RELAP5 User Seminar

Sept. 12-14, 2000 Jackson, Wyoming

Flux Limited Upwind Difference Scheme in RELAP5-3D

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1.0 Introduction

RELAP5-3D is a best estimate nuclear safety code under development at the Idaho National Engineering Laboratory on behalf of the Department of Energy and the International RELAP5 User Group (IRUG). The code extends the capabilities of its predecessor, RELAP5/MOD3, by incorporating multi-dimensional thermal-hydraulics and reactor kinetics capabilities. The purpose of this article is to examine the use of advanced numerics in the multi-dimensional thermal-hydraulics of RELAP5/MOD3. It is shown that with the appropriate use of flux limited upwind difference schemes, RELAP5-3D can not only retain the accuracy and stability of flows that are essentially one dimensional but also have the ability of simulating flows that are three dimensional in nature.

2.0 Numerics for One Dimensional Flows

2.1 RELAP5/MOD3 Scheme

RELAP5/MOD3 seeks to satisfy the one-dimensional single-phase continuity equation to the extent possible. For single-phase one-dimensional steady-state flow, the continuity equation is

$$\frac{d}{dx}(\rho A v) = 0 \tag{1}$$

where ρ, A, and v are the density, flow area, and velocity respectively. In this case,

$$\rho(K)A(K)v(K) = \rho(J-1)A(J-1)v(J-1) = \rho(J)A(J)v(J) \tag{2}$$

and

$$\rho(L)A(L)v(L) = \rho(J+1)A(J+1)v(J+1) = \rho(J)A(J)v(J) \tag{3}$$

where K and L are the from and to volumes of the junction J as shown in **Figure 1**.

$$\text{Hence, } v(K) = 0.5\frac{(\rho(J-1)A(J-1)v(J-1) + \rho(J)A(J)v(J))}{\rho(K)A(K)} \tag{4}$$

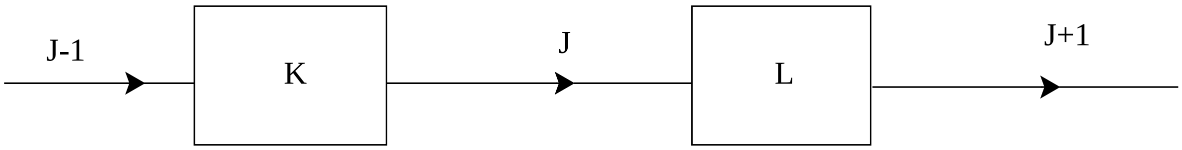

Figure 1 Volume and junction configuration for a single pipe problem

and $$v(L) = 0.5\frac{(\rho(J+1)A(J+1)v(J+1) + \rho(J)A(J)v(J))}{\rho(L)A(L)} \tag{5}$$

By using **(4)** and **(5)** in the following difference formulation of the momentum equation, $$\frac{v^2(L) - v^2(K)}{2\Delta x} = -\frac{1}{\rho}\frac{P(L) - P(K)}{\Delta x} \tag{6}$$

then both the continuity equation and the momentum equation are integrated exactly in the case of single-phase one-dimensional steady-state flows. For stability purposes, the following upwind difference scheme is used

$$\frac{c(J)v(J)v(L) - c(J-1)v(J-1)v(K)}{2\Delta x(J)} = -\frac{1}{\rho}\frac{P(L) - P(K)}{\Delta x(J)} \tag{7}$$

where the area and density ratios c(J) and c(J-1) are chosen so that c(J)v(J) = v(L) and c(J-1)v(J-1) = v(K) for single phase one dimensional steady state flows (i.e. when **(2)** and **(3)** hold), and $\Delta x(J)$ is the mesh size of the control volumed centered at J, or the distance between the centers of volumes K and L.

It should be noted, however, that while the two schemes yield identical results for single phase one dimensional steady state flows, the central differencing scheme shown in **(6)** is more accurate for more general flows. Hence, it is desirable to have a flux limited upwind difference scheme that combines the best features of both schemes. This scheme is discussed in the next section.

