Improvements In Pressure Tube Diametral Creep Predictions And Statistical Error Modeling

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Abstract

The improvements in the uncertainty estimation and model predictions of pressure tube diametral creep in CANDU fuel channels using a statistical error modeling method is presented in this paper. The statistical error modeling was successfully completed using real inspection data from the Bruce B CANDU reactor. The result was a methodology, which ensured a more accurate and realistic approach in predicting pressure tube diameter and estimates of the modeling uncertainties when compared to more commonly used statistical methods.

1. Introduction

The Heat Transport Systems (HTS) of CANDU nuclear power stations are experiencing aging. One of the aging effects is the non-uniform change in the dimension of the pressure tubes (PT) through the mechanism of diametral creep, which are related to the level of irradiation. The changes in the PT diameter affect channel thermal hydraulic characteristics and hence the Critical Heat Flux (CHF). CHF is a key factor in the determination of the Critical Channel Power (CCP), which is in turn used in the calculation of the Neutron Overpower Protection (NOP) system trip set points to ensure that the onset of intermittent fuel sheath dryout is prevented during slow Loss of Regulation (LOR) accidents.

Our work investigates methods to: 1) improve the pressure tube diametral creep model prediction accuracy and 2) derive statistical error models to ensure the most optimal estimates of the CCP variance when the errors in our CCP input parameters are propagated. The proposed approach for improving model predictions and statistical error modeling is demonstrated using actual pressure tube diameter inspection data from Bruce B Nuclear Generating Station (NGS).

Predictive correlations and their respective statistical error models are developed in this work for the purpose of modeling the axial profile of a crept pressure tube. These developed models are the so-called Random-Effects Model (REM) and Fixed-Effects Model (FEM). The prediction accuracy of the REM and FEM are compared against the commonly used Least-squares Regression Model (LRM).

2. Background

2.1 Pressure Tube Characteristics

The pressure tube, as shown in Figure [F-1], is a Zr-2.5%Nb alloy that contains the fuel and the pressurized D_2O coolant within the reactor. Pressure tube diametral creep leads to diametral expansion, and it occurs mostly from irradiation-enhanced creep due to the hoop stress in the pressure tube. It varies axially along the fuel channel, and can be correlated with the axial neutron flux and temperature. Figure [F-1] shows two fuel channel cross-sections: one with a nominal pressure tube diameter and the other with a crept pressure tube.

2.2 Inspection Data of Pressure Tube Diameters

Pressure tube diameters are measured using the so-called Channel Inspection and Gauging Apparatus for Reactors (CIGAR). The data includes measurement of PT diameters along the length of the inspected fuel channel. Inspection data for 37 channels was made available. This set of data covered CIGAR inspections carried out in 2000, 2001, and 2002 from Units 5, 6, and 7. Note that the time (in Effective Full Power Hour[1] (EFPH)) of each inspected fuel channel is known.

2.3 Modelling Pressure Tube Diametral Creep in CANDU Fuel Channels

As shown in Figure [F-2], the local pressure tube diameter depends primarily on two variables, namely time, t (in Effective Full Power Hour (EFPH)), and time-averaged neutron flux ϕ, or alternatively, it depends on the fluence, ψ where:

$$\phi = \frac{\psi}{(3600t)} \tag{1}$$

Lifetime average temperature, T (^oC) above some nominal reference value has also been observed to correlate with changes in PT diameters as shown in Figure [F-2]. Thus, the general functional form to model the axial profile of the PT diameters is restricted to be as follows:

$$S_{ij}^{meas} = a + b\,\psi_{ij} + c\omega_{ij} + e_{ij} \tag{2}$$

where:

i = 1,2, … M = bundle position in a fuel channel
j = 1,2, … J = fuel channel
$S_{ij}^{meas} = \frac{D_{ij}^{m}}{D_o} - 1$ = the measured strain at bundle i, channel j
D_{ij}^{m} = Pressure tube diameter at bundle position i and channel j [mm]
D_o = Nominal pressure tube diameter
ψ_{ij} = Fluence at bundle position i and channel j [n/(m^2 s)]
$\omega_{ij} = \Im(T_{ij}, T_o)$
T_{ij} = Average pressure tube bundle temperature at bundle position i and channel j
T_o = Reference temperature
e_{ij} = error at bundle i and channel j
a, b, c = are the model coefficients

Given the axial location of the measured PT diameter and operational time (in EFPH), the fluence and lifetime average temperature values can be obtained at each measured axial location of the pressure tube using the computer code BTFMAP (channel Boiling Temperature and neutron Fluence MAP).
Three predictive correlations and their respective statistical error models are developed in this work. These predictive models are: 1) Least-squares Regression Model (LRM); 2) Random-Effects Model (REM); and 3) Fixed Effects Model (FEM).

Least-Squares Regression Model (LRM)
From Equation (2), the LRM is described by model coefficients $(a,b,c) = (a_o, b_o, c_o)$ that are constants, which are not specific to any channel, nor any bundle. Thus, the LRM is neither a channel, nor a bundle-specific model (see Table [T-1]). The LRM is commonly used in statistics, which implicitly assumes no error in its independent variables. Physically, the model is unable to capture the variability that may exist in both the channel and bundle. The error structure for the LRM is basic and captured in e_{ij} as errors in all unexplained variabilities associated with the model, measurement, channel, bundle, noise, etc. The LRM error component e_{ij} is simply characterized as follows:

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[1] EFPH is a measure of the age of the pressure tube.

$$e_{ij} \sim N\left(0, \sigma^2\right) \tag{3}$$

Least-Squares Regression Model with Error Model (LRM$^+$)

As discussed in section 1, our primary objectives were to investigate methods to: 1) improve model prediction accuracy; and 2) derive statistical error models to ensure the most optimal estimates of the CCP variance when the errors in our CCP input parameters are propagated. Note that the LRM is restricted to the functional form given in Equation (2) with constant model coefficients given above. Thus, it is not possible to improve the prediction accuracy for the LRM. However, we recognize that the second objective of developing a statistical error model can still be achieved. In contrast to the usual approach in developing the LRM, we recognize that errors do exist in the independent variables, and explicitly model the LRM's deficiencies in capturing the channel-to-channel and bundle-to-bundle variabilities.

