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TITLE: TOWARDS A BETTER HYDRO FOR DYNAMIC MIX CALCULATIONS

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TOWARDS A BETTER HYDRO FOR DYNAMIC MIX CALCULATIONS

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ABSTRACT

A difference equation technique suitable for clean, dynamic mix, and turbulence Lagrangian calculations is shown. This new technique is compared to the standard one for clean one-dimensional calculations of the Noh, Sedov Blast Wave, and Strong Shock Tube test problems, and for a one-dimensional two-phase flow dynamic mix calculation of a modified Noh problem, all test problems involving shocks. The new technique is shown to dramatically reduce the noise in the calculated hydrodynamic quantities of pressure, density, specific internal energy, and Lagrangian interface velocity.

I. INTRODUCTION

Since dynamic mix hydrodynamic calculations typically use a driving term involving the gradient of the pressure, and turbulence calculations depend on gradients of pressure, density and velocity, clearly the less spatial noise there is in a calculation, the more believable are the results. We therefore show in this paper a difference equation technique suitable for clean, dynamic mix, and turbulence calculations, that has a smoothing effect on pressure, density and mean flow velocity. In the next section, we show the effect on clean calculations. In the section following that we extend the technique to mixed problems, and show the effect on a two phase-flow dynamic mix calculation.

All calculations and equations are for one-dimensional Lagrangian hydrodynamics, with an even time difference scheme. For simplicity, all equations-of state (EOS) used in the clean examples are analytic $\gamma = 5/3$ gamma laws, and the mixed example uses a tabular $\gamma = 5/3$ gamma law EOS. The technique, however, is more general and works for any tabular or analytic EOS.

II. CLEAN CALCULATIONS

A. The Basic One-Dimensional Lagrangian Difference Equations

Let:

a = acceleration		v = velocity	
P = pressure		r = radius of Lagrangian interface	
Q, AQ = artificial viscosity terms		E = specific internal energy	
A = area		V = zone volume	
m = zone mass		t = time	

subscript i = designator of a boundary-centered quantity, i^{th} interface
subscript i-$\frac{1}{2}$ = designator of a zone-centered quantity, between the $(i\text{-}1)^{th}$ and i^{th} interfaces

Then the basic difference equations are:

$$a_i = -2[(P_{i+1/2} + Q_{i+1/2} - P_{i-1/2} - Q_{i-1/2})A_i + (AQ_{i+1/2} + AQ_{i-1/2})]/(m_{i+1/2} + m_{i-1/2}) \tag{1a}$$

$$dv_i = a_i dt \tag{1b}$$

$$dr_i = v_i dt \tag{1c}$$

$$m_{i-1/2}dE_{i-1/2} = -(P_{i-1/2} + Q_{i-1/2})(\frac{dV}{dt})_{i-1/2}dt + AQ_{i-1/2}(v_i + v_{i-1}) \tag{1d}$$

$$(\frac{dV}{dt})_{i-1/2} = v_i A_i - v_{i-1} A_{i-1} \tag{1e}$$

For the even-time scheme, predictor-corrector form, the times at which the above terms are to be evaluated are illustrated in Fig. 1. First evaluate P, Q, AQ, A at t_n, then calculate a at t_n, then advance v and r to $t_{n+1/2}$, for the predictor step. For the corrector step re-evaluate P, A at $t_{n+1/2}$, calculate a at $t_{n+1/2}$, re-advance v to $t_{n+1/2}$, advance E to t_n, then advance r to t_n, and then advance v to t_n. Note how E, r and v are all advanced from t_n to t_{n+1}, making this an even-time scheme, as opposed to the time-staggered scheme shown in Fig. 2. While the examples in this paper are all calculated with the two-step even-time scheme of Fig. 1, a simpler one-step even time scheme could also have been used.

It is critical, however, just how P^n and $P^{n+1/2}$ (the values at t_n and $t_{n+1/2}$) are evaluated, for use in Eqs. (1a) and (1d). We will now discuss two possibilities, the standard form and the extrapolated (P^*) form.

B. Standard Form

For the even time scheme, standard form, the pressure used in the basic equations is $P = P(\theta, \rho)$ where ρ = density, θ = temperature, so that table look ups (or analytic EOS functions) give

$$P^n = P(\theta^n, \rho^n) \tag{2a}$$

$$P^{n+1/2} = P(\theta^{n+1/2}, \rho^{n+1/2}), \tag{2b}$$

where

$$\theta^{n+1/2} = \theta^n + (\frac{d\theta}{dt})^{n-1/2}(t_{n+1/2} - t_n) \tag{2c}$$

$$\rho^n = m/V^n, \ \rho^{n+1/2} = m/V^{n+1/2} \tag{2d}$$

and with volume V evaluated from r at the specified time. Note that we have dropped the zonal subscript i-1/2.

