(W) \approx 11$–12 % absolute, whereas a refractive ($\sqrt{\varepsilon'}$) calibration reduces it to ≈ 7–8 %; (ii) the substrate (matrix) explains 95.8 % of CH_4 variance against 1.3 % for W, T, P together, so data-driven models do not transfer between matrices (leave-one-substrate-out RMSE ≈ 10.8 % points ≈ the data SD). A 100-run factorial design with independent pressure control and hold-out validation is proposed.

Keywords: metrological assurance; measurement uncertainty; ANFIS; multivariate measurement; dielectric moisture sensing; biogas; calibration.

1. Introduction

Anaerobic digestion of agricultural waste is controlled by moisture, temperature and pressure of the substrate, but the measured values are only as trustworthy as their metrological characterisation. In biotechnological media three obstacles coincide: (a) the measurand is a living, spatially non-uniform matrix, so the reference method (thermogravimetric drying) itself carries a sampling component; (b) indirect sensors, notably dielectric moisture sensors, respond simultaneously to W, T and bulk density, which violates the one-channel–one-measurand assumption of classical calibration; (c) certified reference materials and traceability chains for moisture of such matrices are, to the author's knowledge, not available. The Guide to the Expression of Uncertainty in Measurement [1] and its supplements [2, 3] provide the formal apparatus, but their application to data-driven (neural or neuro-fuzzy) measurement models is not standardised, while traceability and uncertainty evaluation are mandatory requirements for calibration and testing laboratories [5] (terminology as in [4]). The influence of biomass moisture on

fermentation intensity [10, 11] and the need for metrological support of moisture measurements of agricultural materials [13] were addressed in the author's earlier work. This work frames the three-parameter monitoring as one multivariate measurement system and examines, on real laboratory data, what the metrological characterisation of such a system must contain.

2. Measurement system and model

Fig. 1 shows the structure of the automated measurement system. Sensor outputs $\mathbf{x}$ are conditioned, their covariance $\mathbf{U}_x$ is estimated, and a trained model F returns the vector of measurands $\mathbf{y}$ together with its covariance; a reference branch (gravimetric moisture, reference thermometer and manometer) supplies calibration and validation data, and a self-check block monitors drift and calibration due dates.

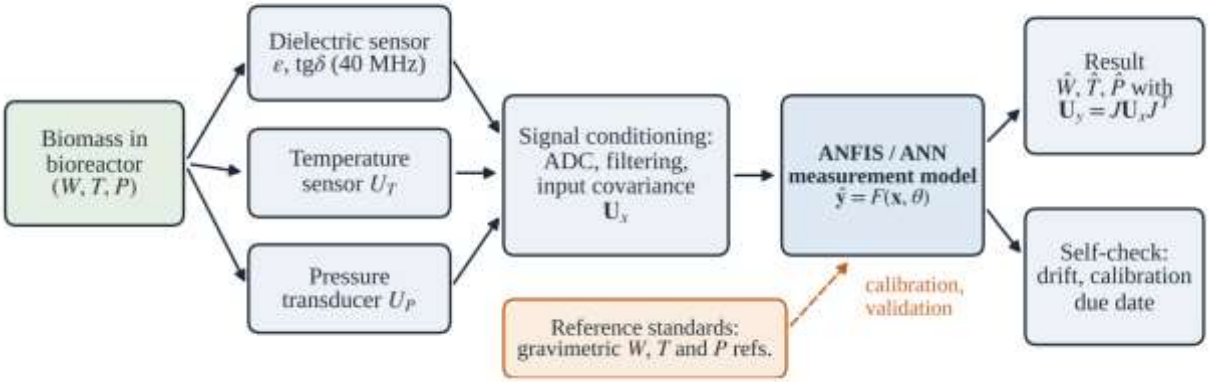


Fig. 1. Structure of the automated complex measurement system with model-based compensation and metrological self-check.

The measurement model is written as

$$\mathbf{y} = (W,\ T,\ P)^T = F(\mathbf{x}, \theta) + \delta, \qquad \mathbf{x} = (\varepsilon',\ \tan\delta,\ U_T,\ U_P)^T \tag{1}$$

where θ are model parameters and δ the model discrepancy. For F we use a first-order Takagi–Sugeno ANFIS [6, 7] (applied to biotechnological objects in [12]) with Gaussian membership functions:

$$\hat{y}_k = \sum_{i=1}^{R} \bar{w}_i\,(\mathbf{p}_{ik}^T\mathbf{x} + r_{ik}), \qquad \bar{w}_i = \frac{w_i}{\sum_j w_j}, \qquad w_i = \prod_m \exp\left[-\frac{(x_m - c_{im})^2}{2\sigma_{im}^2}\right] \tag{2}$$

with R rules, premise parameters (c_{im}, σ_{im}) and consequent parameters ($\mathbf{p}_{ik}$, r_{ik}) estimated by hybrid learning. Because F is differentiable, input covariance is propagated by the law of propagation of uncertainty for several output quantities [3]; for non-linear regimes the Monte Carlo propagation of distributions [2] is used instead:

$$\mathbf{U}_y = J\,\mathbf{U}_x\,J^T + \mathbf{U}_{\text{model}}, \qquad J = \left.\frac{\partial F}{\partial \mathbf{x}}\right|_{\hat{\mathbf{x}}} \tag{3}$$

