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A SYSTEMATIC METHODOLOGY FOR THE REDUCTION OF UNCERTAINTIES IN TRANSIENT THERMAL-HYDRAULICS BY USING IN-BUNDLE MEASUREMENT DATA*

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ABSTRACT

The development of a systematic methodology for the reduction of uncertainties in transient thermal-hydraulics by using in-bundle measurement data is presented. The adjustment of the system parameters and responses and the reduction in their respective uncertainties is treated as a time-dependent constrained minimization problem. An on-line (i.e., real time) large scale optimization scheme is also outlined. Although formulated within the framework of reactor safety analysis, the proposed methodology can be directly applied to other areas, for instance to time-dependent fuel cycle optimization and uncertainty analysis.

INTRODUCTION

The accurate computation of local fluid properties for rod bundle geometries during severe reactor transients (e.g., blowdown) is one of the most challenging problems occuring in reactor safety. The current procedures[1,2] for attempting to solve the transient boundary value convective transport problem in space and time involve coupling of transient thermal-hydraulics analysis and inverse heat conduction codes with experimentally determined hydraulic boundary conditions. A large component of the discrepancies observed[1,2] between in-bundle measured and calculated quantities of interest (henceforth referred to as system responses) is due to the high uncertainties in the experimental boundary conditions. Considerable difficulties are encountered in performing uncertainty analyses of even limited scope[2-4] resulting usually in the imposition of overconservative and costly margins of safety in the design of light water reactors.

The present work outlines a systematic new methodology which incorporates in-bundle measurements and allows computation of transient local fluid conditions with significantly reduced uncertainties. The adjustment of the system parameters and responses, and the reduction of their respective uncertainties, is treated as a time-dependent constrained minimization

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problem which is solved by the method of Lagrange multipliers. An on-line (i.e., real time) large scale optimization scheme is also proposed. Finally a successful application of this methodology to the analysis of an experiment[5] performed within the Oak Ridge National Laboratory's Pressurized Water Reactor Blowdown Heat Transfer (BDHT) Separate Effects Program[6] is presented. Although formulated within the framework of reactor safety analysis, the proposed methodology can be directly applied to other areas, for instance to time-dependent fuel cycle optimization and uncertainty analysis.

THEORY

The methods for reducing the uncertainties in the estimation of nuclear responses through nuclear data "adjustments", which incorporate information from integral benchmark experiments, have been brought to a high degree of sophistication during the last decade.[7] Most of the past applications have been in the field of LMFBR neutronics[8] or conceptual fusion reactor design studies.[9] However, with the coming of age of sensitivity and uncertainty analysis, the direct application of existing procedures to new fields such as energy-economy modeling[10] or transient thermal hydraulics becomes problematic since problem characteristics such as time dependence, nonlinearities and large uncertainties become dominant. In order to reduce computational complexity and prohibitive costs, new concepts such as "on-line" (i.e. real time) strategies have to be introduced, for both adjustment and optimization purposes. Note that in an adjustment procedure, the proper combination of various types of data (responses, parameters, etc.) leads to a systematic reduction of the respective uncertainties as additional information is introduced. By contrast, the optimization procedure's main objective is to reproduce experimental results by computational means. The derivations to follow are sufficiently general to be adapted not only to adjustment but also to optimization problems.

The underlying theory is presented next. Let $\bar{r}^{\nu}$ and $\hat{r}^{\nu}$ denote vectors of expectation values of calculated and adjusted (optimized) system responses at time step ν corresponding, respectively, to the nominal and optimized values of the boundary parameter vectors α^{μ} and $\hat{\alpha}^{\mu}$ at all time steps $\mu \leq \nu$. The formalism assumes the following relationship between the time-dependent responses

$$\hat{r}^{\nu} = \bar{r}^{\nu} + \sum_{\mu \leq \nu} S^{\nu\mu}[\hat{\alpha}^{\mu} - \alpha^{\mu}] \tag{1}$$

where the elements of the sensitivity matrices $S^{\nu\mu}$ are defined as

$$S_{ni}^{\nu\mu} = \begin{cases} \left. \dfrac{\partial \bar{r}_n^{\nu}}{\partial \alpha_i^{\mu}} \right|_{\bar{\alpha}^{\mu}} & \text{if } \mu \leq \nu, \\ 0 & \text{, otherwise.} \end{cases} \tag{2}$$