The error structure for the LRM$^+$, e_{ij} is modeled below in Equations (4) to (7) and found to be appropriate.

$$e_{ij} = \tau_i + \delta_j + \gamma_{ij} \tag{4}$$

where τ_i captures the bundle-to-bundle variabilities, δ_j characterizes the channel-to-channel variabilities, and γ_{ij} describes the remaining unexplained variabilities. The error components for the LRM$^+$ were determined to be appropriately characterized by a normal probability distribution as follows:

$$\tau_i \sim N\left(0, \sigma_\tau^2\right) \tag{5}$$

$$\delta_j \sim N\left(0, \sigma_\delta^2\right) \tag{6}$$

$$\gamma_{ij} \sim N\left(0, \sigma_\gamma^2\right) \tag{7}$$

Estimates of the variances were computed using the Maximum Likelihood Estimation (MLE) method (Reference [1]). Solution of the MLE equations can be found in Appendix A.1.

Random Effects Model (REM)

To improve both the model predictions and error analysis, the REM is developed as a bundle-specific model to preserve the axial functional dependence of the pressure tube diameter by varying the unknown coefficients along a fuel channel. It is able to recognize possible variations (possibly due to different thermalhydraulic conditions or factors associated with fueling) from one bundle to the next in any given fuel channel. However, the REM (like the LRM) does not model the possible spatial variabilities that can exist from channel-to-channel. Thus, the model coefficients for the REM consist of a constant a_o that is generic to all channels, and b_i and c_i that are specific to each bundle location *i*. The following error structure was found to be appropriate for the REM:

$$e_{ij} = \delta_j + \gamma_{ij} \tag{8}$$

where δ_j and γ_{ij} are modeled similarly to the LRM$^+$ given in Equations (6) and (7), respectively. Similar to the LRM$^+$, the variance for the REM error components (discussed in Appendix A.2) are derived using the MLE method. Note that this model assumes, for prediction purposes, that data is available for only a subset of channels under consideration.

Fixed Effects Model (FEM)

Similar to the REM, the FEM is developed to improve both the model predictions and error analysis. In contrast to the REM, the FEM has been developed to provide the best possible estimate of the PT diameter profile, since an appropriate account of the variabilities for each specific channel and bundle are included. As shown in Table [T-1], the model coefficients for the FEM are a_j, b_i, and c_i. That is, the FEM explicitly models the variabilities that can exist from bundle-to-bundle in addition to possible spatial variabilities from channel-to-channel in a reactor core. Thus, the FEM is capable of preserving the axial functional dependence of the pressure tube diameter with the only uncertainty from unexplained variabilities due to system noise, γ_{ij}. Thus, the FEM error model is as follows:

$$e_{ij} = \gamma_{ij} \quad (9)$$

where γ_{ij} is modeled similarly to the LRM^+ given in Equation (7). The variance for the FEM error component is discussed in Appendix A.3. Note that the FEM assumes that data is available for all channels under consideration. Thus, it can not be used for prediction for channels that do not have available measurements.

3. Results

As discussed in Section 1, the objective of this work is to improve the CCP estimates and its uncertainty by: 1) developing more accurate models (i.e., those used in our CCP calculations; and 2) developing statistical error models to ensure that a probabilistic method to propagate errors in the CCP input parameters obtains the most optimal estimate of the CCP variance. We achieve both objectives in developing the REM and FEM, and advance the LRM by developing a model-specific statistical error structure. These results are discussed in this section.

Improvements in the Model Predictions

Our developed predictive models: 1) The Fixed-Effects Model (FEM) and 2) the Random-Effects Model (REM) are compared against the Least-Squares Regression Model (LRM) and the measured data in this section. The residual[2] is computed in Figure [F-3] for the FEM, REM, and LRM. It is evident that the FEM, being a predictive model that is both channel and bundle-specific, provides the most accurate method for estimating the true axial profile for every channel, and at each bundle location. The REM also demonstrated some improvements over the LRM with a standard deviation in its residual of 0.13, compared to 0.17 for the LRM. However, the advantage of the REM is that it provides a more detailed structure of the error, which is then utilized in the determination of the CCP error.

It is evident from Figure [F-4] that the REM provides better predictive ability over the LRM. The REM is a bundle-specific model, and when compared to the LRM (which is neither bundle nor channel specific), demonstrated an improvement in capturing the overall true pressure tube axial profile at every bundle location. In contrast, the LRM was observed to only be able to predict the basic axial profile of the pressure tube. On average, the LRM over-predicted and under-predicted PT diameter approximately an equal amount of time at each bundle location in the fuel channel. The LRM's inability to capture the true PT diameter profile at bundles 9, 10, and 11, is more pronounced when the LRM model is used to make predictions of the axial PT profile with increasing time. The results of the future predictions were that the LRM provided an overly conservative estimate of the pressure tube diameters relative to the REM and FEM. These observations are illustrated in Figure [F-5].

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[2] Residual = Measured Data - Model Prediction

Statistical Error Modeling

Basic modeling methods (i.e., LRM) do not invest efforts in developing advanced statistical error models. Traditionally, the LRM error is modeled as a normal probability distribution with a variance described by the standard deviation of the residual (see Figure [F-3]), with the assumption that no errors exist in its independent variables. This type of error modeling (or lack of) conglomerates all unexplained variabilities (e.g., measurement error, noise, etc.) together, and does not distinguish and quantify one from the other. An advantage of having a detailed error structure is illustrated in Figure [F-6]. As discussed in Section 2.2, our work developed LRM^{+}, which is a more advanced method in capturing the deficiencies in the LRM prediction correlation, and established the following statistical error model:

$$e_{ij} = \tau_i + \delta_j + \gamma_{ij} \qquad (4)$$

The bundle-specific error as shown in Figure [F-6] is able to highlight the strengths and weaknesses of the prediction capabilities of the model. For example, the LRM provides fairly accurate predictions at bundles 6, 8, and 11 for all channels in a core, but it does not provide very accurate predictions at the pressure tube diameter at bundle 1. Errors due to channel variabilities and noise are characterized separately in its own separate probability distribution. Knowing this information is crucial for obtaining optimal estimates of the CCP variance, since we are able to take credit for the strengths in our prediction models, and not unduly penalize ourselves when the model is deficient. Using a probabilistic methodology, such as the Monte-Carlo procedure, the ability to explicitly describe the structure of the errors associated with each prediction model ensures an optimal estimate of the CCP uncertainty when the errors are propagated.

Furthermore, the analysis of variance provides a deeper understanding of the errors, which plays a critical role in quality assurance type problems. For example, the bundle-specific error as shown in Figure [F-6] could lead to identifying different factors, which contributed to the large variability between bundle 1 relative to bundles 6, 8, and 11, and hence lead to improvements in the functional form of the prediction models.