C. Extrapolated Form (P^*)

For the even-time scheme, extrapolated form, we use a different assumption, namely

$$P^n = P^{n+1/2} = P^* \tag{3}$$

in the basic Eqs. (1a) through (1e), to advance all quantities from t_n to t_{n+1}, where P^n, $P^{n+\frac{1}{2}}$ correspond to Fig. 1, and where P^* is the pressure extrapolated from t_n to t_{n+1} using Eqs. (4a)-(4e):

$$E^{n+1} - E^n = -(P^n + P^*)(V^{n+1} - V^n)/2m \tag{4a}$$

$$P^* - P^n = (\gamma - 1)m(E^{n+1}/V^{n+1} - E^n/V^n) \tag{4b}$$

$$\Delta = 1 - (\gamma - 1)\rho E^n/P^n \tag{4c}$$

$$V^{n+1} = V^n + (\frac{dV}{dt})^n(t_{n+1} - t_n) \tag{4d}$$

$$\gamma - 1 = (\frac{\partial P^n}{\partial \theta})_\rho/\rho(\frac{\partial E^n}{\partial \theta})_\rho \tag{4e}$$

where the subscript i-1/2 applies to all quantities. Note that Eq. (4a) is the Hugoniot relation across a shock.

Note also that γ corresponds to the standard specific heat ratio γ of a gamma law equation-of-state if

$$P = (\gamma - 1)\rho E \tag{5a}$$

$$E = E(\theta) \tag{5b}$$

hold, in which case $\Delta = 0$. However, γ is still defined by Eq. (4e) for more complex or tabular equations-of-state, in which case it may not correspond exactly to the standard specific heat ratio.

Solving Eqs. (4a)-(4e) for P^*, and reinserting the subscript i-1/2,

$$P^*_{i-1/2} = \left\{ P\left[1 - \frac{(\gamma - 1)}{2}\frac{dV}{V} + \Delta\frac{dV}{V}\right] / \left[1 + \frac{(\gamma + 1)}{2}\frac{dV}{V}\right] \right\}^n_{i-1/2} \tag{6a}$$

where

$$(\frac{dV}{V})^n_{i-1/2} = (v^n_i A^n_i - v^n_{i-1} A^n_{i-1})(t_{n+1} - t_n)/V^n_{i-1/2} \tag{6b}$$

Thus P^* is the pressure extrapolated from t_n to t_{n+1}, using quantities evaluated at t_n, the beginning of the time step.

D. Comparison of the Standard and Extrapolated (P^*) Forms

To see the advantage of the extrapolated form (P^*) over the standard form, for even-time hydrodynamics, we look at the results for three standard test problems for which analytic solutions are known. For simplicity, we use analytic $\gamma = 5/3$ gamma-law equations-of-state for these clean calculations, and zero in on the noise in the figures. The only difference between the standard and extrapolated (P^*) calculations is in the replacement of $P^n, P^{n+\frac{1}{2}}$ with P^* for the latter.

1. Noh Problem (See Appendix A). We see in Figure 3(a) that for a given form of artificial viscosity, namely the Von Neumann form, the effect of replacing the standard evaluation of pressure (P^n, $P^{n+1/2}$) with the extrapolated value (P^*) is to smooth out the noise in the density without shifting the curve up or down. The solid line is the analytic solution. Similarly in Fig. 3(b), we see the same effect, this time with a covariant tensor viscosity. This illustrates the fact that the smoothing effect caused by replacing P^n, $P^{n+1/2}$ with P^* is not due to P^* mimicking an addition to the artificial viscosity. An actual change in the artificial viscosity causes the calculated curve to shift, as a comparison of Figs. (3a) and (3b) illustrates. For similar comparisons of pressure, specific internal energy and velocity, see Figs. 4(a) and 4(b), Figs. 5(a) and 5(b), and Figs. 6(a) and 6(b).

2. Sedov Blast Wave Problem (See Appendix B). We now use the covariant tensor artificial viscosity only, and calculate v/v_S, P/P_S, and ρ/ρ_S, all versus R/R_S, where v_S, P_S, ρ_S, and R_S are the analytic solutions of velocity, pressure, density, radius at the shock position. The standard even-time solution (Fig. 7(a)) and the extrapolated (P^*) solution (Fig. 7(b)) can be compared (Fig. 7(c)). Note that when $R/R_S = 1$, the curves should all go through 1 for a perfect calculation. Here again the extrapolated P^* calculation smooths out the calculated curve without shifting it materially.

3. Strong Shock Tube Problem (See Appendix C). Continuing to use the covariant tensor artificial viscosity, we show in Fig. 8 the v, E, ρ, P curves versus R. The solid line is the analytic solution. Here again the extrapolated P^* calculation is much smoother.