2.2 Flux Limited Upwind Differencing Scheme

Assume that v(J) is nonnegative. The scheme for the momentum flux representation for single phase flow is as follows,

$$\phi\frac{(v^2(L) - v^2(K))}{2\Delta x(J)} + (1-\phi)\frac{c(J)v(J)v(L) - c(J-1)v(J-1)v(K)}{2\Delta x(J)} \tag{8}$$

$$\phi = \max(0., \min(s(K)/s(L), s(L)/s(K))) \tag{9}$$

$$s(K) = \frac{\rho(J)A(J)v(J) - \rho(J-1)A(J-1)v(J-1)}{\Delta x(K)} \tag{10}$$

$$s(L) = \frac{\rho(J+1)A(J+1)v(J+1) - \rho(J)A(J)v(J)}{\Delta x(L)} \tag{11}$$

Here $\Delta x(K)$ and $\Delta x(L)$ are the mesh sizes of the volumes K and L respectively. For general two phase flows, the mass flux $\rho A v$ in **(4)**, **(5)**, **(9)**, and **(10)** is replaced by $\alpha\rho A v$ for each phasic momentum equation where α, ρ, and v are the phasic void, density, and velocity in each phase. The flux limiter ϕ is one for linear mass flows and zero for oscillatory massflows. This is motivated by the observation that the central differencing scheme given by **(4)**, **(5)**, and **(6)** already computes the exact solution when $\rho(x)A(x)v(x)$ is a linear function in x. Hence, there is no need to use the upwind scheme in this case. The more nonlinear the mass flow rate is, the more upwinding is used in the scheme and both stability and accuracy are achieved by a compact and easy to use scheme. This scheme will be called the R5 flux limited upwind scheme. It is available only for the semi-implicit scheme of RELAP5-3D as an option to the user. The default scheme is still the RELAP5/MOD3 scheme. The scheme is not needed for the nearly implicit scheme since central differencing applied implicitly is stable and is therefore the default scheme in the general release version of the code.

3.0 Numerics for Multi-Dimensional Flows

In three dimensional flows, the momentum flux in the momentum equations has more terms than in the one dimensional case. For example, The momentum flux in cylindrical coordinates in the radial direction is

$$\rho\left(v_r\frac{\partial v_r}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta} + v_z\frac{\partial v_r}{\partial z} - \frac{v_\theta^2}{r}\right) \qquad (12)$$

The purpose of this article is to examine the use of the flux limited upwind scheme

for the normal derivatives in each coordinate direction, i.e. $v_r\frac{\partial v_r}{\partial r}$

in the radial direction in the radial momentum equation and $v_z\frac{\partial v_z}{\partial z}$ in the z direction in the z momentum equation and so on.

The cross derivative terms are computed by very simple upwind differencing schemes. We note that because the path of integration for the radial momentum equation for example is in the radial direction while the differencing is in the z or azimuthal directions, highly accurate results cannot be obtained by accurate representation of the cross derivative alone. More accurate integration formulas involving the use of variables at points that are not immediate neighbors of the mesh point P where the derivatives are evaluated, Reference **1**, have to be used. They will be examined in a later work.

3.1 Flux Limited Upwind Differencing Scheme

The R5 flux limited upwind scheme is used in all coordinate directions in cartesian coordinates and in the z and azimuthal directions in cylindrical coordinates to compute the normal derivatives in the momentum equations. It is available only for the semi-implicit scheme of RELAP5-3D as an option to the user. The default scheme is the RELAP5/MOD3 scheme. It is not needed for the nearly implicit scheme since the central differncing scheme there is stable and is the default scheme for the IRUG version. It's not used in the radial direction in cylindrical coordinates because the development of R5 flux limited upwind scheme assumes that the flow in the radial direction is hyperbolic, i.e. velocity is proportional to 1/r, where r is the distance to the origin. The volume average velocities v(K) and v(L) given by **(4)** and **(5)** are overweighted by the velocity at the junction farther away from the center regardless of the direction of the flow. This is undesirable since in general the flow field in the radial direction does not have a singularity in the origin or center of the cylinder and can be approximated by a linear or a parabolic function. Hence, a simpler scheme based on the classical first order upwind difference scheme is used in the radial direction except when there is a drain hole in the center in which case the R5 flux limited scheme is used.

