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REFINEMENT OF THE MASS CONSERVATION ALGORITHM USED IN CATHENA

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ABSTRACT

The need to correct mass conservation errors is an integral part of the numerics underlying CATHENA. In the past, it was found necessary for stability reasons to neglect mass conservation errors when the code ran at the minimum time step or a `re-do` *occurred. This could potentially lead to significant discrepancies in fluid inventory during some simulations. In CATHENA MOD-3.5b/Rev 0, a revised mass conservation strategy was implemented that addresses the weaknesses of the previous strategy. Mass is now conserved at all times, and a redistribution strategy has been implemented to ensure numerical stability when rapidly varying conditions could lead to node overfilling. This work outlines the refined algorithm, and illustrates its effectiveness.*

1 INTRODUCTION

CATHENA (Canadian Algorithm for THErmalhydraulic Network Analysis) is a computer program designed for the analysis of two-phase flow and heat transfer in piping networks. The CATHENA thermalhydraulic code was developed by AECL, Whiteshell Laboratories, primarily for the analysis of postulated accident conditions in CANDU® reactors.

The thermalhydraulic model employed in CATHENA uses a one-dimensional, non-equilibrium two-fluid model consisting of six partial differential equations for mass, momentum and energy conservation; three for each phase. A first-order finite-difference representation is used to solve the differential equations, utilizing a semi-implicit one-step method in which the time step is not limited to the material Courant number. At each time step, the coupled linear finite-difference equations representing the thermalhydraulic network to be modelled form a sparse matrix which is written and solved. Details of the thermalhydraulic model employed in CATHENA and the numerical solution used to implement it can be found in reference [1].

2 MASS CONSERVATION ERROR CORRECTION ALGORITHM

One of the consequences of the linearized numerical algorithm employed in CATHENA to solve the thermalhydraulic conservation equations is need for a mass correction term. Since the density of the liquid and gas phases is not a linear function of pressure and phase enthalpy, a truncation error in

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mass and energy can develop over a time step. An additional error may also result during transitions between two-phase and single-phase conditions since the void fraction must be limited to values between zero and unity.

To prevent this truncation error from accumulating, a mass correction term is calculated at each time step for each phase for each thermalhydraulic node and is applied in the subsequent time step. The error correction ε term can be expressed as follows for both the gas and liquid terms:

$$\varepsilon_k^{n+1} = \left(\alpha_k^n \rho_k^{\overline{n+1}} - \alpha_k^{n+1}\rho_k^{n+1}\right) + \rho_k^n \left(\alpha_k^{n+1} - \alpha_k^{\overline{n+1}}\right) \tag{1}$$

where $k = f$ for liquid and $k = g$ for the gas phase, n represents the time step, ρ_k is phase density, and α_k is the void fraction. The $\alpha_k^n \rho_k^{\overline{n+1}}$ term in Equation (1) represents the mass in the system at time step $n+1$ as calculated using the dependent variables and the linearized property routines. The $\alpha_k^{n+1}\rho_k^{n+1}$ term represents the actual phase mass in the system as calculated using the derived value for ρ_k. The difference between these two terms represents the mass error incurred as a result of the linearizing the property routines in CATHENA.

The $\rho_k^n(\alpha_k^{n+1} - \alpha_k^{\overline{n+1}})$ term in Equation (1) represents the phase mass error incurred due to truncation of the void fraction term. Here $\alpha_k^{\overline{n+1}}$ is the value of void fraction as obtained through the solution of the finite difference equations, and α_k^{n+1} is the "clipped" value of void fraction at one or zero which results if the calculated finite-difference solution result is outside these limits, as defined by:

$$\alpha_k^{n+1} = \min\left[\max\left[\alpha_k^{\overline{n+1}}, 0.0\right], 1.0\right] \tag{2}$$

The mass error ε_k is calculated at the end of the time step and is applied as a correction term in the new time step as shown schematically in Figure 1. The mass correction term is applied as a source term in the mass conservation equations in the next time step.