III. DYNAMIC MIX CALCULATIONS

A. Extension of Extrapolation Technique to Mixed Zones

Having smoothed out the noise in a clean calculation, we would like to try the technique in a dynamic mix problem, and see what effect the smoothing has on the calculated mixing. However, we shall first need an extension of the extrapolation scheme defined earlier, from a single material to a mixture of materials. So from Eq. (6a) we define

$$\frac{P^*}{P} = f(\gamma, \frac{dV}{V}, \Delta) \quad , \qquad (7a)$$

where

$$f(\gamma, \frac{dV}{V}, \Delta) = \left[1 - \frac{(\gamma-1)}{2}\frac{dV}{V} + \Delta\frac{dV}{V}\right] / \left[1 + \frac{(\gamma+1)}{2}\frac{dV}{V}\right] \tag{7b}$$

Then if we have a mixed zone with two materials in pressure equilibrium, designated by a and b, we have

$$\frac{P^*}{P} = f(\gamma^a, \frac{dV^a}{V^a}, \Delta^a) \tag{8a}$$

$$= f(\gamma^b, \frac{dV^b}{V^b}, \Delta^b) \tag{8b}$$

where

$$V^a + V^b = V \tag{9a}$$

$$dV^a + dV^b = dV \tag{9b}$$

Equations 7 to 9 can then be algebraically manipulated to yield

$$\frac{dV^a}{V^a} = \frac{dV}{V} / [\frac{V^a}{V} + \frac{V^b}{V} g(\gamma^a)/g(\gamma^b)] \tag{10a}$$

where

$$g(\gamma) = \frac{(\gamma+1)}{2}\frac{P^*}{P} + (\frac{\gamma-1}{2}) - \Delta \tag{10b}$$

Since γ^a, γ^b, V^a, V^b, Δ^a, Δ^b, V, dV can all be calculated at time t_n, the unknowns can now be regarded as P^* and dV^a, so that Eqs. (8a) and (10a) can be iterated to solve for P^*, in each zone.

We are now ready to see what effect the smoothing has on the calculated mixing, and shall try it out on a two-phase-flow calculation of dynamic mixing. Since the two-phase flow equations allow both mixing and demixing, and the term driving the interpenetration velocity is linear in the gradient of the pressure, we could guess that the noise in the pressure would cancel out, at least approximately. We shall now test this speculation with another test problem, a modified Noh problem.

B. Comparison of the Standard and Extrapolated (P^*) Forms, for the Modified Noh Problem (See Appendix D).

We now examine the effect of replacing P^n, $P^{n+1/2}$ with P^* for a two-phase-flow dynamic mix calculation of a modified Noh problem. This problem is similar to the Noh problem, with tabular $\gamma = 5/3$ gamma law equations of state used, except that the material is now divided into two regions, with the outer one of density 2, the inner one of density 1. Note that until the shock formed at the origin reaches the interface, the calculations are clean. While we unfortunately do not have an analytic solution for this modified Noh problem, we can still compare the standard even time hydro calculation with the extrapolated even time P^* calculation.

In Fig. 9 we see P, ρ, hmixfr (hmixfr = fraction of zone mass that is the heavier material) as calculated by the two different methods, the standard method and the extrapolated P^* method. Note that while the standard calculation continues to be noisy in pressure, the difference in hmixfr as calculated by the two methods is relatively small, at least for this simple test problem.

IV. CONCLUSION

The use of the P^* extrapolation in the even-time hydro equations decreases the noise present in the standard calculation, for clean test problems involving shocks. Extension of this method to the two-phase-flow dynamic mix even-time hydro equations continues to decrease the noise in pressure, density, and Lagrangian interface velocity. For the two-phase flow problem considered here, there was little sensitivity of the mix distribution to the noise in the calculation. While the examples shown here were for a two-step (predictor-corrector) form of even-time hydro, other calculations with one-step even-time hydro are quite similar.

V. ACKNOWLEDGMENT

The suggestion that the use of the extrapolated pressure P^* would decrease the noise in even-time clean hydrodynamic calculations was made by P. P. Whalen, who has done considerable work on this scheme. He has also extended it to two-dimensional hydrodynamics. The extension of the P^* prescription to mixed zones is the author's work.