$S_{ni}^{\nu\mu}$ are evaluated on a sensitivity hypersurface at an appropriate point $\bar{\alpha}^{\mu}$. In nonlinear cases $\bar{\alpha}^{\mu}$ is determined by an iterative scheme, while in linear problems $\bar{\alpha}^{\mu}$ equals α^{μ}. Denoting the in-bundle measurements by r^{ν} and the actual variations in the boundary parameters and responses by

$$x^{\nu} = \hat{\alpha}^{\nu} - \alpha^{\nu} \tag{3}$$

$$y^{\nu} = \hat{r}^{\nu} - r^{\nu} \tag{4}$$

$$d^{\nu} = \bar{r}^{\nu} - r^{\nu} \tag{5}$$

respectively, a Bayesian inference approach[11] or alternately a maximum likelihood estimation (normal pdf's) leads to the requirement that the quadratic form

$$Q = \left[\tilde{y} \vdots \tilde{x} \vdots \dots\right] \cdot \begin{bmatrix} C_{rr} & C_{r\alpha} & \dots \\ C_{\alpha r} & C_{\alpha\alpha} & \dots \\ \dots & \dots & \dots \end{bmatrix}^{-1} \cdot \begin{bmatrix} y \\ \hline x \\ \hline \vdots \end{bmatrix} \tag{6}$$

be minimized subject to constraints which describe the functional relationship between boundary parameters and system responses:

$$y^{\nu} = \sum_{\mu \leq \nu} S^{\nu\mu} \cdot x^{\mu} + d^{\nu} \qquad \nu = 1, \dots NT \tag{7}$$

In Equation (6) $\tilde{y}$ and $\tilde{x}$ denote transposed partitioned vectors

$$\tilde{y} = (\tilde{y}^{1}, \dots, \tilde{y}^{\nu}, \dots, \tilde{y}^{NT}); \quad \tilde{x} = (\tilde{x}^{1}, \dots, \tilde{x}^{\nu}, \dots, \tilde{x}^{NT}) \tag{8}$$

while C_{rr} and $C_{\alpha\alpha}$ represent the partitioned uncertainty matrices of experimental responses and boundary parameters, respsectively, e.g.,

$$C_{\alpha\alpha} = \begin{bmatrix} C_{\alpha\alpha}^{1} & C_{\alpha\alpha}^{(1,2)} \dots & \dots \\ C_{\alpha\alpha}^{(1,2)} & C_{\alpha\alpha}^{2} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & C_{\alpha\alpha}^{NT} \end{bmatrix} \tag{9}$$

The covariance matrices $C_{\alpha\alpha}^{(\nu,\mu)}$ describe correlations between the uncertainties in the boundary parameters at distinct time steps, while the $C_{r\alpha}$'s [cf. Eq. (6)] account for correlations between experimental responses and boundary parameters. Additional features (e.g., methods uncertainties[8]) can readily be incorporated into the optimization process by replacing the symbols [...] in Eq. (6) with appropriate vectors and corresponding covariance matrices.

The system of equations (6-7) can be treated as a constrained minimization problem and solved by the method of Lagrange mutipliers. For example, if all off-diagonal covariance submatrices are zero, the solution is

$$x^{\nu} = -C_{\alpha\alpha}^{\nu} \cdot \tilde{S}^{\nu\nu} \cdot \lambda^{\nu}; \qquad y^{\nu} = C_{rr}^{\nu} \cdot \lambda^{\nu} \tag{10}$$

where

$$\lambda^{\nu} = [C_{rr}^{\nu} + S^{\nu\nu} \cdot C_{\alpha\alpha}^{\nu} \cdot \tilde{S}^{\nu\nu}]^{-1} \cdot h^{\nu} \tag{11}$$

with

$$h^{\nu} = d^{\nu} - \sum_{\mu<\nu} S^{\nu\mu} \cdot C_{\alpha\alpha}^{\mu} \cdot \tilde{S}^{\mu\mu} \cdot \lambda^{\mu} \tag{12}$$

Note the fundamental role[12,13] of the Lagrange multipliers λ^{ν}. It appears not only in the expressions for the adjustments of the boundary parameters and responses [cf. Eq. (10)], but it can also be shown that the covariance matrices associated with x^{ν} and y^{ν} are given by expressions involving the covariance matrix associated with λ^{ν} ($C_{\lambda\lambda}^{\nu}$); in particular:

$$C_{xx}^{\nu} = C_{\alpha\alpha}^{\nu} \cdot \tilde{S}^{\nu\nu} \cdot C_{\lambda\lambda}^{\nu} \cdot S^{\nu\nu} \cdot C_{\alpha\alpha}^{\nu} \tag{13}$$

$$C_{yy}^{\nu} = C_{rr}^{\nu} \cdot C_{\lambda\lambda}^{\nu} \cdot C_{rr}^{\nu} \tag{14}$$

