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# Performance Comparison of Higher-Order Numerical Schemes Applied to 1D Thermal-Hydraulic System Analysis Code

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## 1. Introduction

For the realistic thermal-hydraulic analysis of nuclear reactor systems and the Korean regulatory activity, MARS (Multi-dimensional Analysis of Reactor Safety) code has been developed as a best-estimate code. In MARS code, the governing equations are based on the two-phase two-field model (continuous liquid and vapor). So, the governing equations consist of two phasic continuity equations, two phasic momentum equations, two phasic energy equations and a continuity equation of non-condensable gases. These governing equations are discretized using the first-order semi-implicit scheme.

Furthermore, the existing nuclear system analysis codes such as RELAP5, COBRA-TF, TRAC, MARS and SPACE use the first-order numerical scheme in both space and time discretization. However, the first-order scheme is highly diffusive and less accurate due to the first order of truncation error. So, the numerical diffusion problem which make the gradients to be smooth in the regions where the gradients should be high can occur during the analysis, which often predicts less conservatively than the reality. So, the second-order scheme is more accurate than the first-order scheme if the same number of meshes are used. Therefore, the first-order scheme is not always desirable in many applications of nuclear system analysis. For instance, during an accident condition, the pressure of a reactor system can fluctuate dramatically. This may result in the peak cladding temperature dramatic increase due to strong heat transfer between coolant and structures, since quick flashing or condensation may occur which are the results of pressure fluctuation [1]. Therefore, the nuclear system analysis code needs high predictive capability.

For this study, the in-house code has been developed for application of the higher-order numerical schemes on 1D thermal-hydraulic system analysis code. Using this code, performance of higher-order numerical scheme is evaluated in terms of accuracy and stability.

## 2. Methods & Results

For this study, MARS code will be used as the reference code to identify the numerical diffusion problem which can arise in the first-order scheme. The higher-order scheme will be also tested for the numerical diffusion and dispersion problems as well. A single phase transient analysis code which is possible to calculate in the first-order and the higher-order scheme but mimics MARS solver is built in MATLAB environment. Fig. 1 shows algorithm of single-phase transient analysis code. The 1st and 2nd order backward Euler schemes are implemented as the temporal discretization. As the spatial discretization, the 1st and 2nd order upwind schemes, centered differencing scheme and Lax-Wendroff scheme are implemented to evaluate the accuracy, the numerical diffusion issues and stability. In this study, all of test cases are limited in single-phase flow to see only the effect of the numerical scheme only. Under the two phase flow condition, various models and correlations such as the wall/interfacial heat transfer coefficient and the wall/interfacial friction coefficient are determined by the flow regime. So, these coefficients are not smooth between different flow regimes sometime. This can generate noise and instability in the code results, which makes it challenging to observe numerical scheme effect alone. By using this code, this study will be conducted to evaluate effect of numerical diffusion and dispersion problems and to identify the accuracy improvement and the change of the stability criterion in system analysis code through a simple pipe flow simulation.