4. Conclusion

Improvements in the predictive abilities using the Random Effects Model (REM) and Fixed Effects Model (FEM) over the more commonly used application of the Least-squares Regression Model (LRM) are illustrated in this paper. This improvement can be understood since both the REM and FEM preserve the inherent axial dependence in the pressure tube, whereas the LRM does not. Furthermore, advanced statistical error models are also developed in this work for all three correlations. These developed statistical error models significantly improve our understanding of the prediction uncertainties over more commonly used statistical methods, which implicitly assume the independent variables are exact. Furthermore, the improved modeling predictions and a structured statistical error model are crucial for obtaining optimal estimates of the CCP variance (and hence NOP trip setpoints), since this ensures the propagation of errors in our CCP input parameters will obtain the most optimal estimate of the CCP variance.

5. References

1. Stuart, A., Ord., J.K., “Kendall’s Advanced Theory of Statistics, volume 2, Classical Inference and Relationship Fifth edition”, Oxford University Press, New York, 1991.

6. Acknowledgements

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Table [T-1] - Pressure Tube Diametral Creep Correlations

Pressure Tube Diameteral Creep Models	Functional Form and Error Model
Least-squares Regression Model (LRM) (without error modeling)	$S_{ij}^{meas.} = a_o + b_o \psi_{ij} + c_o \omega_{ij} + e_{ij}$
Least-squares Regression Model (LRM^{+}) (with error modeling)	$S_{ij}^{meas.} = a_o + b_o \psi_{ij} + c_o \omega_{ij} + \tau_i + \delta_j + \gamma_{ij}$
Random Effects Model (REM)	$S_{ij}^{meas.} = a_o + b_i \psi_{ij} + c_i \omega_{ij} + \delta_j + \gamma_{ij}$
Fixed Effects Model (FEM)	$S_{ij}^{meas.} = a_j + b_i \psi_{ij} + c_i \omega_{ij} + \gamma_{ij}$

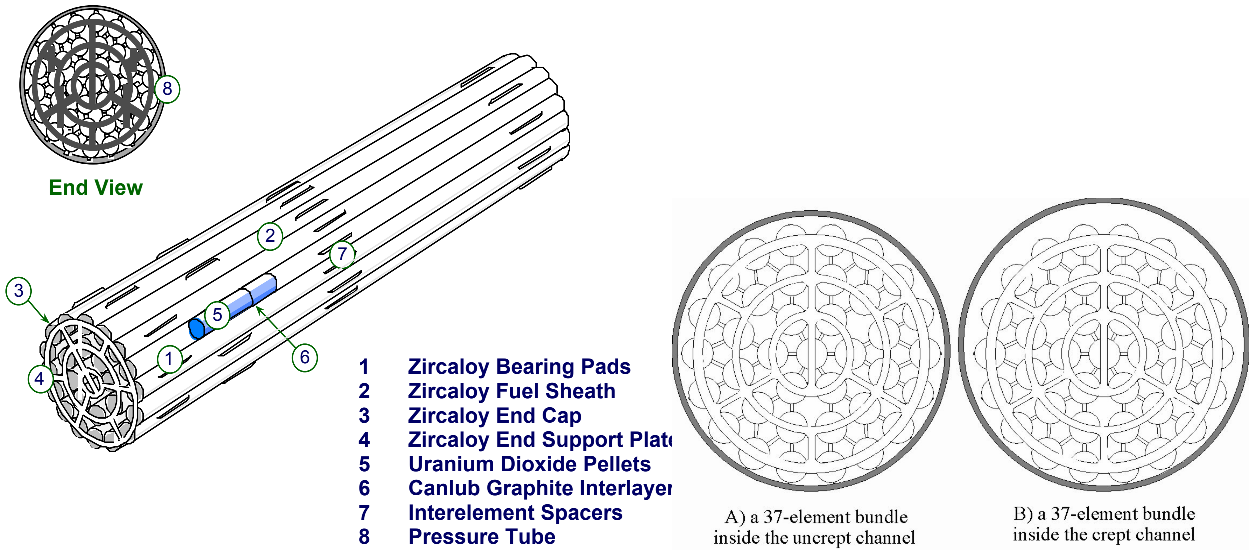

FIGURE [F-1]: (LEFT) CANDU fuel bundle contained within the fuel channels; (RIGHT) Schematic Diagrams of Fuel-Channel Configuration in (A) Nominal and (B) Diametral Crept Pressure Tubes

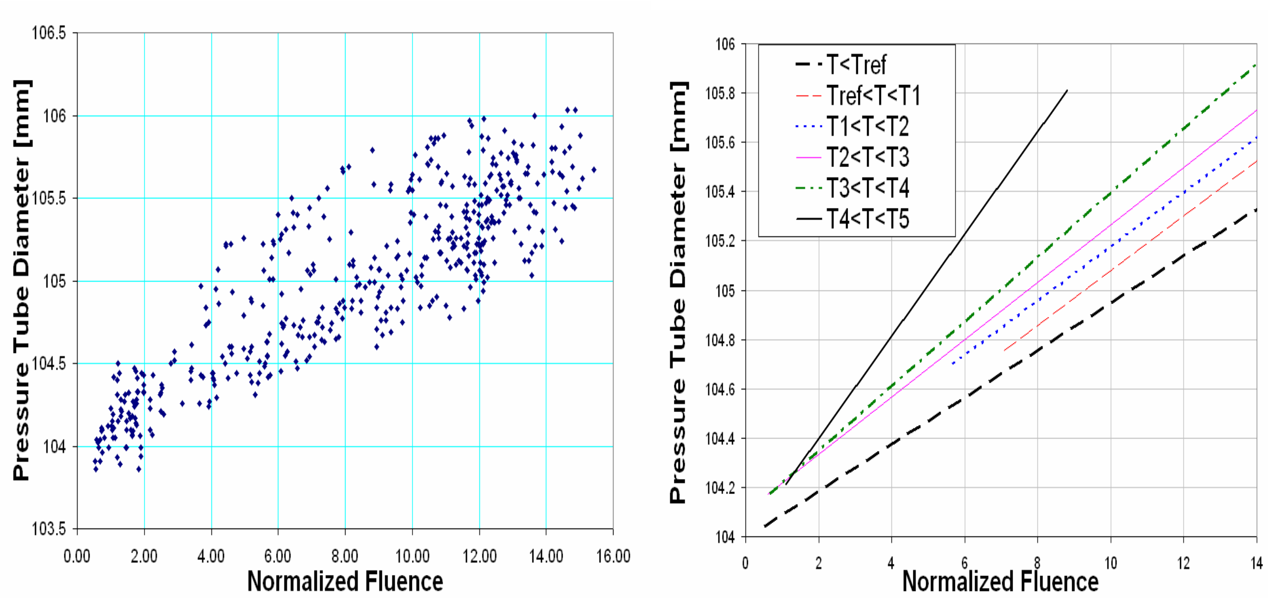

FIGURE [F-2]: (LEFT) Pressure Tube (PT) diameter as a function of fluence; (RIGHT) PT diameter as a function of fluence and time averaged local temperature. Note that the PT diameter is observed to increase proportionally to increasing Temperatures above the reference Temperature (i.e., Tref)