The covariance matrix $C_{\lambda\lambda}^{\nu} \equiv \langle \Delta\lambda^{\nu} \tilde{\Delta}\lambda^{\nu} \rangle$ is obtained from

$$C_{\lambda\lambda}^{\nu} = [C_{rr}^{\nu} + S^{\nu\nu} C_{\alpha\alpha}^{\nu} \tilde{S}^{\nu\nu}]^{-1} C_{hh}^{\nu} [C_{rr}^{\nu} + S^{\nu\nu} C_{\alpha\alpha}^{\nu} \tilde{S}^{\nu\nu}]^{-1} \tag{15}$$

In the above expression $C_{hh}^{\nu} \equiv \langle \Delta h^{\nu} \tilde{\Delta} h^{\nu} \rangle$ denotes the covariance matrix associated with the inhomogeneous source term of the Lagrange equations, i.e.

$$C_{hh}^{\nu} = \langle \Delta d^{\nu} \tilde{\Delta} d^{\nu} \rangle - \sum_{\mu<\nu} S^{\nu\mu} C_{\alpha\alpha}^{\mu} \tilde{S}^{\mu\mu} \langle \Delta\lambda^{\mu} \tilde{\Delta} d^{\nu} \rangle$$

$$- \sum_{\mu<\nu} \langle \Delta d^{\nu} \tilde{\Delta\lambda}^{\mu} \rangle \, S^{\mu\mu} \, C^{\mu}_{\alpha\alpha} \, \tilde{S}^{\nu\mu} \tag{16}$$

$$+ \sum_{\mu<\nu} S^{\nu\mu} \, C^{\mu}_{\alpha\alpha} \, \tilde{S}^{\mu\mu} \, C^{\mu}_{\lambda\lambda} \, S^{\mu\mu} \, C^{\mu}_{\alpha\alpha} \, \tilde{S}^{\nu\mu}$$

In deriving Eq. (16) use was made of the relationship $\langle \Delta\lambda^{\mu} \tilde{\Delta\lambda}^{\eta} \rangle = C^{\mu}_{\lambda\lambda}\delta_{\mu\eta}$, which is consistent with the assumptions leading to the solution form (10). The covariance matrix of the best estimates for the boundary parameters is then simply

$$C^{\nu}_{\hat{\alpha}\hat{\alpha}} = C^{\nu}_{\alpha\alpha} - C^{\nu}_{xx} \tag{17}$$

For the best response estimates it is similarly

$$C^{\nu}_{\hat{r}\hat{r}} = C^{\nu}_{rr} - C^{\nu}_{yy} \tag{18}$$

"Recalculated" responses $\hat{\bar{r}}^{\nu} = \bar{r}\,[\hat{\alpha}^{1},\ldots,\hat{\alpha}^{\nu}]$ can be computed by using $\{\hat{\alpha}^{\mu},\mu\leq\nu\}$ as the new "nominal" values for the boundary parameters. The adequacy of the solution is tested by ensuring, at each time step ν, that

$$\underset{n}{\mathrm{Max}} \left| \frac{\hat{\bar{r}}^{\nu}_{n} - \hat{r}^{\nu}_{n}}{\hat{r}^{\nu}_{n}} \right| < \varepsilon_{r} \quad \text{or} \quad \underset{n}{\mathrm{Max}} \left| \frac{\hat{\bar{r}}^{\nu}_{n} - r^{\nu}_{n}}{r^{\nu}_{n}} \right| < \varepsilon_{r} \tag{19}$$

are satisfied, according to whether the problem is of adjustment - or optimization - type, respectively. It sould be pointed out that whenever significant parameter adjustments are to be expected, because of poorly known initial parameter values, or in highly nonlinear problems, the linearity assumption, on which the conventional adjustment algorithms are based, is likely to break down, i.e. the above test (Eq. 19) fails. Such problems have then to be solved iteratively, so that even when no a priori response-parameter correlations are assumed, they appear after the first iteration and necessitate a more general formalism.[13,14]

ON-LINE ADJUSTMENT AND OPTIMIZATION STRATEGY: AN OUTLINE

Since the implementation of the algorithm developed in the previous section requires the availability of sensitivities of the form $S^{\nu\mu}$, this algorithm becomes less practical as the number of time intervals of interest increases. For example the algorithm would clearly be practical for fuel management optimization problems, where typically only a few intervals ["cycles"] are of interest. In transient thermal-hydraulics problems several hundred time intervals of interest are generally involved. Even if the concepts of sensitivity theory for nonlinear systems[15] are employed [such that one computer run per response at time step ν gives the sensitivities with respect to all system parameters at time step μ, $\mu \leq \nu$], $\nu(\nu+1)/2$ runs would still be needed per time dependent response in order to determine all the required sensitivities.