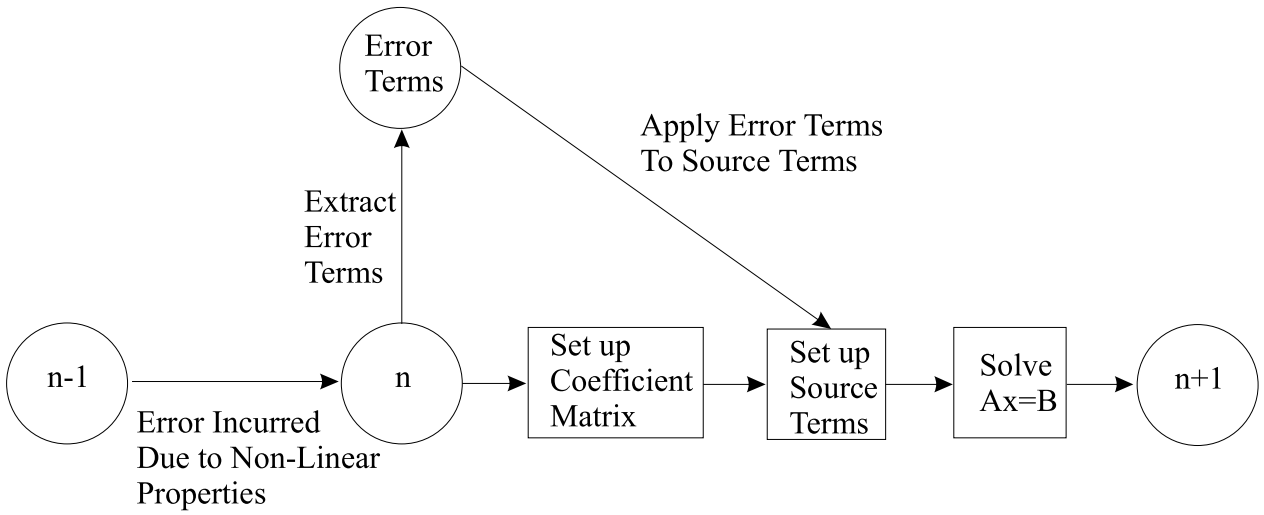

FIGURE 1: Overview of CATHENA Mass Error Correction Scheme.

It was found that the application of the mass error term could cause numerical instabilities under certain conditions. As shown in Figure 1, the mass truncation incurred from step $n-1$ to n is applied

as part of the equations used to advance the code from step n to $n+1$. However, if step $n-1$ to n is much larger than step n to $n+1$ problems may occur. For example, a rapid transient could decrease the time step and/or cause a `re-do` to occur. In this case, a potentially large error correction incurred from step $n-1$ to n could be applied over a very small time step from step n to $n+1$. This correction can cause instabilities in the solution by adding a large source term into the mass conservation relationships for the next time step.

An automatic timestep controller controls the size of time step CATHENA uses to advance the solution. The timestep controller monitors the change in critical state variables from one time step to another. If the change in these variables exceed pre-defined limits, the timestep controller decreases the subsequent solution timestep to minimize numerical errors in the solution. Conversely, if the change in these variables is smaller than pre-defined limits, the timestep controller can increase the subsequent solution timestep to minimize the computational time requirements. If the variable changes are bounded by the pre-defined limits, the timestep controller does not change the subsequent solution timestep.

In cases where the solution undergoes a particularly violent change, the timestep controller also has the ability to cause CATHENA to execute a `re-do`. In this case, the solution is rejected, and the step is "re-done" using 1/4 the previous time step. In particularly severe cases, several `re-dos` can occur in sequence, and the solution time step can be drastically reduced. This procedure can be repeated until the solution time step reaches the allowed minimum time step.