APPENDIX A

Spherical Noh Problem

Initial conditions:

- sphere of radius 1.0 m
- 100 equal-spaced zones
- density = 1.0 kg/m^3
- specific internal energy = 10^{-21} J/kg. (We used this small finite value of specific internal energy to avoid zero temperatures.)
- velocity = -1.0 m/s, all zone interfaces

Boundary Condition:

- outer boundary velocity = -1.0 m/s at all times

  The problem was run to 0.6 second, using an analytic $\gamma = 5/3$ gamma-law EOS, hydro only (no heat conduction, no radiation), for four cases:
- Von Neumann artificial viscosity, standard even time hydro
- Von Neumann artificial viscosity, P^* even time hydro
- covariant tensor artificial viscosity, standard even time hydro
- covariant tensor artificial viscosity, P^* even time hydro

Discussion:

We have used

$$Q = \rho\left(1.2\frac{dV}{dt}/A\right)^2$$

for the Von Neumann form[1] of artificial viscosity. For the covariant tensor form of artificial viscosity, $Q_{i+\frac{1}{2}}$, $\Delta Q_{i+\frac{1}{2}}$ correspond to the Q_j, $\Delta Q_j(A_{j+\frac{1}{2}} - A_{j-\frac{1}{2}})/2$

of Eqs. 9′ and 10 on page 318 of Ref. 2. Note that we have set their $C_Q = 1.2^2$ for all zones except the inner one, for which we use $C_Q = 1.2^2/3$, following a recommendation by Ref. 3. The analytic solution to the Noh problem can be found in Ref. 4.

APPENDIX B

Spherical Sedov Blast Wave Problem

Initial conditions:

- sphere of radius 1.2 m
- 120 equal-spaced zones, of thickness .01 m
- density = 1.0 kg/m^3
- specific internal energy of 10^{-21} J/kg in outer 118 zones, and 14727.34 J/kg in inner 2 zones
- velocity = 0., all zone interfaces

Boundary Condition:

- outer boundary velocity = 0. at all times

  The problem was run to 1.0 second, using an analytic $\gamma = 5/3$ gamma-law EOS, hydro only, for two cases:
- covariant tensor artificial viscosity, standard even-time hydro
- covariant tensor artificial viscosity, P^* even-time hydro

Discussion:

For the analytic solution, see Ref. 5 (problem of an intense explosion). For $\gamma = 5/3$, we used a value of λ (as defined in Ref. 5) equal to 1.1517, a number calculated by Ref. 6. We then selected the product of the initial specific internal energy and volume of the central hot spot to be λ^{-5}, so that the analytic solution would go through radius = 1 at time = 1, in the appropriate units. The analytic curves we plot were provided by Ref. 7.

APPENDIX C

Strong Shock Tube Problem

Initial conditions:

- planar geometry
- 30 zones, constant mass ratio of 0.7337, density of 10^3 kg/m^3, specific internal energy of 10^{11} J/kg, r = 0. to 0.03m (Note mass-matching at material interface).
- 60 equal mass zones, density of 1.0 kg/m^3, specific internal energy of 10^5 J/kg, r = 0.03m to 0.09m
- velocity = 0., all zone interfaces

Left and Right Boundary Conditions:

- velocity = 0. at all times

  The problem was run to 6.0 seconds, using analytic $\gamma = 5/3$ gamma law EOS, hydro only, for two cases:
- covariant tensor artificial viscosity, standard even time hydro
- covariant tensor artificial viscosity, P^* even time hydro

Discussion:

The test problem was devised by Ref. 8, and is discussed in Ref. 9, where the analytic solution can be found.

APPENDIX D

Modified Spherical Noh Problem

Initial conditions:

- sphere of radius 1.0 m
- 50 equal-spaced zones, density of 1.0 kg/m^3, specific internal energy of 10^{-21} J/kg, from r=0. to r=0.5 m
- 100 equal-spaced zones, density of 2.0 kg/m^3, specific internal energy of 5.0 $\times$ 10^{-22} J/kg, from r=0.5 m to r=1.0 m (Note mass-matching at material interface.)
- velocity = -1.0 m/s, all zones

Boundary Condition:

- outer boundary velocity = -1.0 m/s at all times.
  The problem was run to 0.6 second, using a tabular γ=5/3 gamma-law EOS, hydro only, with two-phase-flow dynamic mixing, a Newtonian drag force (with a Newtonian drag coefficient of 0.44 and a particle diameter of 3000 microns), for two cases:
- covariant tensor artificial viscosity, standard even-time hydro
- covariant tensor artificial viscosity, P^* even-time hydro