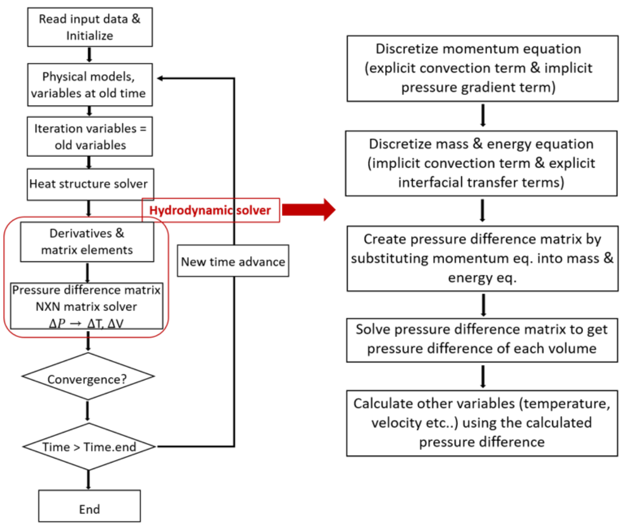


Fig. 1. Algorithm of single phase transient analysis code

### *2.1 Numerical Tests*

A single phase pipe flow with a sine pulse of temperature is modeled by MARS and the NTS codes separately and the results are compared to each other. Fig. 2 shows the configuration of single phase pipe flow with a sine pulse of temperature. In this test, the fluid flows at 1m/s through the pipe with cross sectional area of 0.5m$^2$ and 20m in length. The initial temperature and pressure of the fluid is 300K and 101,325Pa, respectively. The temperature of the injected fluid is changed with time as shown in Fig. 3. The pulse width is 5sec and the interval is 1.5 sec. This simulation is performed for several numbers of meshes to compare MARS with the NTS code. A sensitivity test for other higher-order scheme is conducted. Table 1 shows the higher-order numerical schemes used for the sensitivity tests.

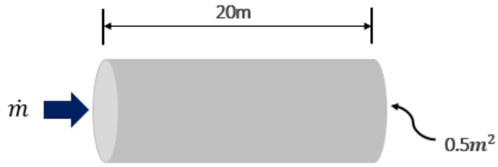


Fig. 2. Configuration of single phase pipe flow with sine pulse of temperature

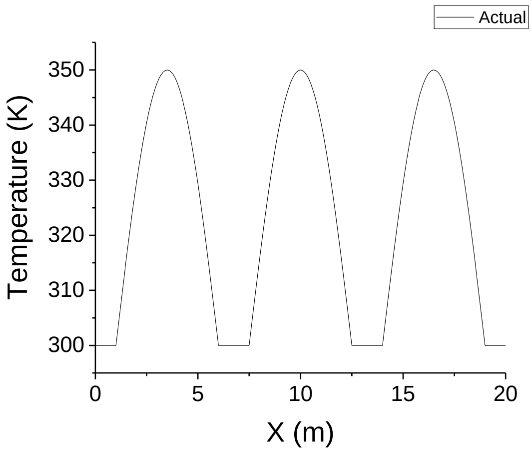


Fig. 3. Temperature profile of fluid injected at pipe inlet

Table I: Higher-order Numerical Schemes for Sensitivity Tests

| Temporal scheme | Spatial scheme |
|---|---|
| 1st order backward Euler scheme | 1st order upwind scheme |
| | 2nd order upwind scheme |
| 2nd order backward Euler scheme | Centered differencing scheme |
| | Lax-Wendroff scheme |

*2.2 Results*

Figs. 4-6 show the results of higher-order numerical schemes for sensitivity. The mesh size and the time step is 0.5m and 0.01sec, respectively. Fig. 4 shows the comparison of the 1st order and 2nd order spatial schemes when the 1st order temporal scheme is fixed. In the 1st order spatial scheme, the temperature profile is deteriorated due to the numerical diffusion. However, the accuracy is improved in the 2nd order spatial scheme as shown in Fig. 4. Figs. 5 and 6 show the comparison of the 1st order and 2nd order temporal schemes when the 1st order or 2nd order spatial numerical scheme is fixed. In this case, the improvement of accuracy is not expected when the temporal scheme is higher order. However, the temperature below 300K or above 350K is predicted locally in the 2nd order numerical scheme. Since the input temperature range is 300 to 350K, it is impossible to predict the temperature below 300K or above 350K. To compare quantitatively these results in terms of the accuracy, $R^2$-value for each numerical schemes is calculated. These results are indicated in Table II. The 1st order temporal scheme and 2nd order Lax-Wendroff scheme shows the best accuracy as shown in Table II.