3.2 Special Formulation for Flow in the Radial Direction

The following formulation is used in the radial direction in cylindrical coordinates.

$$\phi\frac{(v^2(L) - v^2(K))}{2\Delta x(J)} + (1-\phi)\frac{v(J)(v(J) - v(J-1))}{\Delta x(K)} \tag{13}$$

$$\phi = \max(0.(\min(s(K)/s(L), s(L)/s(K)))) \tag{14}$$

$$s(K) = \frac{v(J) - v(J-1)}{\Delta x(K)} \tag{15}$$

$$s(L) = \frac{v(J+1) - v(J)}{\Delta x(L)} \tag{16}$$

Here v(K) and v(L) are the classical volume centered velocities, i.e.

$$v(K) = \frac{v(J) + v(J-1)}{2} \tag{17}$$

$$v(L) = \frac{v(J) + v(J+1)}{2} \tag{18}$$

and the flux limited scheme is a linear combination of the classical first order upwind differencing scheme and second order central differencing scheme. A similar scheme was used in References **2** and **3**. The main difference is that a symmetric flux limiter is used here while References **2** and **3** used a nonsymmetric limiter.

This scheme will be called the classical flux limited upwind scheme.

4.0 Stability of the Flux Limited Upwind Scheme

The scheme is stable because of the following considerations. If the solution is a linear function, the scheme is obviously stable because it reproduces the exact solution. If instead the solution is oscillatory, i.e. the slope of the solution changes sign within the [J-1, J+1] interval, then the upwind scheme is used and the scheme is again stable. Hence, we need only to consider the case when the slope of a non-linear solution does not change sign within the [J-1, J+1] interval.

We examine the behavior of a mesh solution function of unit magnitude in this case. The mesh solution function can be written as a linear combination of a linear mesh function and an oscillatory one, i.e.

$$f(x) = g(x) + \alpha h(x) \tag{19}$$

where g(x) is a linear mesh function and h(x) is an oscillatory mesh function that is zero at the junctions J-1 and J+1 and 1 at the junction J as shown in **Figure 2**. The graph of the mesh solution function f(x) consists of the line segments AP and PB in the intervals [J-1, J] and [J, J+1] respectively. The graph of the linear mesh function g(x) consists of the line segments AQ and QB in the intervals [J-1, J] and [J, J+1] respectively. Because the mesh function is of unit magnitude, the y coordinate of the point B is one.