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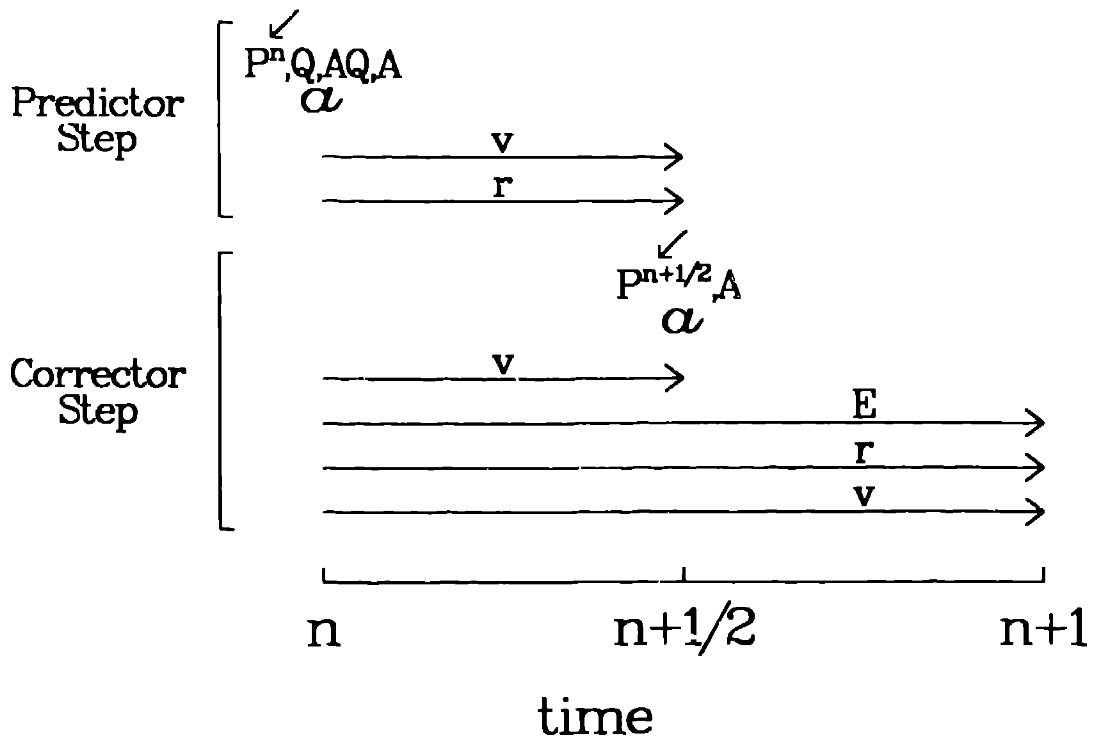

Fig. 1. Predictor-corrector even-time scheme.

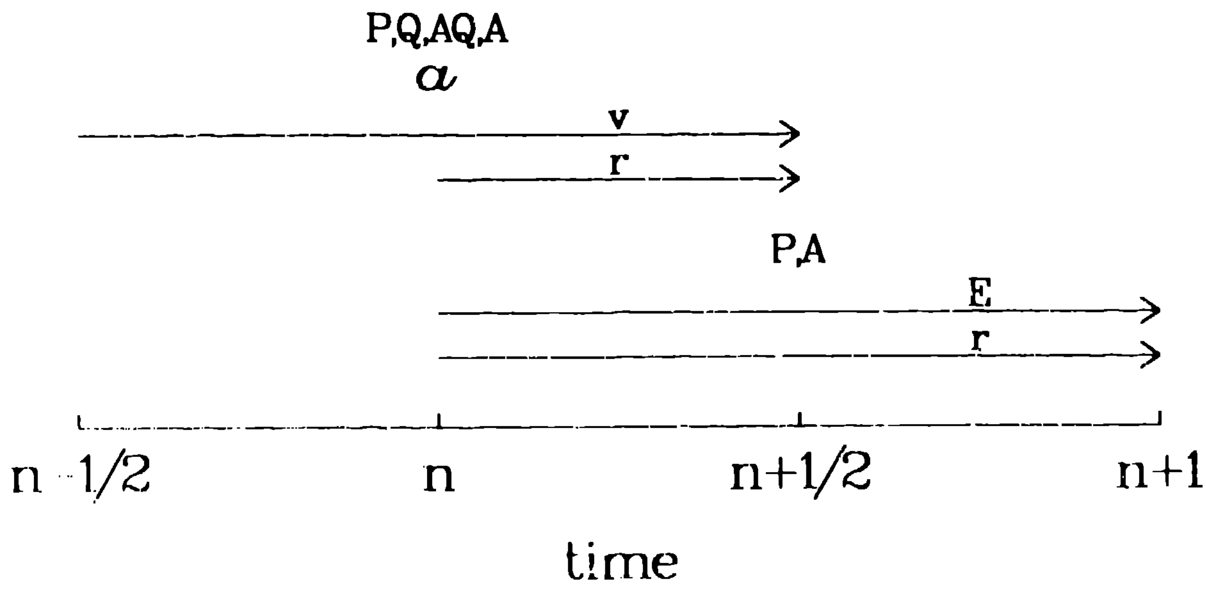

Fig. 2. Time staggered scheme.