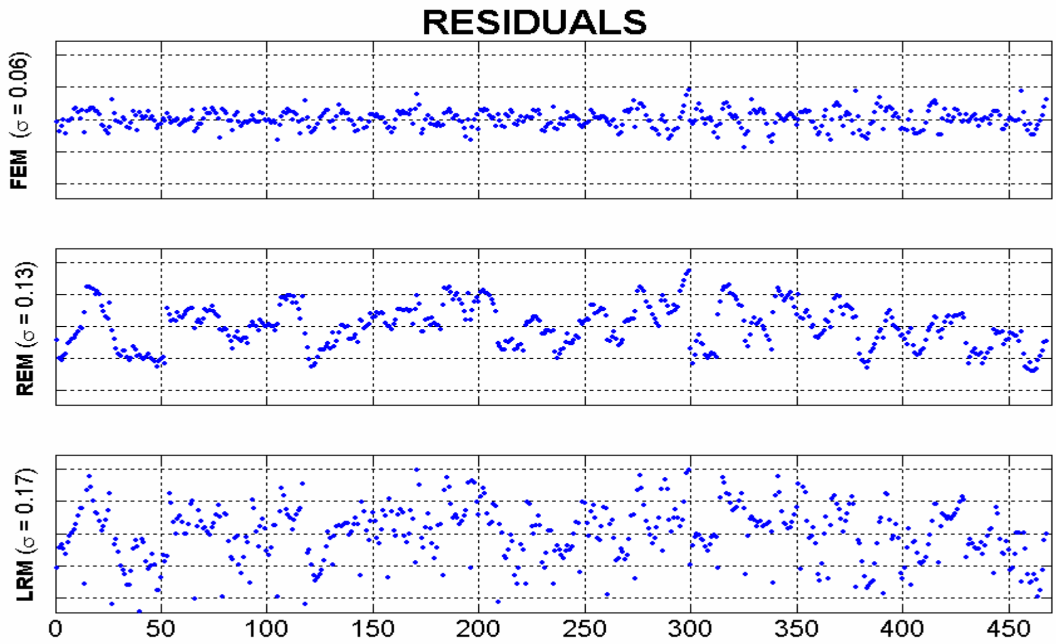

FIGURE [F-3]: Comparison of the residuals of the different predictive models

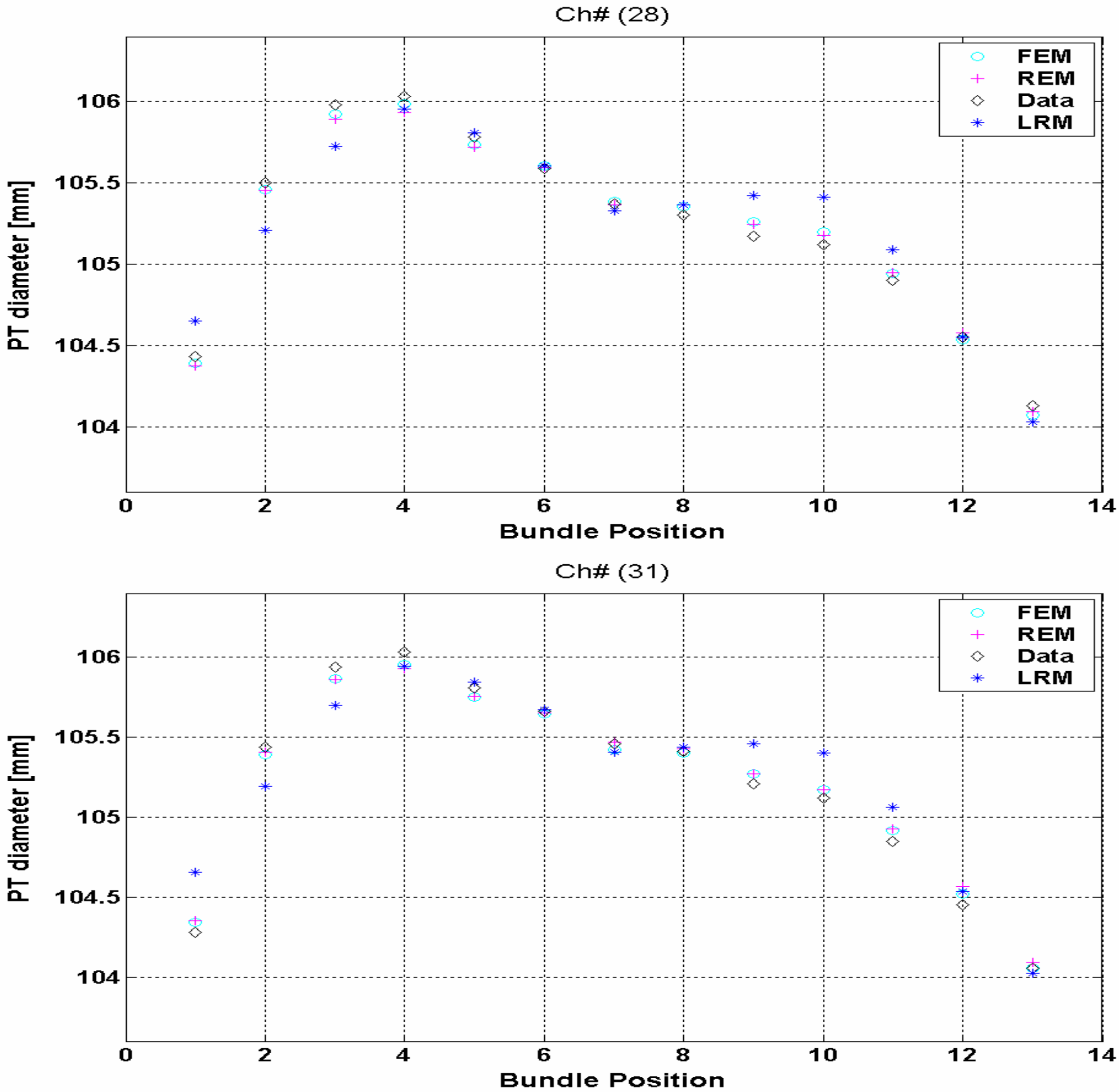

FIGURE [F-4]: Comparing the LRM, REM, and FEM's ability to model the true axial profile of a pressure tube