In versions of CATHENA prior to MOD-3.5b/Rev 0, a simple solution was chosen to avoid potential problems caused by the application of the mass correction term. Assuming numerical instabilities occured primarily when the code was running at the minimum allowed timestep or performing a `re-do`, no mass conservation correction was performed under these conditions. However, this technique can cause undesirable mass discrepancies in the system under investigation if a significant number of `re-dos` or solutions steps at minimum timesteps are encountered.

3 REVISED MASS CONSERVATION ERROR CORRECTION ALGORITHM

For CATHENA MOD-3.5b/Rev 0, a revised mass conservation error algorithm was implemented. Since CATHENA is a two-phase code, both the liquid and vapour mass conservation equations have mass error correction terms. For the vapour phase, it was assumed that the relatively high vapour compressibility will accommodate a correction term of any size without causing numerical difficulties. As a result, the vapour mass error is always added back into the node from which it originated.

Figure 2 shows a flow chart of the revised mass correction algorithm for the liquid phase. First, each node is checked to see if the addition of the mass error correction term will overfill the node.

3.1 Overfilling Calculation

A node is considered overfull if the addition of the mass error correction term might cause the pressure or void fraction to change enough to reduce the subsequent time step.

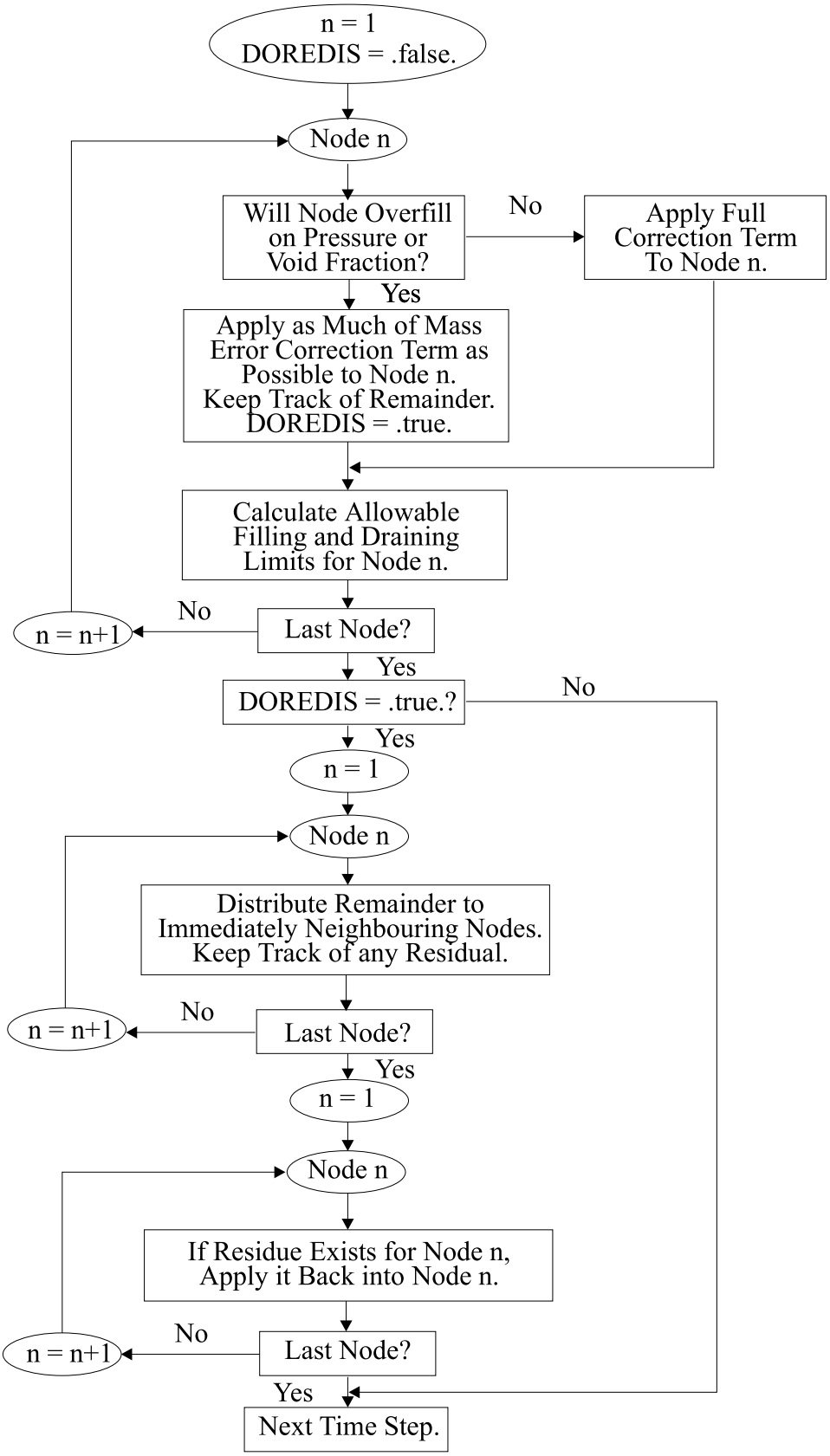

FIGURE 2: Detailed Schematic of CATHENA Liquid Mass Conservation Error Correction Algorithm.

If the node is filled with a single-phase liquid, the change in pressure of the node (ΔP_{node}) in response to the addition of the mass error correction term can be estimated as follows:

$$\Delta P_{node} \simeq \frac{\Delta \rho_f}{\left.\frac{\partial \rho_f}{\partial P_f}\right|_h} \tag{3}$$

where the change in mass is represented as a change in node liquid density $\Delta \rho_f$. The liquid isenthalpic compressibility $\left.\partial \rho_f / \partial P_f\right|_h$ is an available quantity in the CATHENA steam property tables.