In order to circumvent this difficulty an adjustment and/or optimization scheme in real time is described in Fig. 1. It involves an interactive relationship between a transient thermal hydraulics code (e.g. RELAP), the ORION sensitivity generation module[16] and the NOGA optimization and adjustment code.[17] On-line acquisition of experimental data is available as a possible option; in practice the time scale of the specific transient problem under investigation governs the implementation of the latter capability. It should be emphasized that the sensitivities generated by the proposed scheme for system parameters perturbed at time step ν, implicitly account for the optimized values of the parameters at all previous time steps, and hence considerably reduce the overall cost of the adjustment or optimization process.

The current paper is mainly concerned with the development of a systematic methodology for the reduction of uncertainties in transient thermal-hydraulics by incorporating in-bundle measurment data. It should be pointed out however, that the procedure clearly has the capability of estimating the nominal uncertainties of the calculated responses by simply combining sensitivities and nominal system parameter covariances. This latter aspect is directly comparable to the current methods[2,3,4,18] for estimating uncertainties in transient thermal hydraulic problems, where in general statistically determined "response surfaces" are used. These response surfaces are obtained by curve-fitting quantities of interest computed by perturbing the system parameters in a prescribed way [i.e., latin hypercube sampling, factorial designs, etc.]. Many sophisticated statistical algorithms [e.g. moment matching] exist for estimating the statistical properties and uncertainty distributions of the responses. In those algorithms the response surface functions as surrogate for the original computer code, "engineering judgement" being used to drastically limit the number of parameters, since only comparatively few can be considered in practice. In current response surface procedures the treatment of time dependence is approximated by assuming that the surface curvature coefficients are constant over large time intervals. The availability of an optional on-line response surface generation capability in the ORION module is expected to provide a practical means to validate algorithms currently in use.

The formalism of the on-line adjustment and optimization methodology, including treatment of nonlinearities and response parameter correlations, will be presented elsewhere.[14] Preliminary results for a representative nonlinear transient thermal hydraulics problem will be discussed in the following section.

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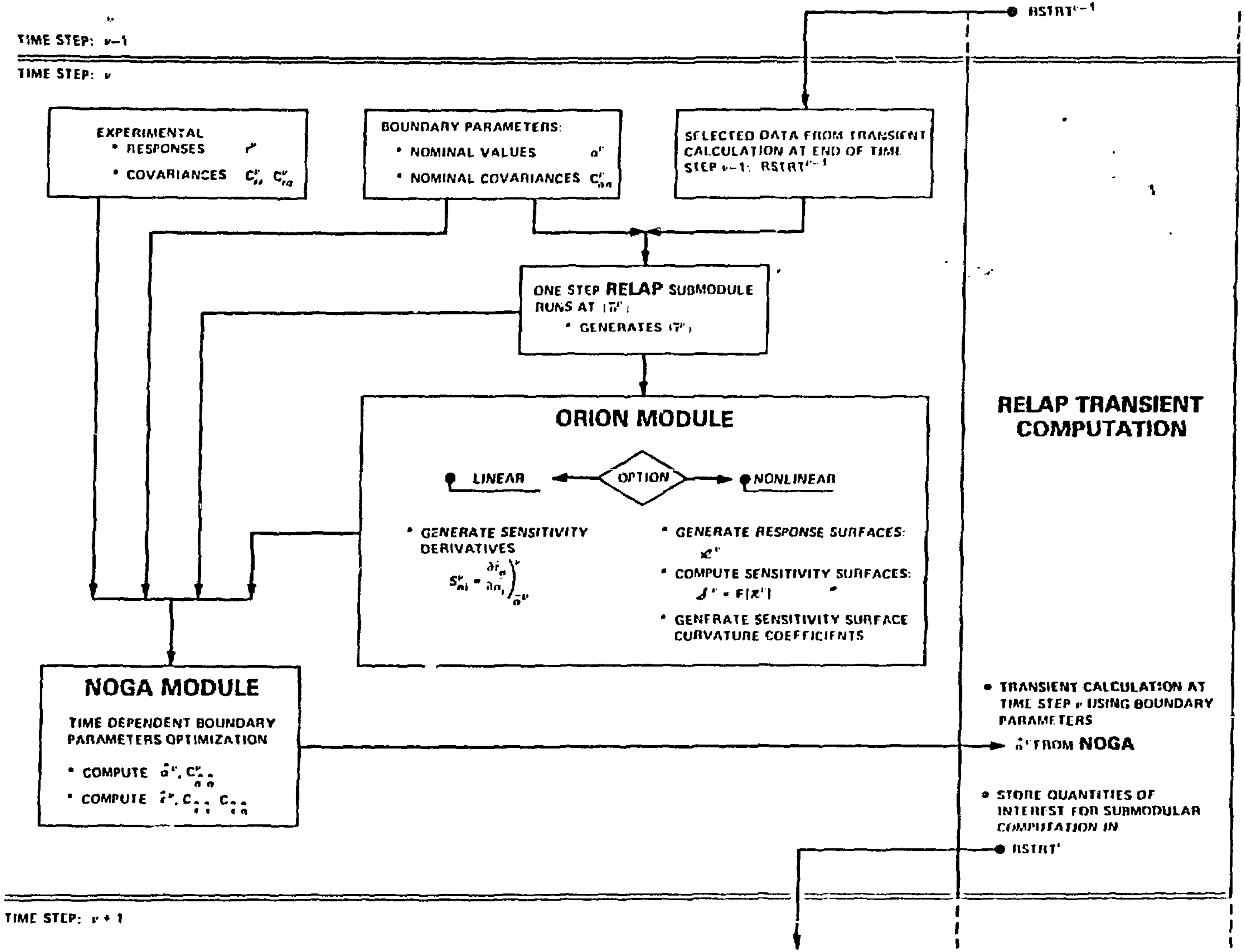
Figure 1