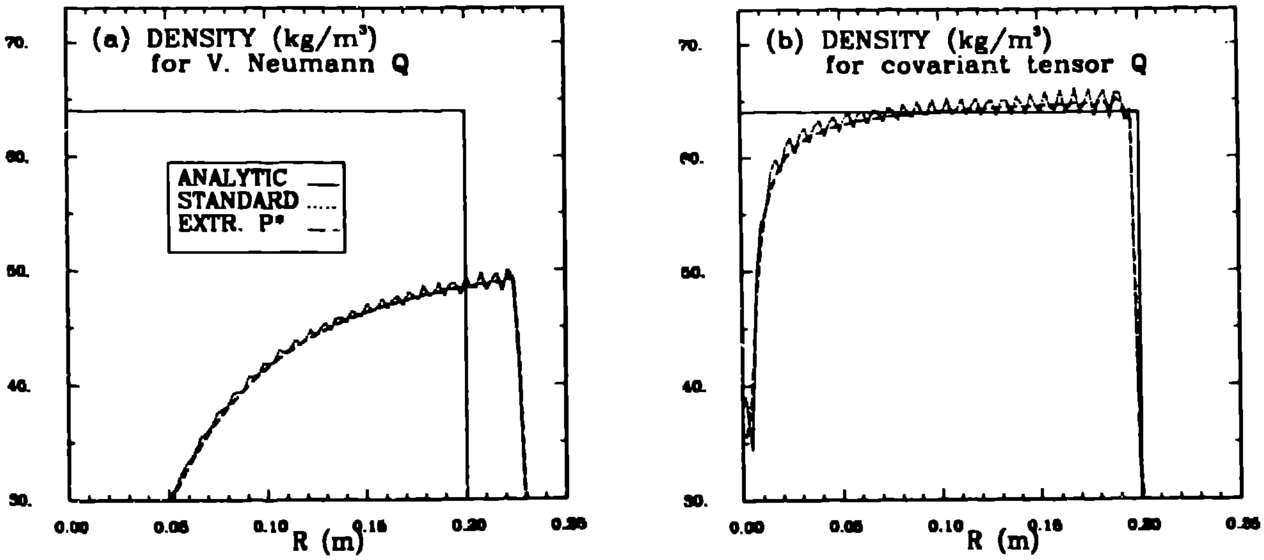

Fig. 3. Spherical Noh problem, density, at time = 0.6 second, using (a) Von Neumann artificial viscosity and (b) covariant tensor artificial viscosity.

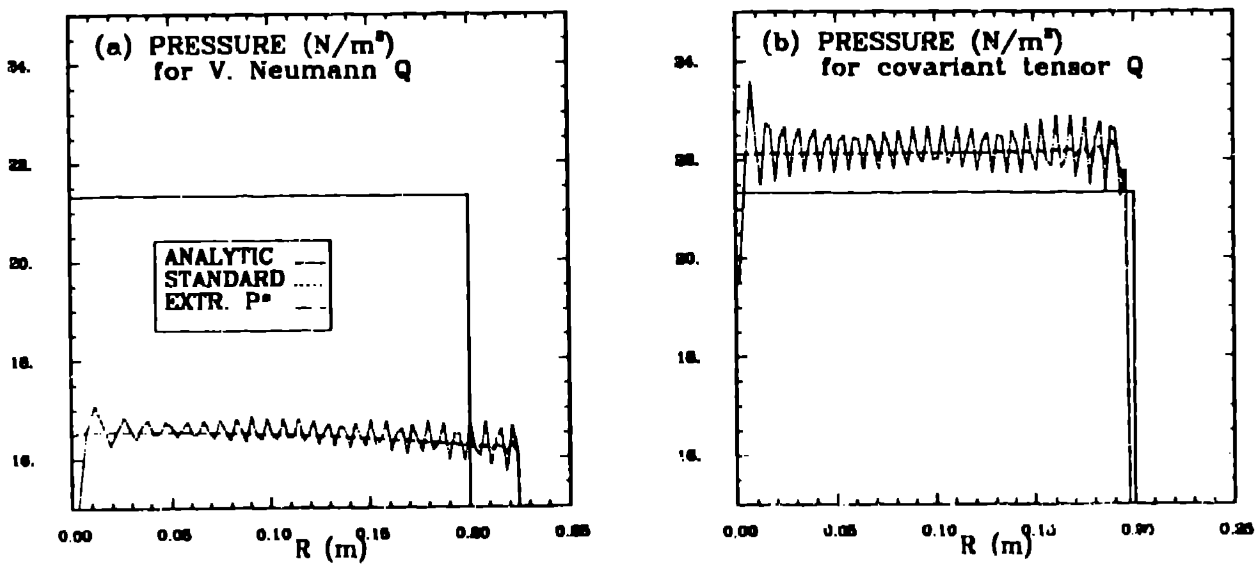

Fig. 4. Spherical Noh problem, pressure, at time = 0.6 second, using (a) Von Neumann artificial viscosity and (b) covariant tensor artificial viscosity.