If the node is in two-phase flow, the vapour phase can be displaced by the liquid, and the change in the node void fraction ($\Delta \alpha_{node}$) in response to the addition of mass from the error correction term can be estimated using the following expression:

$$\Delta \alpha_{node} \simeq \frac{\Delta \rho_f}{\rho_f}(1 - \alpha_g) \tag{4}$$

where α_g is the void fraction, and ρ_f is the density of the liquid.

Keeping in mind that the error correction term could be positive or negative, the largest allowed pressure perturbation as a result of a mass error correction is:

$$\left|\Delta P_f\right| \leq |x_P \Delta P_{TSC}| \tag{5}$$

where ΔP_f is the maximum pressure change allowed by adding the mass error correction term, ΔP_{TSC} is the maximum change in pressure allowed without causing the time step controller to decrease the time step, and x_P is the pressure time controller factor (constant, range: $0 \rightarrow 1$).

Similarly, the largest allowed void fraction perturbation as a result of a mass error correction is:

$$\Delta \alpha_g \leq \max[x_\alpha \Delta \alpha_{TSC}, \Delta \alpha_g(\text{fill})] \tag{6}$$

if the node is being filled, and

$$-\Delta \alpha_g \geq \min[-x_\alpha \Delta \alpha_{TSC}, -\Delta \alpha_g(\text{empty})] \tag{7}$$

if the node is being emptied, where $\Delta \alpha_g$ is the maximum void fraction change allowed on adding the mass error correction term, $\Delta \alpha_{TSC}$ is the maximum change in void fraction allowed without causing the time step controller to decrease the time step, x_α is the void fraction time controller factor (constant, range: $0 \rightarrow 1$), and $\Delta \alpha_g$(fill/empty) is the change in void fraction needed to fill or empty the node respectively.

The constant factors x_P and x_α are both set to 0.5. In other words, the values of ΔP_f and $\Delta \alpha_g$ are allowed to come to within a factor of 0.5 of reducing time step through changes in pressure and void fraction respectively, as estimated by equations (3) and (4).