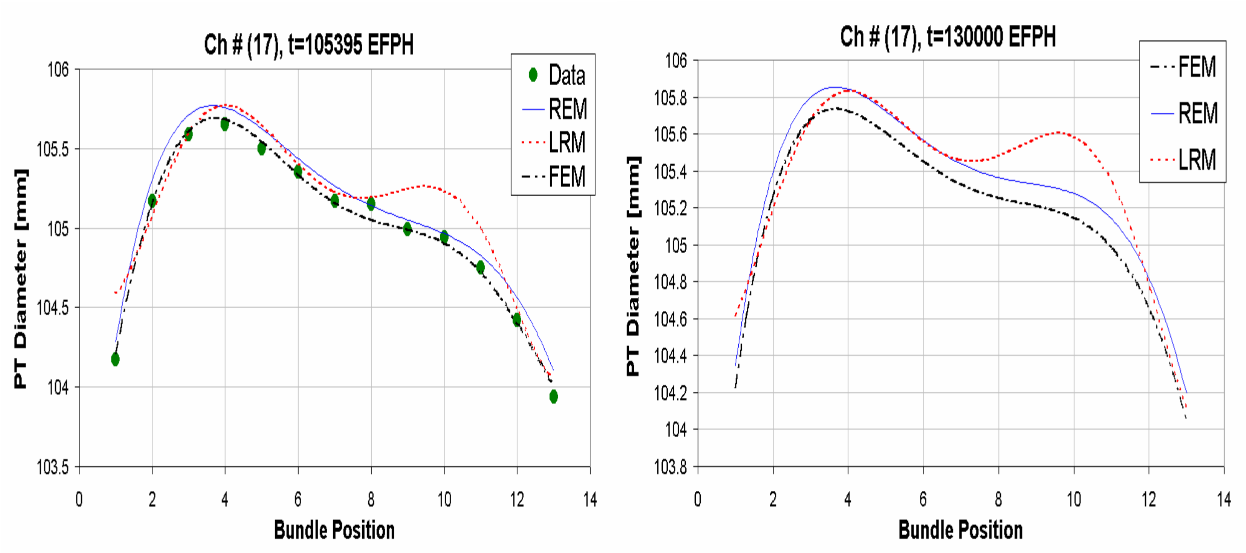

FIGURE [F-5]: Comparing the model predictions results and used to predict in time. (LEFT) Model predictions at t = 105395 EFPH; (RIGHT) Model predictions at t = 130000 EFPH.

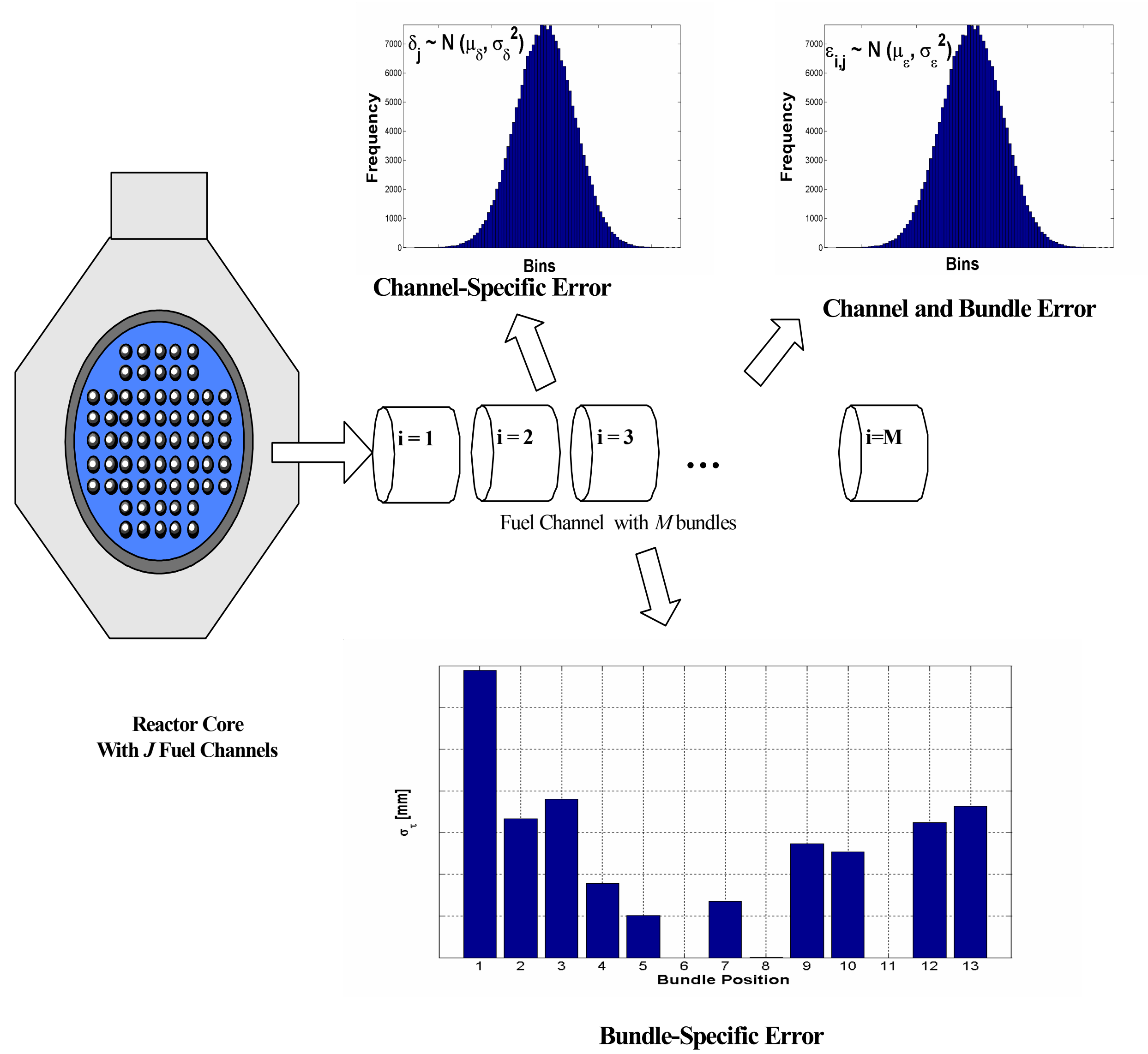

FIGURE [F-6]: Statistical error modeling of the Least-Squares Regression Model (LRM)