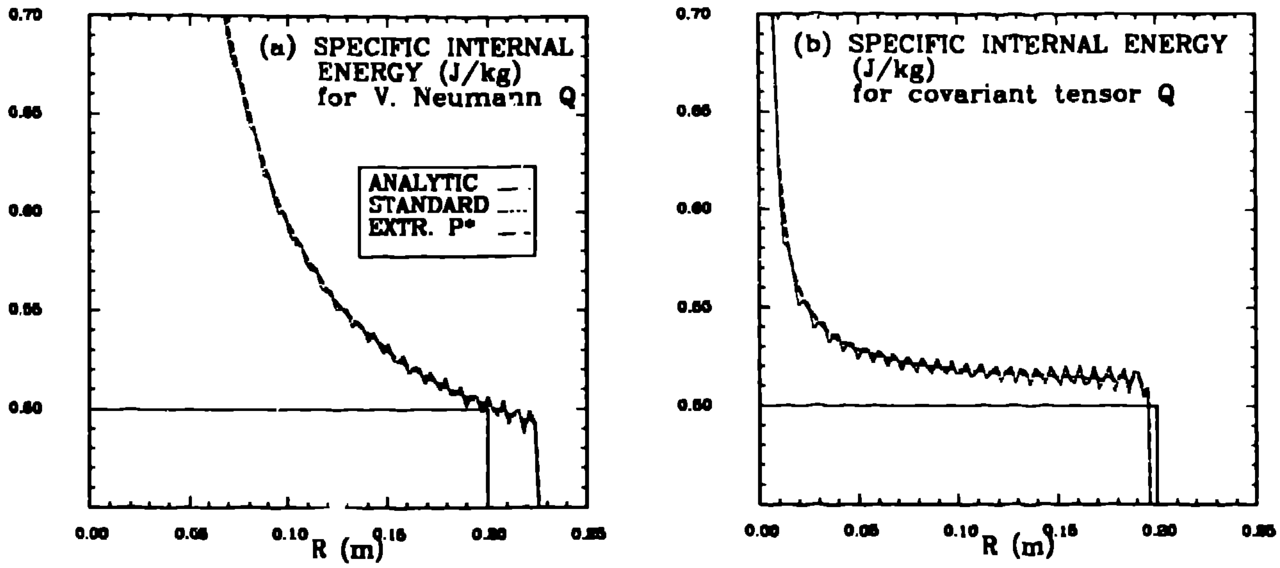

Fig. 5. Spherical Noh problem, specific internal energy, at time = 0.6 second, using (a) Von Neumann artificial viscosity and (b) covariant tensor artificial viscosity.

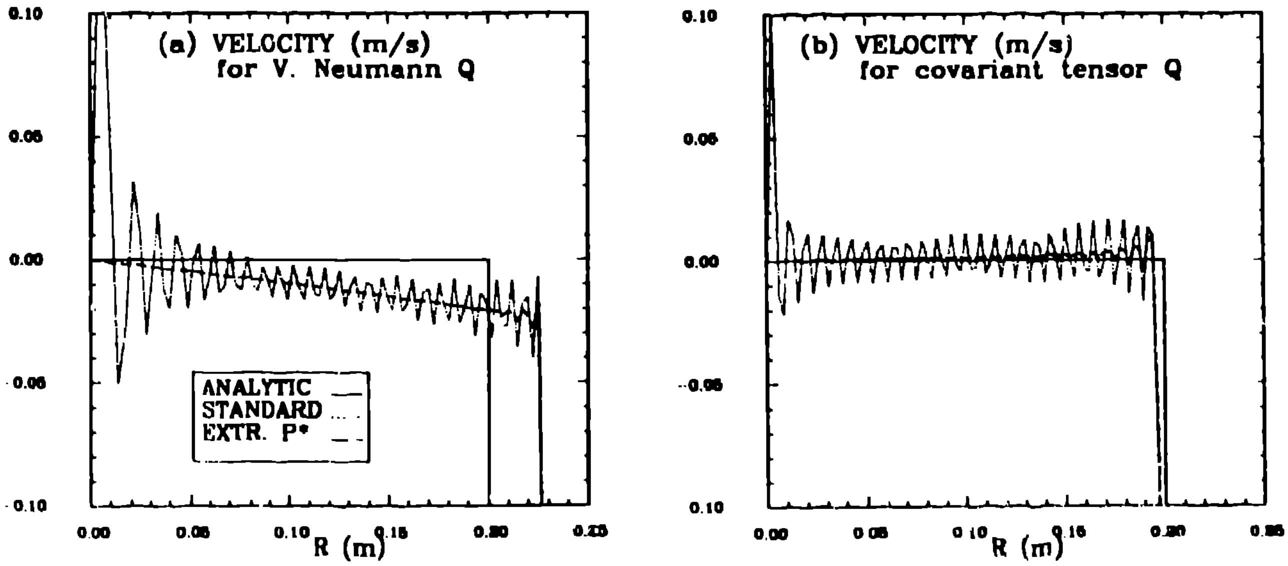

Fig. 6. Spherical Noh problem, velocity, at time = 0.6 second, using (a) Von Neumann artificial viscosity and (b) covariant tensor artificial viscosity.