The algorithm implemented in CATHENA also accounts for combinations of Equations (5) and (6) or (7). For example, the addition of the mass conservation error term could fill the node by displacing the last bit of void within the limits allowed by Equation (6), and then continue to overpressurize it within the limits allowed by Equation (5).

3.2 Application of Mass Error Correction Term

If the node will not overfill, the entire mass error correction term for the thermalhydraulic node being examined is applied back into the node. If the node might overfill, as much of the mass error correction term as possible is applied to the node. Any liquid mass that cannot be added back into the present node within the limits allowed by Equations (5) through (7) is saved for possible later re-distribution.

3.3 Fill and Drain Limits

As shown in Figure 2, after the mass correction error term has been applied to the maximum extent possible in the present node, a calculation is made using Equations (3) through (7) to determine how much more could be filled or drained from this node without disturbing the time step controller. These upper and lower limits are saved for use by the redistribution algorithm.

3.4 Mass Redistribution

Once an attempt has been made to apply the mass error correction term to all nodes, a check is made to determine if mass redistribution is required. If it was not possible to add the full mass error correction term back into any one of the original nodes without anticipating a pressure excursion, an attempt is made to redistribute this mass into neighbouring nodes.

The algorithm only allows mass to be redistributed into immediately adjacent nodes. In cases where two or more nodes are attached to a node, preference is given to nodes that have two-phase. If a neighbouring node is a boundary condition, all of the remaining mass is assumed to be redistributed to this node. A check is also made to ensure none of the links attaching neighbouring nodes are closed due to the presence of large resistances (k's) or closed valves. All redistributions are subject to the fill and drain limits previously calculated to avoid potential perturbation of the timestep controller.

3.5 Residual Mass Error Correction Term

Finally, as shown in Figure 2, a mass error correction term may still remain which cannot be distributed to the immediately adjacent nodes. This residue is placed back in the originating node, regardless of the limits established by Equations (3) through (7).

4 TEST OF MASS CONSERVATION ALGORITHM

To test the revised mass conservation algorithm, a test problem was needed that involved potentially violent phenomena. A simulation of such a test problem may spend a significant fraction of its time at the minimum time step, and result in a large number of `re-do`s. Using the previous mass conservation strategy, a potentially significant mass error could accumulated as the mass error correction terms are neglected at the minimum time steps and during `re-do`. The revised mass conservation algorithm should correct this mass error.

A test problem that fits these requirements is a hot horizontal tube refill experiment [2]. Figure 3 shows a schematic of the experimental facility. A horizontal pipe was electrically heated, and subsequently cooled through the introduction of highly subcooled liquid from one end of the pipe. A CATHENA model of this experiment was constructed. The condensation and subcooled boiling phenomena experienced in the experiment tend to frequently drive the simulation down to the minimum time step, and rapid changes in void fraction, pressure, and phase enthalpies cause frequent `re-do`s to occur. CATHENA calculate models were used to determine the relative mass imbalance incurred by CATHENA as the simulation proceeds. The relative mass imbalance, RMI, is expressed as:

$$RMI = \frac{\Delta M_{CMI}}{M_{TOT}} \tag{8}$$

where ΔM_{CMI} is the cumulative mass imbalance and M_{TOT} is the total mass in the system.

As shown by the solid line in Figure 4, a significant relative mass imbalance was incurred before the implementation of the present mass error correction algorithm. After implementation of the mass error correction algorithm outlined in Section 3, the RMI is reduced by several orders of magnitude. Small momentary residual mass imbalances still occur at isolated points in the simulation as shown by the spikes in the broken line in Figure 4, but they do not accumulate as before. These small residual spikes may be the result of momentary rounding errors in the finite-difference matrix solution or the calculate models used to calculate the actual mass in the system.