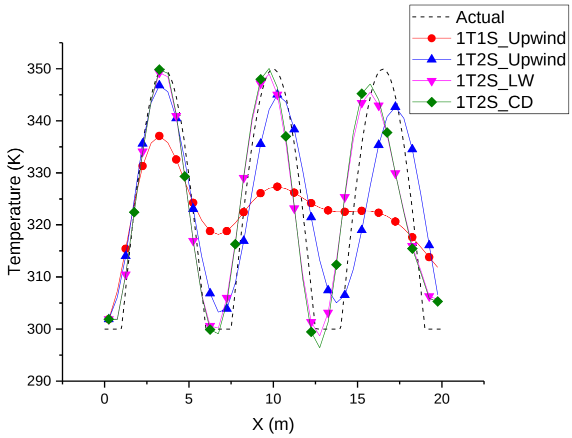


Fig. 4. Sensitivity results of the spatial numerical schemes

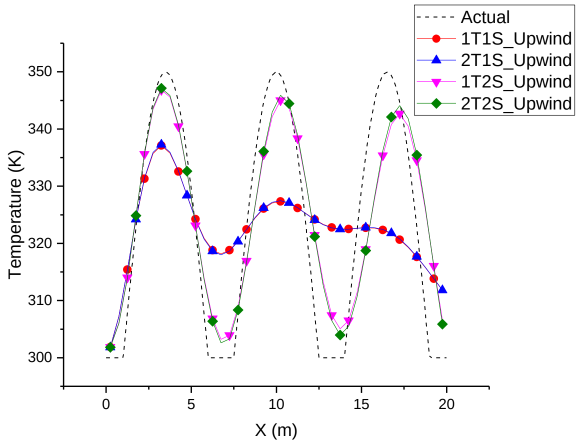


Fig. 5. Sensitivity results of the temporal numerical schemes for the 1st order or 2nd order upwind scheme

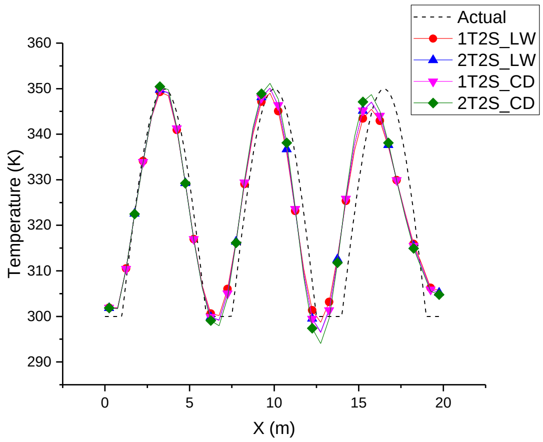


Fig. 6. Sensitivity results of the temporal numerical schemes for Lax-Wendroff(LW) or centered differencing(CD) scheme

Table II: $R^2$-value for each numerical schemes

| | 1T1S Upwind | 2T1S Upwind | 1T2S Upwind | 2T2S Upwind |
|---|---|---|---|---|
| $R^2$ | 0.911 | 0.906 | 0.993 | 0.996 |
| | 1T2S LW | 2T2S LW | 1T2S CD | 2T2S CD |
| $R^2$ | 0.997 | 0.995 | 0.993 | 0.973 |

LW is Lax-Wendroff scheme, CD is centered differencing scheme and 1T1S means the 1st order temporal and 1st order spatial scheme. Based on this rule, legends '2T1S' and '2T2S' are designated to indicate different numerical schemes.

To evaluate the stability of each numerical scheme, the maximum Courant number is compared in Table III. The maximum Courant number is decreased when the only temporal scheme is advanced as shown in Table III. In case of 1T2S LW, the maximum Courant number is similar to 1T1S Upwind. Therefore, 1T2S LW case is the best in terms of the numerical stability.

In this case, when the temporal scheme is higher order, the accuracy is not improved and the stability is reduced. To identify this problem, the theoretical stability is calculated by the Lax analysis, which is the practical method to calculate the stability of numerical scheme. In this problem, the velocity and pressure is constant. So, since this case is the same with solving only the energy equation, the Lax analysis is applied to the energy equation.

$$\frac{\partial}{\partial t}(\rho_k U_k) + \frac{1}{A}\frac{\partial}{\partial x}(\rho_k U_k v_k A) = -\frac{P}{A}\frac{\partial}{\partial x}(v_k A) + Q_{wk} + DISS_k \quad (1)$$

where ρ, U, A, v, P are density, internal energy, flow area and velocity, $Q_w$ is wall heat transfer rate and DISS is the dissipation term.