3. Calibration of the dielectric channel and its uncertainty

The dielectric channel (high-frequency moisture meter, cf. [10]) was calibrated against gravimetric moisture on one drying series of a biomass sample (n = 7, W = 0–71 %, permittivity at 40 MHz, vector network analyser). A mixing law of the refractive type [8]

predicts that $\sqrt{\varepsilon'}$ rather than ε' is linear in the water fraction, whereas $\varepsilon'(W)$ is often approximated by a linear or low-order polynomial relation (cf. the empirical polynomial for soil in [9]). We compare the linear and the $\sqrt{\varepsilon'}$ forms. The moisture estimate from a reading ε'_0 and its standard uncertainty follow the classical inverse-prediction scheme:

$$\sqrt{\varepsilon'} = a + bW, \qquad \hat{W}_0 = \frac{\sqrt{\varepsilon'_0} - a}{b} \tag{4}$$

$$u^2(\hat{W}_0) = \frac{s^2}{b^2}\left[1 + \frac{1}{n} + \frac{(\hat{W}_0 - \bar{W})^2}{S_{WW}}\right], \qquad U_{95} = t_{0.975,\, n-2}\, u(\hat{W}_0) \tag{5}$$

where s is the residual standard deviation, n the number of calibration points and $S_{WW} = \Sigma(W_i - \bar{W})^2$. The results are given in Table 1 and Fig. 2.

Table 1. Comparison of calibration models for the dielectric channel (n = 7, one drying series; preliminary).

Model	s, in model units	Leave-one-out RMSE	$U_{95}(W)$, % absolute
$\varepsilon' = a + bW$ (linear)	2.35 (ε')	3.29 (ε')	10.8–12.0
$\sqrt{\varepsilon'} = a + bW$	0.203 ($\sqrt{\varepsilon'}$)	0.255 ($\sqrt{\varepsilon'}$)	7.3–8.3

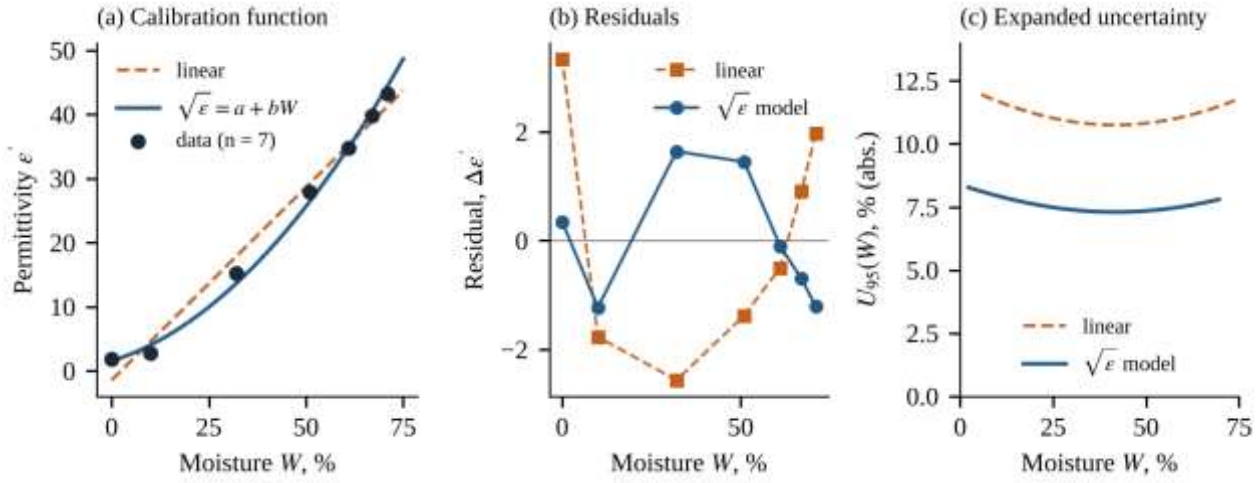


Fig. 2. Dielectric calibration: (a) data and fitted functions; (b) residuals in ε' units, the linear model shows a systematic (curved) pattern; (c) expanded uncertainty of moisture from eq. (5) over the calibrated range.

The linear model gives a negative intercept ($a = -1.44$, i.e. $\varepsilon' < 1$ at $W = 0$), is physically inconsistent and leaves a systematic residual pattern (Fig. 2b), which reveals a model error component that is absent from a purely statistical uncertainty. The $\sqrt{\varepsilon'}$ calibration removes most of this pattern and lowers $U_{95}(W)$ by about one third. Even so, an expanded uncertainty of ≈ 7–8 % absolute is far above what process control needs; it is dominated by the small number of points and by the use of a single drying run. It is a measured,

quantified deficiency of the calibration design, not of the sensor principle, and it fixes the requirement for replicated calibration at independent moisture levels.