5 SUMMARY AND CONCLUSIONS

Prior to CATHENA MOD-3.5b/Rev 0, mass was not strictly conserved during `re-do` and at minimum timestep size, potentially leading to errors in fluid inventory during a simulation. A revised mass conservation error correction algorithm has been successfully implemented in CATHENA. Mass is now conserved at all times, and a redistribution strategy to nearest neighbouring nodes has been implemented to ensure numerical stability during simulations containing rapidly varying conditions. As shown by the test results, the major source of mass conservation error has been corrected. Some residual mass error remains, possibly as a result of numerical rounding errors in the matrix solution or the calculate models. These residual errors are negligible however, and do not accumulate.

ACKNOWLEDGEMENTS

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REFERENCES

1. B.N. Hanna, “CATHENA: A thermalhydraulic code for CANDU analysis”, Nuclear Engineering and Design, 180 (1998) 113-131. 1
2. A. Abdul-Razzak, A.M.C. Chan, and M. Shoukri, "Rewetting of Hot Horizontal Tubes", Nuclear Engineering and Design, 138 (1992) 375–388. 7

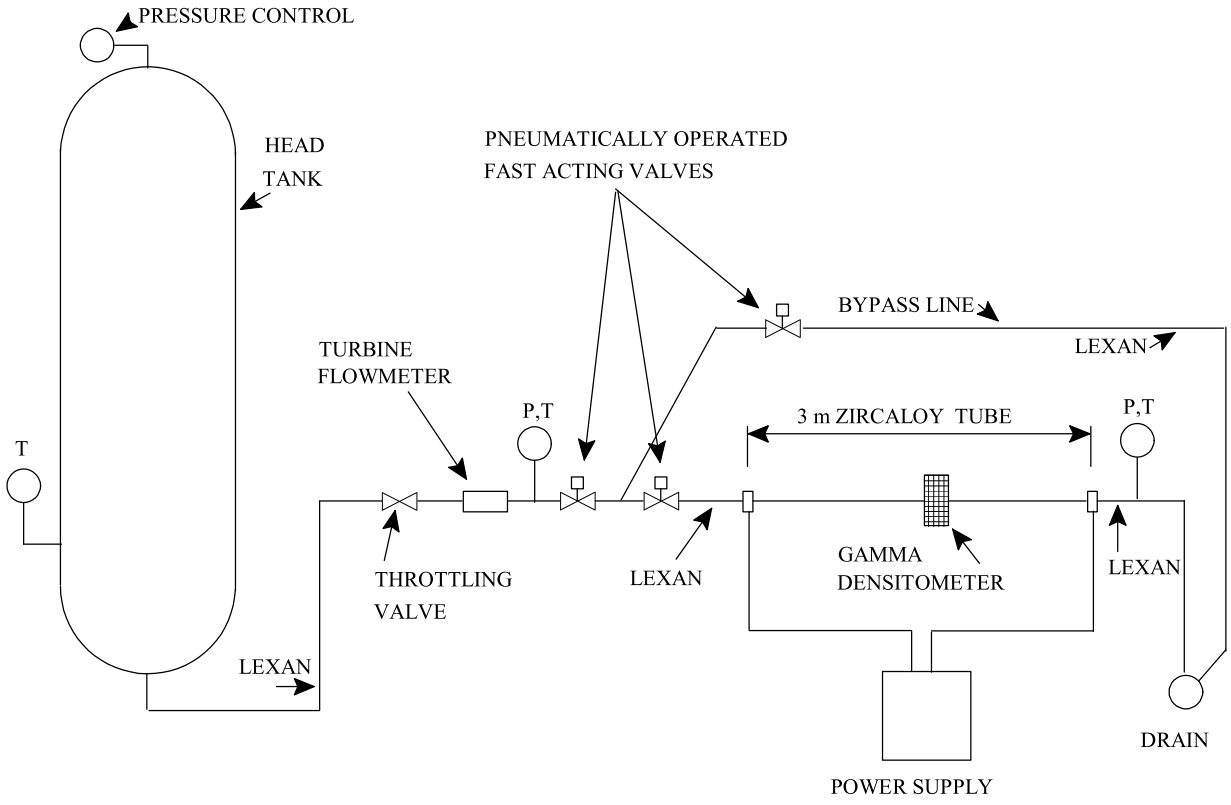

FIGURE 3: Schematic of Refill Test Loop.