Appendix –Prediction Correlations and Error Model Components

A.1 Least-Squares Regression Model with Error Modelling (LRM+)

From Table [T-1], the LRM+ is expressed in vector form as follows:

$$S = U_N a_o + \psi\, b_o + \omega\, c_o + (u_J \otimes I_M)\tau + (I_J \otimes u_M)\delta + \gamma$$

where:

i = 1,2, … M = bundle position in a fuel channel
j = 1,2, … J = fuel channel
N = total number of S_{ij} (M * J)
U_N = column vector of ones, size [N x 1]
u_J = column vector of ones, size [J x 1]
u_M = column vector of ones, size [M x 1]
I_M = identity matrix of size [M x M]
τ = is a column vector of $\tau_i, i = 1,2,3...M$, size [M x 1]
δ = is a column vector of $\delta_i, i = 1,2,3...J$, size [J x 1]

Let: $e = (u_J \otimes I_M)\tau + (I_J \otimes u_M)\delta + \gamma$

where ⊗ is the tensor product. Assuming independence among the error components:

$$Var(\mathrm{e}) = \sigma_\gamma^2 I_N + \sigma_\delta^2 E_N + \sum_{i=1}^{M} \sigma_\tau^2 G_i = V$$

where:

E_N = matrix of ones, size [N x N]; E_M = matrix of ones, size [M x M];

$E_N = I_J \otimes E_M = I_J \otimes (U_M U_M^T)$, $G_i = (u_J u_J^T \otimes E_i)$

Note:

$$V = \sigma_\gamma^2 \left(I_N + \frac{\sigma_\delta^2}{\sigma_\gamma^2} E_N + \frac{\sigma_\tau^2}{\sigma_\gamma^2} \sum_{i=1}^{M} G_i \right) = \sigma_\gamma^2 V_\gamma ; \qquad V = \sigma_\delta^2 \left(\frac{\sigma_\gamma^2}{\sigma_\delta^2} I_N + E_N + \sum_{i=1}^{M} \frac{\sigma_{\tau_i}^2}{\sigma_\delta^2} G_i \right) = \sigma_\delta^2 V_\delta$$

$$V = \sigma_{\tau_i}^2 \left(\frac{\sigma_\gamma^2}{\sigma_{\tau_i}^2} I_N + \frac{\sigma_\delta^2}{\sigma_{\tau_i}^2} E_N + \sum_{k=1}^{M} \frac{\sigma_{\tau_k}^2}{\sigma_{\tau_i}^2} G_k \right) = \sigma_{\tau_i}^2 V_{\tau_i}$$

The multivariate probability density function L is used as the objective function for estimating the unknown parameters ($\beta, \sigma_\delta^2, \sigma_\gamma^2, \sigma_\tau^2$) using Maximum Likelihood Estimation (MLE):

$$L(\beta, \sigma_\delta^2, \sigma_\gamma^2, \sigma_\tau^2) = (2\pi)^{-\frac{1}{2}N} |V|^{-1/2} \exp\left(-\frac{1}{2} \mathbf{e}^T V^{-1} \mathbf{e} \right),$$

where |V| is the determinate of the variance matrix V. The maximum of the likelihood function L is found by taking the derivative ln(L) with respect to each parameter in L, and setting the partial derivatives to zero as follows:

Let: $\Im = -2 \ln L(\beta, \sigma_\tau^2, \sigma_\delta^2, \sigma_\gamma^2$

$$\frac{\partial \Im}{\partial \beta} = -2 X^T V^{-1} (\mathbf{S} - \mathrm{X}\beta) = 0 ; \qquad \frac{\partial \Im}{\partial \sigma_\gamma^2} = trace(V^{-1}) - e^T V^{-2} e = 0 ;$$

$$\frac{\partial \Im}{\partial \sigma_\delta^2} = \mathrm{trace}\{\mathrm{V}^{-1} E_N\} - \mathbf{e}^{\mathrm{T}} V^{-1} E_N V^{-1} e = 0 ; \qquad \frac{\partial \Im}{\partial \sigma_{\tau_i}^2} = \mathrm{trace}\{\mathrm{V}^{-1} G_i\} - \mathbf{e}^{\mathrm{T}} V^{-1} G_i V^{-1} e = 0$$

To obtain unbiased estimators of the error components $\sigma_\gamma^2, \sigma_\delta^2$ and $\sigma_{\tau_i}^2$, an unbiasing factor is obtained as follows:

$$E\left\{\frac{\hat{\sigma}_\gamma^2}{\sigma_\gamma^2}\right\} = \frac{1}{trace\{V^{-1}\}} E\{\hat{e}^T V^{-2} \hat{e}\}; \qquad E\left\{\frac{\hat{\sigma}_\delta^2}{\sigma_\delta^2}\right\} = \frac{1}{trace\{V^{-1} E_N\}} E\{\hat{e}^T V^{-1} E_N V^{-1} \hat{e}\}$$

$$E\left\{\frac{\hat{\sigma}_{\tau_i}^2}{\sigma_{\tau_i}^2}\right\} = \frac{1}{trace\{V^{-1} G_i\}} E\{\hat{e}^T V^{-1} G_i V^{-1} \hat{e}\}$$

Thus, an explicit solution (using the fixed-point iteration algorithm) can be used to solve for the unbiased estimates of the error components:

$$\therefore \hat{\hat{\sigma}}_\gamma^2 = \frac{\hat{\sigma}_\gamma^2}{E\left\{\frac{\hat{\sigma}_\gamma^2}{\sigma_\gamma^2}\right\}} = \frac{\hat{\sigma}_\gamma^2}{trace(V^{-2} HVH)} trace\{V^{-1}\} \qquad \therefore \hat{\hat{\sigma}}_\delta^2 = \frac{\hat{\sigma}_\delta^2}{trace\{V^{-1} E_N V^{-1} HVH\}} trace\{V^{-1} E_N\}$$

$$\therefore \hat{\hat{\sigma}}_{\tau_i}^2 = \frac{\hat{\sigma}_{\tau_i}^2}{trace\{V^{-1} G_i V^{-1} HVH\}} trace\{V^{-1} G_i\}$$

where:

$$HVH = Var(e_o) = E\{e_o e_o^T\} = \left(I_N - X(X^T X)^{-1} X^T\right) Var(e) \left(I_N - X(X^T X)^{-1} X^T\right)$$

$$e_o = S - X\beta_o = X\beta - X\beta_o + e = -X\Delta\beta_o + e = \left(I_N - X(X^T X)^{-1} X^T\right) e$$