ON-LINE INCORPORATION OF INBUNDLE MEASUREMENTS IN THE DETERMINATION OF TRANSIENT LOCAL FLUID CONDITIONS



PRELIMINARY ASSESSMENT OF THE METHODOLOGY FOR A TRANSIENT UPFLOW OF HIGH PRESSURE WATER

The methodology discussed so far has been applied to the analysis of a transient upflow film boiling heat transfer experiment,[5] performed within the Oak Ridge National Laboratory's Pressurized Water Reactor Blowdown Heat Transfer (BDHT) Separate Effects Program.[6] A primary objective of this program is the calculation of transient heat transfer coefficients. The source of experimental data needed to meet this objective is the Thermal Hydraulic Test Facility (THTF), a non-nuclear pressurized water loop containing an array of full length electrically heated rods. Its standard configuration is shown in Fig. 2. Figure 3 is a simplified diagram showing the position of THTF piping and instrumented spool pieces relative to the test section.

In the experiment to be discussed the transient was initiated by breaking the outlet rupture disk assembly (Fig. 3) at time t = 0.0's. Although the THTF has a rupture disk assembly at the outlet and inlet, by breaking at the outlet only and installing an orifice at the pressurizer, unidirectional flow through the test section, inlet spool pieces, outlet nozzle spool piece and vertical outlet spool piece, throughout the transient was assured. The unidirectional flow in the instrumented spool pieces and rod bundle facilitated the calculation of fluid conditions in the rod bundle during the transient. Simultaneous with the breaking of the outlet rupture disk, the pump was tripped and bundle power was ramped up from ~4 to ~6.5 MW. During the transient, data was taken by a computer-controlled data acquisition system (DAS) capable of scanning 2000 instruments at a rate of 20 data points per instrument per second. Simultaneous with acquiring data the DAS also monitored the sheath thermocouples to determine the trip time for ramping power down.

The capability of predicting "accurately" (i.e. with reduced uncertainties) the transient local fluid conditions in the THTF test section where experimental measurements are not available constitutes an important mission of the BDHT program. Presently, the heater rod surface conditions are supplied by the inverse heat conduction code ORINC[19] which uses the individually recorded rod amperage, voltage and thermocouple responses as input. Bundle fluid conditions are calculated using the homogeneous two-phase flow, thermodynamic equilibrium computer code RLPSFLUX.[20] RLPSFLUX is a locally modified version of RELAP4 Mod 5 Update 2,[21] which uses the ORINC calculated rod surface heat fluxes in place of the standard RELAP4/MOD5 heat transfer package. RLPSFLUX also uses measured conditions in THTF instrumented spool pieces as hydraulic boundary conditions. Figure 4 is the noding diagram of the THTF test section for the calculation of bundle fluid conditions used in this paper. At Junction 18 (J18 on Fig. 4), which models the test section inlet, the boundary condition supplied was mass flux and enthalpy versus time. The boundary condition used at the test section outlet was pressure versus time specified in Volume 17 (circled 17 on Fig. 4). The film boiling correlations being evaluated were not used in the calculation of the bundle fluid conditions, since the energy input to the fluid from the heater rods versus time (as calculated by ORINC) was specified.