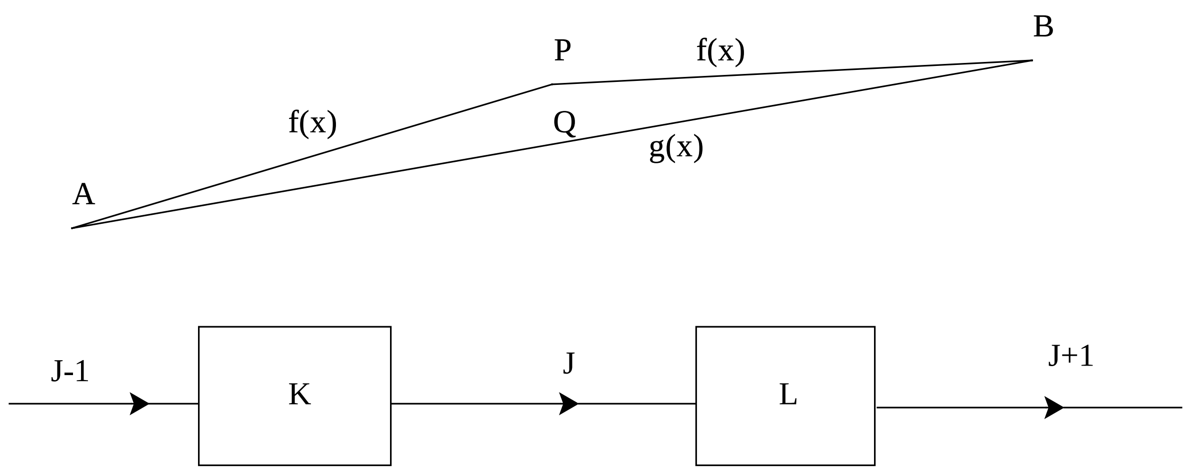

Figure 2 Representation of a nonlinear mesh function in the interval

The point N in **Figure 3** has the same x coordinate as the points P and Q and the same y coordinate as the point A. The points M and R have the same x coordinate as the point B and the same y coordinates as the points P and Q respectively. Let L(XY) denote the length of the line segment XY. Then the oscillatory ratio α in **(19)** is equal to L(PQ). Assume that the mesh spacing is uniform, i.e. L(PM) = L(AN). Then the flux limiter ϕ is given by ratio of the slopes L(BM)/L(PM) to

L(PN)/L(AN) and it is equal to L(BM)/L(PN). The upwind weighting factor 1 - ϕ is given by ratio of L(PN)-L(BM) to L(PN). Noting thatL(QN) = L(BR) by congruent triangles, we have L(PN) - L(BM) = L(PQ) + L(QN) - (L(BR) - L(PQ)) = 2L(PQ) + L(QN) - L(BR) = 2L(PQ). Hence, the upwind to central differencing ratio 1 - ϕ / ϕ is given by 2L(PQ)/L(BM). Because L(BM) is always less than or equal to two (the y coordinate of B is one while that of M is between minus one and one), this ratio is always bigger than or equal to α, the oscillatory ratio. Hence, the scheme is stable since with the exception of the linear case, it is always overweighted in the upwind scheme than is absolutely necessary. The more nonlinear the mesh solution function is, the more overweighted in the upwind scheme the flux limited scheme is. This enables the scheme to be both accurate and robust.