Since: $\Delta\beta_o = \beta_o - \beta$; $\qquad \beta_0 = (X^T X)^{-1} X^T S = (X^T X)^{-1} X^T (X\beta + e) = \beta + (X^T X)^{-1} X^T e$

A.2 Random Effects Model

From Table [T-1], the REM can be expressed in vector form for every channel and every bundle location as follows:

$$S = \mathbf{U}_N a + \Psi b + \Omega c + (I_J \otimes U_M)\delta + \gamma = [\boldsymbol{U}_N, \Psi, \Omega] \begin{pmatrix} \mathbf{a} \\ \boldsymbol{b} \\ \boldsymbol{c} \end{pmatrix} + \boldsymbol{U}\delta + \gamma = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e}$$

where: $\Omega = (diag(\omega_{\cdot 1}) \cdots diag(\omega_{\cdot J}))^T$; $\Psi = (diag(\psi_{\cdot 1}) \cdots diag(\psi_{\cdot J}))^T$; $\mathrm{U} = (I_J \otimes U_M)$;

U_N = column vector of ones, size [N x 1]; U_M = column vector of ones, size [M x 1]

$\delta = (\delta_1 \cdots \delta_J)^T$; $\qquad \gamma = (\gamma_{\cdot 1} \cdots \gamma_{\cdot J})^T$; $\qquad \gamma_{\cdot J} = (\gamma_{1J} \cdots \gamma_{MJ})^T$

b = $(b_1 \cdots b_M)^T$; $\qquad$ c = $(c_1 \cdots c_M)^T$; $\qquad$ e= $(e_{\cdot 1} \cdots e_{\cdot J})^T$;

Assuming independence among the error components, the variance of the error component given as:

$$Var(\mathrm{e}) = \sigma_\delta^2 UU^T + \sigma_\gamma^2 I_N = \sigma_\gamma^2 I_N + \sigma_\delta^2 E_N$$

Since: $UU^T = (I_J \otimes U_M)(I_J \otimes U_M)^T = (I_J \otimes U_M)(I_J \otimes U_M^T) = E_N$

Like before, the multivariate probability density function L is used as the objective function for estimating the unknown parameters ($\beta, \sigma_\delta^2, \sigma_\gamma^2$) using Maximum Likelihood Estimation (MLE):

$$L(\beta, \sigma_\delta^2, \sigma_\gamma^2) = (2\pi)^{-\frac{1}{2}N} |V|^{-1/2} \exp\left(-\frac{1}{2}\mathbf{e}^T V^{-1} \mathbf{e}\right),$$

where |V| is the determinate of the variance matrix V. The maximum of the likelihood function L is found by taking the derivative ln(L) with respect to each parameter in L and setting the partial derivatives to zero as follows:

Let: $\Im = -2\ln L(\beta, \sigma_\delta^2, \sigma_\gamma^2)$

$$\frac{\partial \Im}{\partial \beta} = -2X^T V^{-1}(\mathbf{S} - \mathrm{X}\beta) = 0\,; \qquad \frac{\partial \Im}{\partial \sigma_\delta^2} = \frac{d\left(\ln|V|\right)}{d\sigma_\delta^2} + e^T \frac{dV^{-1}}{d\sigma_\delta^2} e = 0$$

$$\frac{\partial \Im}{\partial \sigma_\gamma^2} = \frac{\partial}{\partial \sigma_\gamma^2}\ln|V| + \mathbf{e}^{\mathrm{T}} \frac{\partial V^{-1}}{\partial \sigma_\gamma^2}\mathbf{e} = 0\,; \qquad \frac{\partial \Im}{\partial \sigma_\delta^2} = \mathrm{trace}\left\{\mathrm{V}^{-1}\frac{\partial V}{\partial \sigma_\delta^2}\right\} - e^T V^{-1}\frac{\partial V}{\partial \sigma_\delta^2} e$$

$$\therefore trace\left\{V^{-1}\right\} - \mathbf{e}^{\mathrm{T}} V^{-2}\mathbf{e} = 0 \qquad \therefore trace\left(V^{-1}E_N\right) - e^T V^{-1} E_N V^{-1} e = 0$$

The error components can be solved explicitly using the Sherman-Morrison formula:

$$A^{-1} = \frac{1}{\sigma_\gamma^2}\left[I_M - \frac{1}{M+\kappa}U_M U_M^T\right] \text{where:} \qquad \kappa = \frac{\sigma_\gamma^2}{\sigma_\delta^2}$$

This calculation can be achieved since:

$$U = I_J \otimes U_M$$

$$V = \sigma_\gamma^2 I_N + \sigma_\delta^2 U U^T = \sigma_\gamma^2(I_J \otimes I_M) + \sigma_\delta^2(I_J \otimes U_M)(I_J \otimes U_M^T) = I_J \otimes \left[\sigma_\gamma^2 I_M + \sigma_\delta^2 U_M U_M^T\right]$$

let: $A = \sigma_\gamma^2 I_M + \sigma_\delta^2 U_M U_M^T\,;$ $\qquad V = I_J \otimes A \qquad \therefore V^{-1} = I_J \otimes A^{-1}$

Thus, it can be shown that:

$$trace\left(V^{-1}\right) = \mathrm{J\ trace(A^{-1})} = J\frac{1}{\sigma_\gamma^2}\left[M - \frac{1}{M+\kappa}trace(U_M U_M^T)\right] = J\frac{1}{\sigma_\gamma^2}\left[M - \frac{M}{M+\kappa}\right] = \frac{N}{\sigma_\gamma^2}\left[1 - \frac{1}{M+\kappa}\right]$$

$$V^{-2} = \left(I_J \otimes A^{-1}\right)\left(I_J \otimes A^{-1}\right) = I_J \otimes \left\{\frac{1}{\sigma_\gamma^4}\left(I_M - \frac{U_M U_M^T}{M+\kappa}\right)\left(I_M - \frac{U_M U_M^T}{M+\kappa}\right)\right\} = \frac{1}{\sigma_\gamma^4}\left(I_N + \frac{(-M-2\kappa)}{(M+\kappa)^2}E_N\right)$$

$$trace(V^{-1}E_N) = trace\left\{\frac{1}{\sigma_\gamma^2}\left[I_J \otimes \left(I_M - \frac{U_M U_M^T}{M+\kappa}\right)\right]\left[I_J \otimes \left(U_M U_M^T\right)\right]\right\} = \frac{N}{\sigma_\gamma^2}\frac{\kappa}{M+\kappa} = \frac{N}{\sigma_\delta^2(M+\kappa)}$$

$$V^{-1}E_N V^{-1} = \frac{1}{\sigma_\gamma^4}\left[I_J \otimes (I_M - \frac{U_M U_M^T}{M+\kappa})\right]\left[I_J \otimes \left(U_M U_M^T\right)\right]\left[I_J \otimes (I_M - \frac{U_M U_M^T}{M+\kappa})\right] = \frac{1}{\sigma_\delta^4}\left[\frac{1}{(M+\kappa)^2}\right]\left[I_J \otimes \left(U_M U_M^T\right)\right]$$