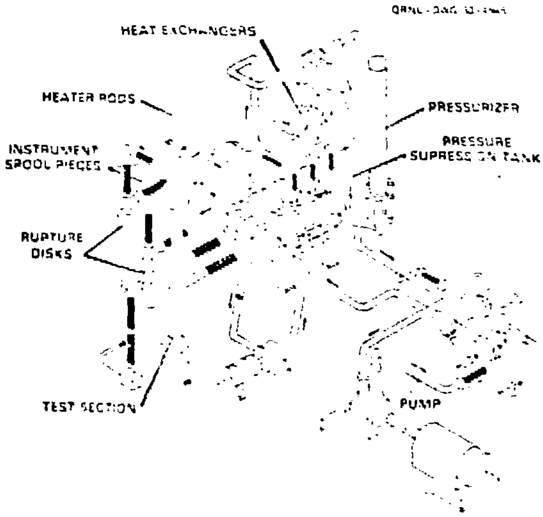


Fig. 2 THTF in standard configuration.

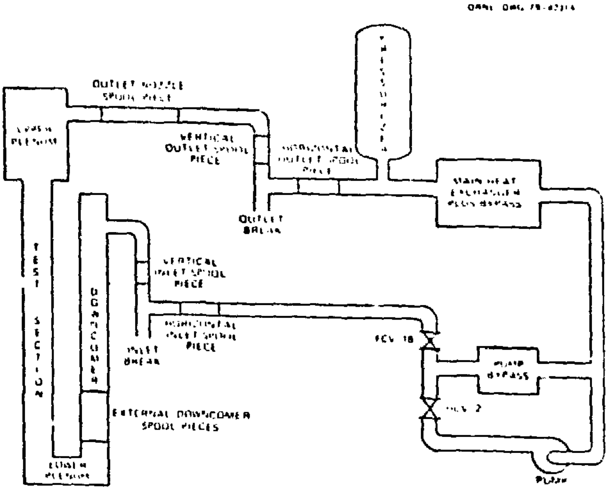


Fig. 3 Diagram of THTF.

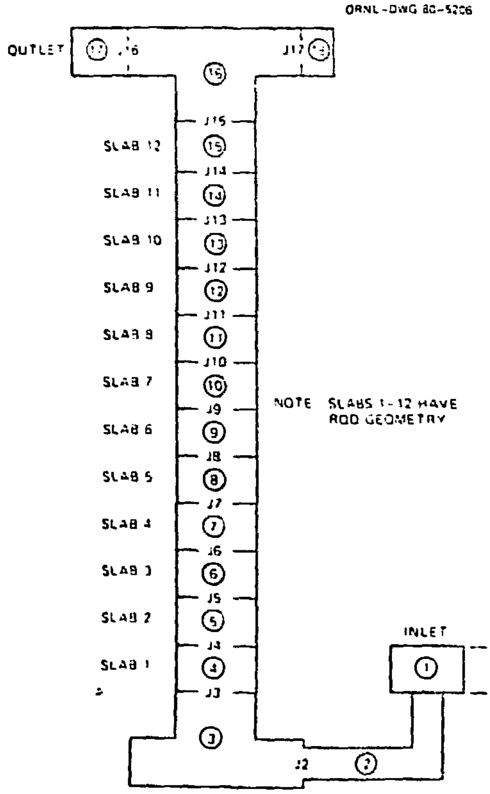


Fig. 4 Node diagram of RELAP4 THTF Test Section Model

Fig. 5-a. Experimental [illegible] and Nominal [illegible] Mass Flow Responses at [illegible]

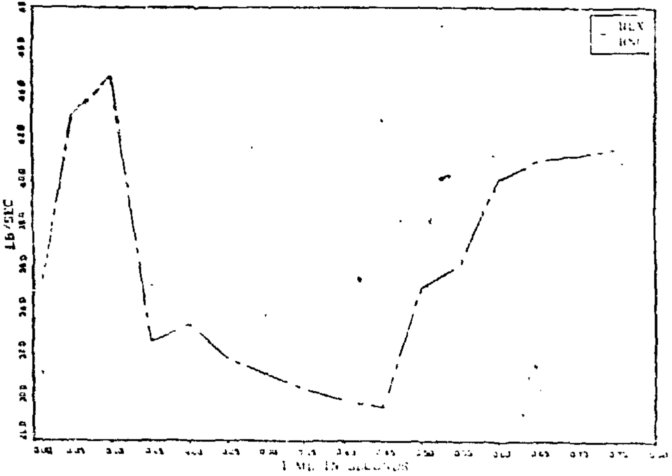


Fig. 5-b. [illegible] Mass Flow Responses at [illegible] Junction [illegible] Response Surface [illegible]