Equation (1) is the energy equation using the single phase transient analysis code. This equation is simply discretized using the 1st order and 2nd order temporal scheme with the spatial scheme like equation (2) and (3).

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + \frac{< f^n u^{n+1} >_{i+1/2} - < f^n u^{n+1} >_{i-1/2}}{\Delta x} = R_i^n \quad (2)$$

$$\frac{1}{\Delta t}\left(\frac{3}{2} f_i^{n+1} - 2 f_i^n + \frac{1}{2} f_i^{n-1}\right) + \frac{< f^n u^{n+1} >_{i+1/2} - < f^n u^{n+1} >_{i-1/2}}{\Delta x} = R_i^n \quad (3)$$

where f = $\rho_k U_k$. The angle brackets denote the fluxes for each spatial scheme. These discretized equations are rearranged like equation (4).

$$f_i^{n+1} = a_i f_{i-1}^n + b_i f_i^n + c_i f_{i+1}^n + R_i^n \quad (4)$$

where $a_i$, $a_i$ and $a_i$ are expressed by the Courant number. Then, for all the node,

$$F^{n+1} = A_N F^n + R_N \quad (5)$$

where

$$F^n = \begin{pmatrix} f_1^n \\ f_2^n \\ f_3^n \\ \vdots \\ f_N^n \end{pmatrix},$$

$$A_N = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ a_1 & b_1 & c_1 & \cdots & \cdots & 0 \\ 0 & a_2 & b_2 & c_2 & \cdots & 0 \\ 0 & \cdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & a_{N-2} & b_{N-2} & c_{N-2} \\ 0 & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix}$$

From the Lax analysis, ‖ $A_N$ ‖ implies the stability criterion. Thus, in the 1st order temporal and 1st order upwind scheme, the maximum Courant number, which is the stability criterion, is 1 as shown in Table III. However, in the 2nd order temporal scheme which is equation (3), the coefficient of $f_i^{n+1}$ is 3/2. Compared to the 1st order temporal scheme, the inverse of this coefficient is multiplied to equation (4). Therefore, ‖ $A_N$ ‖ is 2/3 in the 2nd order temporal scheme as shown in 2T1S Upwind of Table III. The more detail discussion will be presented during the conference.

Table III: Maximum Courant number for each numerical schemes

| No. node | 1T1S Upwind | 2T1S Upwind | 1T2S Upwind | 2T2S Upwind |
|---|---|---|---|---|
| 20 | 0.9987 | 0.7786 | 0.2989 | 0.1599 |
| 40 | 1.0197 | 0.6198 | 0.2599 | 0.1200 |
| 80 | 0.9999 | 0.5999 | 0.2400 | 0.1280 |
| Average | 1.0061 | 0.6661 | 0.2633 | 0.1360 |

| No. node | 1T2S LW | 2T2S LW | 1T2S CD | 2T2S CD |
|---|---|---|---|---|
| 20 | 0.9968 | 0.4596 | 0.2302 | 0.1201 |
| 40 | 0.9997 | 0.1700 | 0.1420 | 0.0760 |
| 80 | 0.9999 | 0.1560 | 0.1200 | 0.0600 |
| Average | 0.9998 | 0.2619 | 0.1641 | 0.0854 |

## 3. Conclusions

This study evaluated the feasibility of the higher-order numerical scheme for the next generation nuclear system analysis code. The accuracy is improved in the 2nd order spatial scheme. However, the numerical stability is decreased and the accuracy is not expected to improve when the only temporal scheme is advanced. Therefore, the 1st order temporal scheme and 2nd order Lax-Wendroff scheme showed the best performance in terms of the accuracy and the numerical stability.

For further research, the dependency of numerical stability on the boundary conditions, initial conditions and geometry will be studied.

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