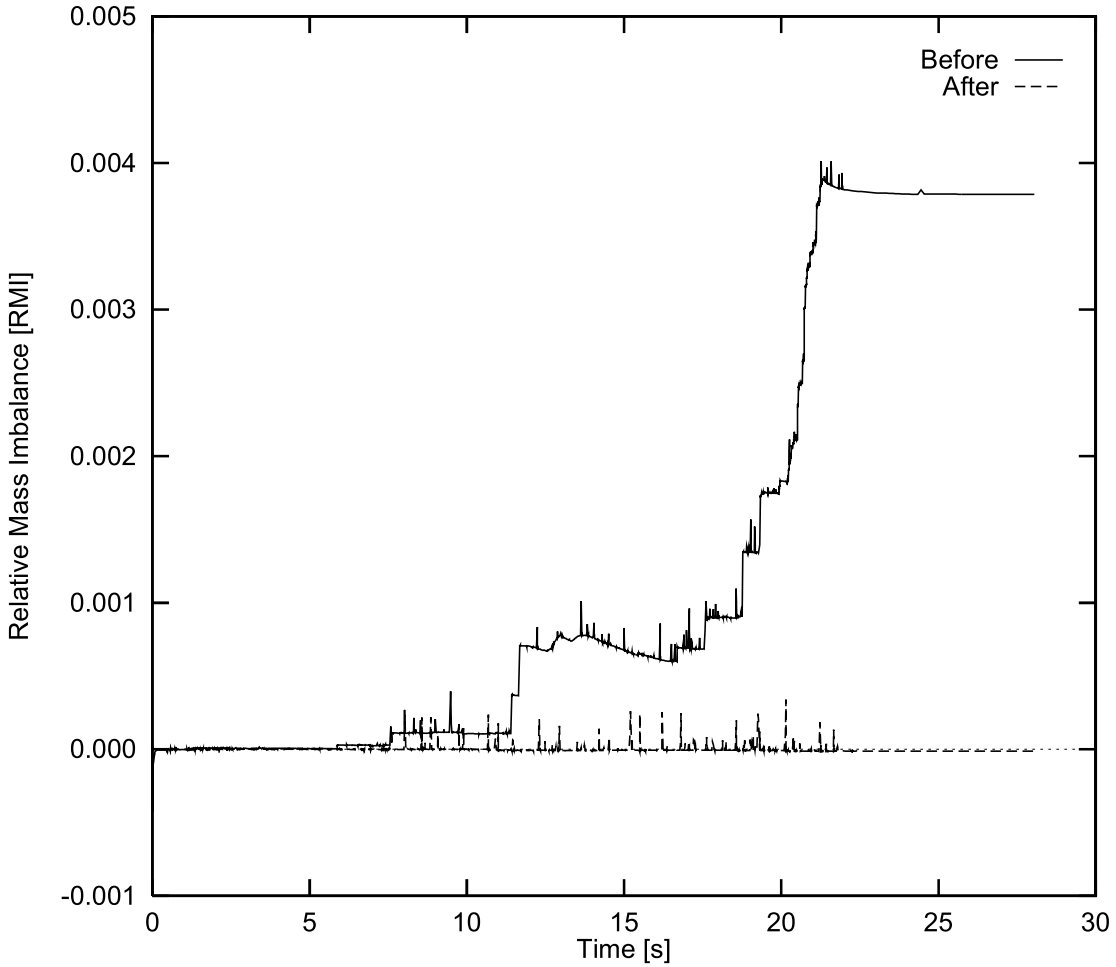

FIGURE 4: Mass Imbalance, Before and After Implementation of New Mass Conservation Error Correction Algorithm.