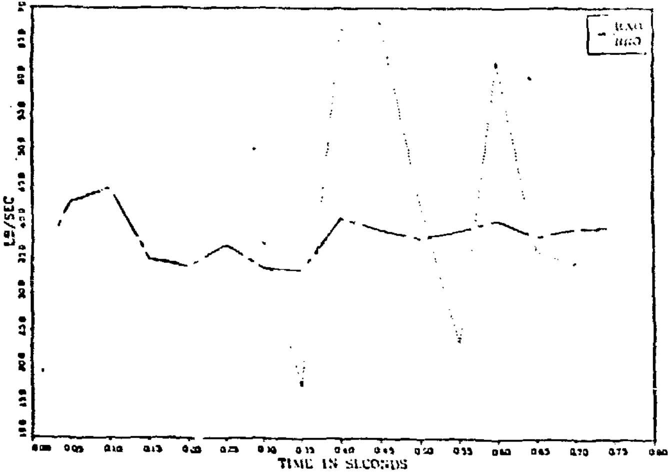


Fig. 5-c. Adjusted (RAN) and Recalculated (RRN) Mass Flow Responses at THIF Junction in FOR Test 3.05.SAR, Using On-Line Computed Sensitivities.

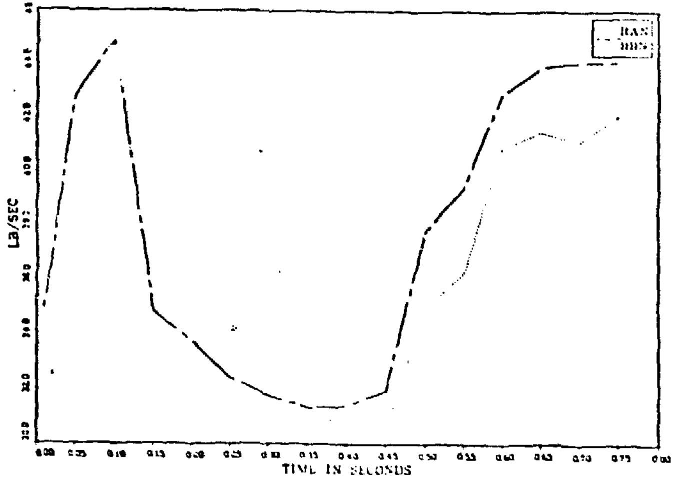


Fig. 6 Standard Deviation of the Experimental (SDE), Nominal (SDC) and On-Line Adjusted (SDA) Mass Flow Responses at THIF Junction in FOR Test 3.05.SAR.

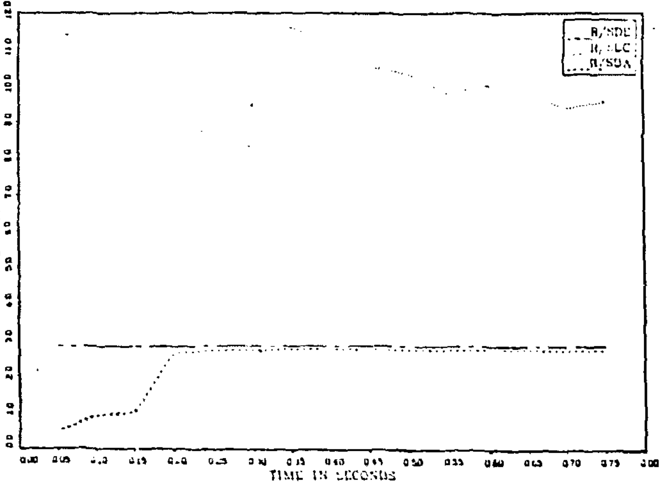


Fig. 7-a. Sensitivities (RS = [illegible] Response Surface Type, OL = On-Line) of Mass Flow Response at THIF Junction to Inlet Mass Flow for Test 3.05.SAR