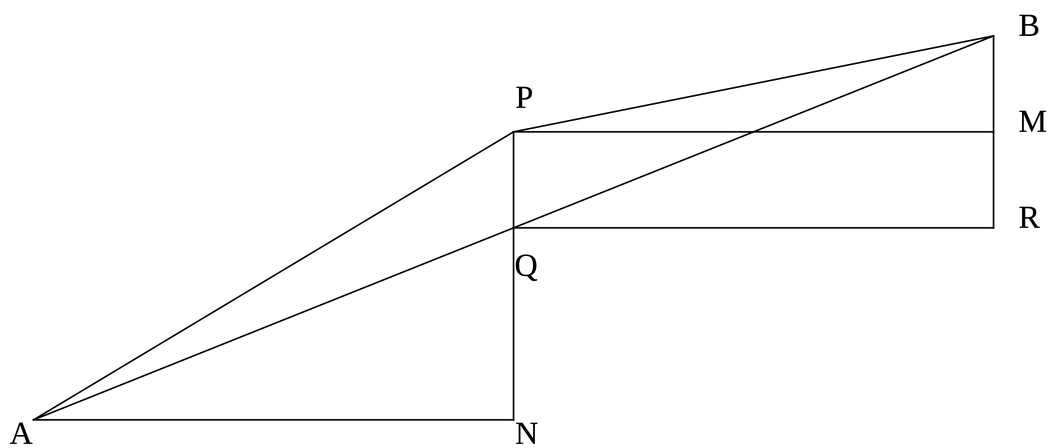

Figure 3 Auxilliary diagram for the stability proof

5.0 Test Results

5.1 Test Results for the One Dimensional Radial Flow Problem

This problem is used to compare the accuracy of the following three schemes, the classical first order upwind differencing scheme and the two flux limited upwind differencing schemes on a very simple one dimensional problem. The problem is actually cast as a three dimensional problem. It has only one three dimensional component that has six azimuthal sectors, one axial level, and either three or eight radial rings and a hole in the center. In the three radial rings case e.g., each azimuthal sector has three radial volumes with the first volume being the innermost ring and the third volume the outermost volume. The first volume is connected to a time dependent volume in the center via a single junction. Pressure and temperature are prescribed at the time dependent volume. The third volume is connected to a time dependent volume via a time dependent junction where velocity is prescribed. Hence, the three dimensional problem is actually a collection of six separate single phase one dimensional problems where a pressure of 5.0e5 Pa is prescribed at the outlet but velocity at 0.8667 m/s is prescribed at the inlet for all the six 1D problems. The volume centered pressures are plotted in **Figure 4**.

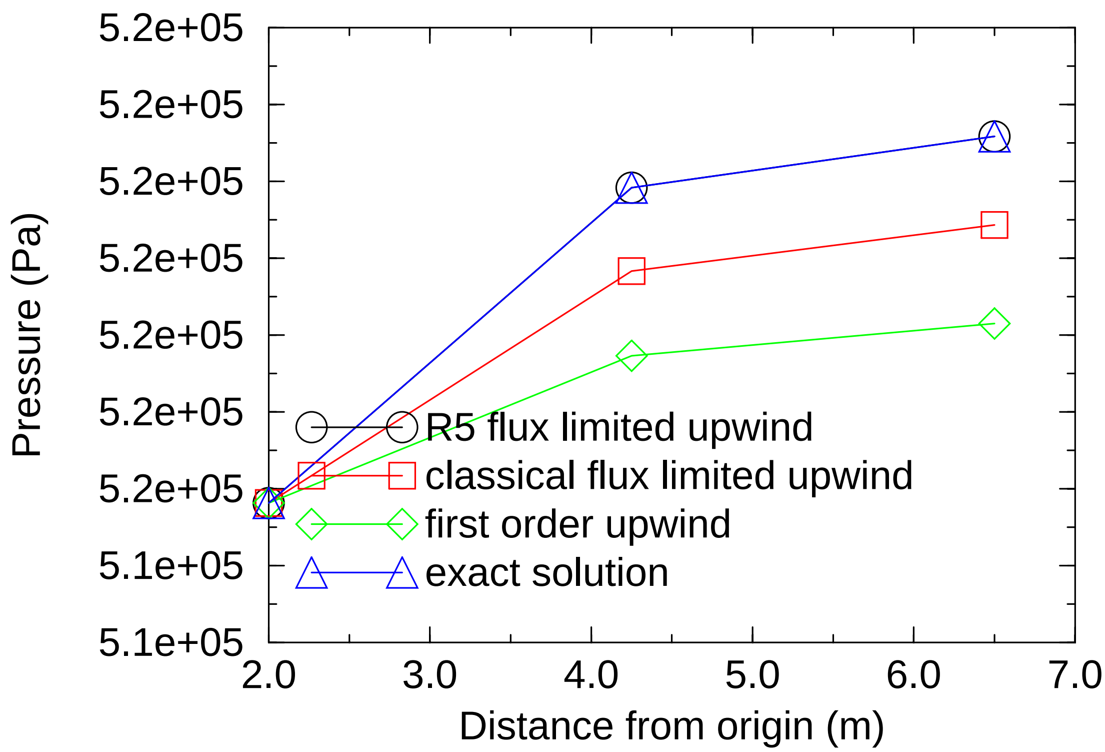

Figure 4 Comparison of the accuracy of three difference schemes for the radial flow problem

Because the flow is strictly one dimensional, the R5 gives the exact solution whereas the classical first order upwind scheme is the least accurate since it's only of first order accuracy.

5.2 Test Results for flow through a cylindrical wedge from the bottom

This is a very simple problem designed to test whether the numerical schemes allow a steady flow through a cylindrical wedge shaped region to be held steady at all time. The flow is forced from the bottom to go up a three dimensional cylindrical region modeled as a three dimensional component in cylindrical coordinates. The flow is kept steady so that in principle all three difference schemes considered in the last section should yield identical results.