The solution to the set of equations is thus:

$$X^T V^{-1}\mathrm{S} = X^T V^{-1} X\beta \qquad \therefore \hat{\beta} = \left(X^T V^{-1} X\right)^{-1} X^T V^{-1}\mathrm{S}$$

Estimates of σ_δ^2 and σ_γ^2 are derived from the MLS as follows:

$$trace(V^{-1}) - e^T V^{-2} e = 0$$

$$\frac{N}{\sigma_\gamma^2}\left[1 - \frac{1}{M+\kappa}\right] = e^T \frac{1}{\sigma_\gamma^4}\left(I_N + \frac{(-M-2\kappa)}{(M+\kappa)^2}E_N\right)e$$

$$\sigma_\gamma^2 + \sigma_\delta^2 = \frac{1}{N}e^T e$$

From the MLS:

$$trace\left(V^{-1}E_N\right) = e^T V^{-1} E_N V^{-1} e$$

$$\sigma_\delta^2 = \frac{\hat{e}^T\left[I_J \otimes U_M U_M^T\right]\hat{e}}{N(M+\kappa)}\,; \qquad \therefore M\sigma_\delta^2 + \sigma_\gamma^2 = \frac{1}{N}e^T E_N e$$

thus, the estimates of σ_δ^2 and σ_γ^2 are given as the following:

$$\hat{\sigma}_\delta^2 = \frac{1}{N(M-1)}\hat{e}^E\left(E_N - I_N\right)\hat{e} \qquad \text{and} \qquad \hat{\sigma}_\gamma^2 = \frac{1}{N(M-1)}\hat{e}^E\left(MI_N - E_N\right)\hat{e}$$

where: $\qquad \hat{e} = e = S - X\hat{\beta}$

A.3 Fixed-Effects Model

From Table [T-1], the FEM can be expressed in vector form as follows:

$$S_{\cdot j} = \begin{pmatrix} S_{1j} \\ S_{2j} \\ S_{3j} \\ \vdots \\ S_{Mj} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} a_j + \begin{pmatrix} \psi_{1j} & 0 & 0 & 0 & 0 \\ 0 & \psi_{2j} & 0 & 0 & 0 \\ 0 & 0 & \psi_{3j} & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \psi_{Mj} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_M \end{pmatrix} + \begin{pmatrix} \omega_{1j} & 0 & 0 & 0 & 0 \\ 0 & \omega_{2j} & 0 & 0 & 0 \\ 0 & 0 & \omega_{3j} & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \omega_{Mj} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_M \end{pmatrix} + \begin{pmatrix} e_{1j} \\ e_{2j} \\ e_{3j} \\ \vdots \\ e_{Mj} \end{pmatrix}$$

$$S_{\cdot j} = U_M a_j + diag(\psi_{\cdot j})b + diag(\omega_{\cdot j})c + e_{\cdot j}$$

$$S = \begin{pmatrix} S_{\cdot 1} \\ S_{\cdot 2} \\ S_{\cdot 3} \\ \vdots \\ S_{\cdot J} \end{pmatrix} = \begin{pmatrix} U_M & 0 & 0 & 0 & 0 \\ 0 & U_M & 0 & 0 & 0 \\ 0 & 0 & U_M & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & U_M \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_J \end{pmatrix} + \begin{pmatrix} diag(\psi_{\cdot 1}) \\ diag(\psi_{\cdot 2}) \\ diag(\psi_{\cdot 3}) \\ \vdots \\ diag(\psi_{\cdot J}) \end{pmatrix} b + \begin{pmatrix} diag(\omega_{\cdot 1}) \\ diag(\omega_{\cdot 2}) \\ diag(\omega_{\cdot 3}) \\ \vdots \\ diag(\omega_{\cdot J}) \end{pmatrix} c + \begin{pmatrix} e_{\cdot 1} \\ e_{\cdot 2} \\ e_{\cdot 3} \\ \vdots \\ e_{\cdot J} \end{pmatrix}$$

let:

$\Omega = \left(diag(\omega_{\cdot 1}) \cdots diag(\omega_{\cdot J})\right)^T$; $\Psi = \left(diag(\psi_{\cdot 1}) \cdots diag(\psi_{\cdot J})\right)^T$; $\psi_{\cdot J} = \left(\psi_{1J} \cdots \psi_{MJ}\right)^T$

$\delta = \left(\delta_1 \cdots \delta_J\right)^T$; $\gamma = \left(\gamma_{\cdot 1} \cdots \gamma_{\cdot J}\right)^T$; $\gamma_{\cdot J} = \left(\gamma_{1J} \cdots \gamma_{MJ}\right)^T$

b = $\left(b_1 \cdots b_M\right)^T$; c = $\left(c_1 \cdots c_M\right)^T$; e= $\left(e_{\cdot 1} \cdots e_{\cdot J}\right)^T$;

$$S = \left(I_J \otimes U_M\right)a + \Psi b + \Omega c + e$$

$$X = [\left(I_J \otimes U_M\right), \Psi, \Omega]$$

$$\hat{\beta} = (X^T X)^{-1} X^T S$$

where ⊗ is the tensor product, N is the product of M and J, and P = 2M+1. The vector **S** is of size [Nx1], $\hat{\beta}$ of size [P x 1] are the model coefficients, **X** is of size [N x P] and **e** is an [Nx1] column vector of "error" random variables. The variance of the error component is described as:

$$E(e) = 0$$

$$Var(e) = \sigma_\gamma^2 I$$

It can be shown that an unbiased estimate of the variance is given by the following:

$$\hat{\sigma}_\gamma^2 = \left(\frac{1}{n-p}\right) e^T e$$