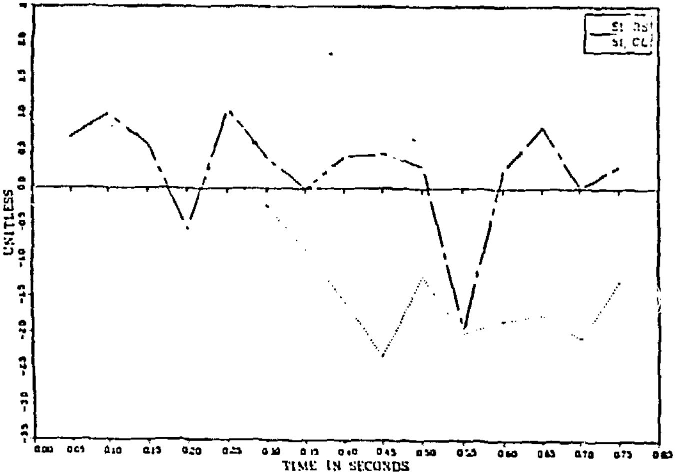
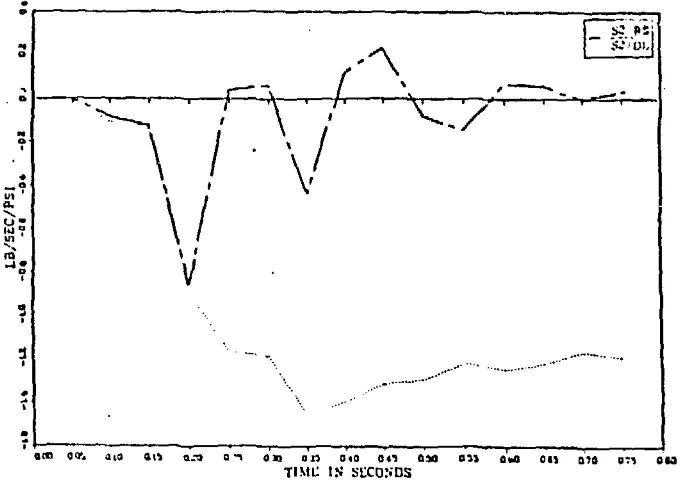


Fig. 7-b. Sensitivities (RS = [illegible] Response Surface Type; OL = On-Line) of Mass Flow Response at THIF Junction to Outlet Pressure for Test 3.05.SAR



For a preliminary assessment of the methodology, the incorporation of in-bundle measurement data was limited to the specification of a single experimental response. The mass flow at Junction 16 (see Fig. 4) was chosen, since the pressure measured in the outlet nozzle spool piece was used as a boundary condition in the model. Two sets of sensitivities were generated for the corresponding calculated response. The first set was obtained[13] by perturbing the system boundary parameters uniformly in time according to a star point design pattern. Quadratic response surfaces were generated on a much denser time grid ($\Delta t = .05s$) than generally reported elsewhere.[2-4] The possibility of performing off-line uncertainty analysis, with sensitivities computed at significantly lower costs than would be required to develop a complete $S^{\nu\mu}$ data base, could thus be assessed. The second set of sensitivities was generated using the on-line scheme outlined in Section 3 of the present paper. The experimental and nominal calculated values of the mass flow response are plotted on Fig. 5.a. The adjusted and recalculated values resulting from the off-line scheme are given in Fig. 5.b. The on-line adjustment results are shown in Fig. 5.c. The standard deviations of the experimental, nominal and on-line adjusted responses are plotted on Fig. 6. Finally Fig. 7 shows the first order sensitivities for off-line and on-line adjustemnt, evaluated at the nominal values of the inlet mass flow and outlet pressure boundary parameters.

SUMMARY AND CONCLUSIONS

A systematic methodology for the reduction of uncertainties in transient thermal-hydraulics by using in-bundle measurement data was presented. The adjustment of the system parameters and repsonses and the reduction in their respective uncertainties was treated as a time-dependent constrained minimization problem. The solution algorithm, defined as "off-line" adjustment and/or optimization, requires the availability of sensitivities of the form $S_{ni}^{\nu\mu}$ relating the variations in the responses {n} to perturbations in the system parameters {i} for given time intervals ν and μ. The algorithm was found to be particularly attractive in situations in which only a limited number of time intervals are of interest, such as fuel management multicriterion optimization studies. The cost of generating a sensitivity data base $S_{ni}^{\nu\mu}$ increases rapidly with the number of time intervals of interest. An attempt to use sensitivities computed by response surface generation techniques appears to cast some doubt about the capability of the latter techniques, as currently implemented, to fully estimate the uncertainties [or be used in uncertainty reduction procedures] in transient thermal-hydraulic problems where strong time-coupling effects are dominant. As a promising feasable alternative, an on-line (i.e. real time) large scale adjustment and optimization scheme was outlined and successfully applied to a transient upflow of high pressure water. The improvement in responses recalculated with on-line adjusted boundary parameters is striking. Although preliminary covariance data were used, even the linear approximation reduced the original discrepancies by more than 50% with a corresponding reduction in the uncertainties. More detailed results will be reported in a forthcoming publication,[14] which will also include the treatment of nonlinearities and response parameter correlations.

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