4. Matrix effect and validation of data-driven models

To test what can be learned from W, T, P with a neural or regression model, 127 laboratory records of the author's earlier experiments (cf. [10, 11]) were analysed (8 substrates; W = 60–80 %, T = 40–55 °C, P = 0.113–0.126 MPa; biogas yield and CH_4 content; one value of 0.95 m³/kg, evidently a typing error, excluded). Pressure turned out to be collinear with moisture (Pearson $r = 0.84$) because it was not set independently, and each setting was measured once. Models were compared by the coefficient of determination and by cross-validated errors

$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}, \qquad \mathrm{RMSE}_{\mathrm{LOSO}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(y_i - \hat{y}_i^{(-g(i))}\right)^2} \tag{6}$$

where $g(i)$ is the substrate of record i, so that LOSO (leave-one-substrate-out) predicts an unseen matrix. Results are in Fig. 3 and Table 2.

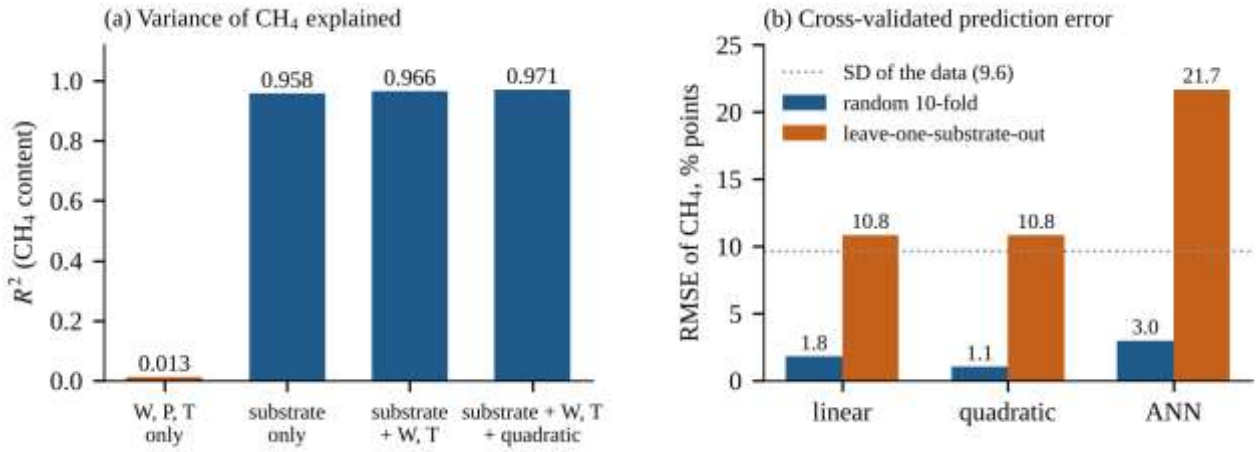


Fig. 3. (a) Share of CH_4 variance explained by different predictor sets; (b) cross-validated RMSE of CH_4 content for linear, quadratic and ANN (8 hidden neurons) models.

Table 2. Cross-validated RMSE for two outputs (substrate indicator + W, P, T as inputs).

Model	CH_4, random 10-fold, % pts	CH_4, LOSO, % pts	Yield, random 10-fold, m³/kg	Yield, LOSO, m³/kg
Linear	1.80	10.85	0.017	0.068
Quadratic	1.05	10.83	0.010	0.068
ANN (8 neurons)	2.98	21.69	0.195	0.455
SD of data	9.61	9.61	0.061	0.061

The substrate alone explains 95.8 % of CH_4 variance, W, P, T only 1.3 %; within a substrate, temperature raises CH_4 by ≈ 0.15 % points per °C, the moisture effect is negligible in the 60–80 % range. When the matrix is unseen the error equals or exceeds the standard deviation of the data (LOSO RMSE 10.8 vs SD 9.6), and the ANN, trained on 127 points, is inferior to a quadratic regression in both validation schemes. Consequently, a data-driven model can serve as a measurement model only when (i) the matrix is represented by measured descriptors or the model is characterised matrix-by-matrix, and (ii) validation is performed on data not used for training, with reported uncertainty. Agreement of a model with its own training data, which is sometimes reported as zero error, carries no metrological information.

5. Conclusions and further work

(1) Three-parameter biomass monitoring is treated as one multivariate measurement problem with an explicit model, input covariance and model-discrepancy term. (2) A $\sqrt{\varepsilon'}$ dielectric calibration is physically consistent and reduces the expanded uncertainty of moisture from ≈ 11–12 % to ≈ 7–8 % absolute compared with a linear function; the remaining uncertainty is determined by the calibration design. (3) The matrix explains almost all the variability of the process outputs, and neural or ANFIS models do not transfer across matrices; their metrological characterisation must therefore be matrix-specific and based on hold-out validation. (4) Next, a 100-run factorial experiment is planned with moisture, temperature and pressure set independently, replicated centre points for repeatability, gravimetric reference with calibrated balance, and Monte Carlo propagation [2, 3] through the ANFIS/ANN model.

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