Instead it is found that only the two flux limited upwind schemes give the correct results. The first order upwind differencing is not accurate enough to force the velocities to satisfy the continuity equation and eventually the flow spins up in the radial direction. This is further evidence that the flux limited schemes are stable.

5.3 Thermally Stratified Flow in a Horizontal Pipe

In this test problem, subcooled water at 430 K are forced into the left end of a horizontal pipe modeled as a 3D component that originally was filled with warm water at 470 K. The cylindrical pipe is 7m in diameter and 9 m in height. While the warm water was forced to the right, the flow also becomes thermally stratified. This 3D effect is captured by the RELAP5-3D code although no comparison to the data is made here. The result are given in **Figure 5**.

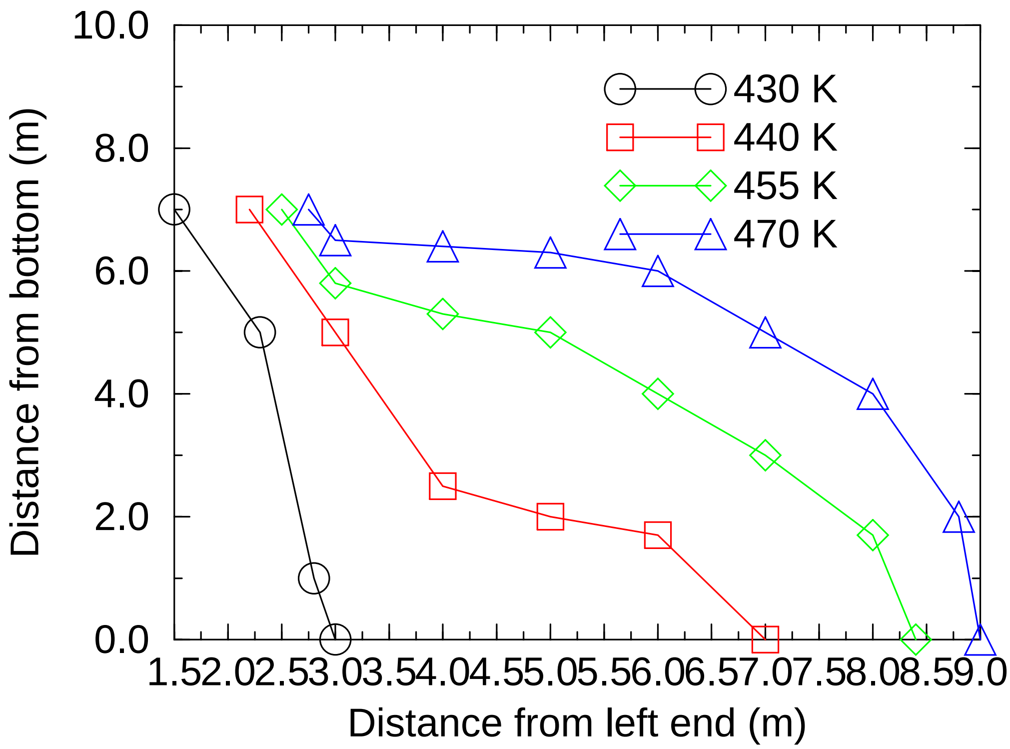

Figure 5 Comparison of temperatures (K) at different distances from the bottom of a 7 m diameter horizontal cylinder

6.0 References

1 Shieh, A, Bernoulli Corrected Upwind Difference Schemes, Software Design, Implementation, and Verification Document, Idaho National Engineering and Environmental Laboratory, R5M3BET-001, June 1997.

2 Tiselj, I. and Petellin, S., “First and Second Order Accurate Schemes for Two-Fluid Models”, to appear in ASME-Journal of Fluids Engineering.

3 LeVeque, R., “Numerical Methods for Conservation Laws”, Lectures in Mathematics, ETH, Zurich, Birkhauser, Verlag 1992, Basel.