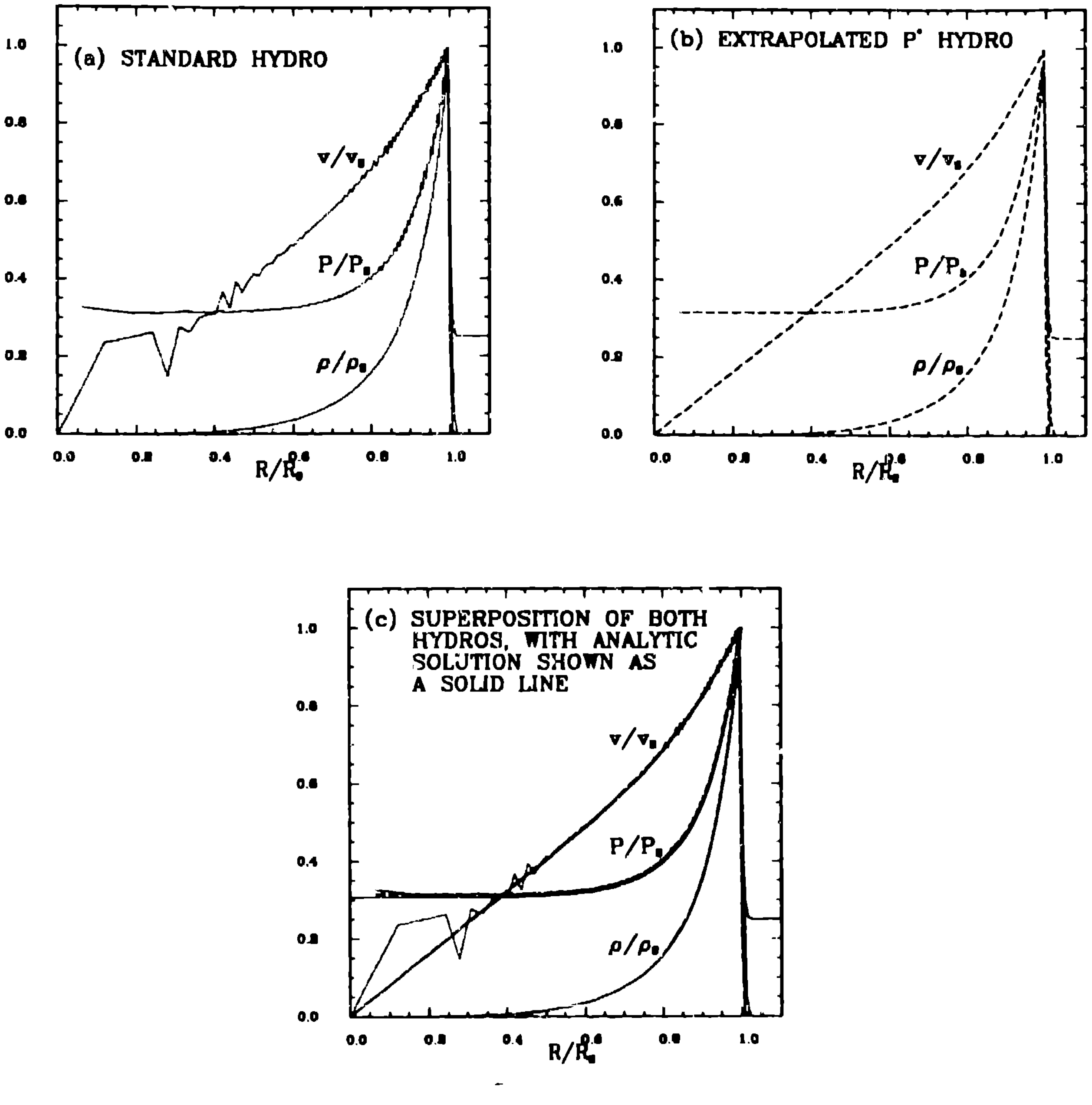

Fig. 7. Spherical Sedov Blast Wave problem, for (a) standard hydro, (b) extrapolated P^* hydro, and (c) a superposition of the two hydros with analytic solution shown as a solid line, at time = 1.0 second.

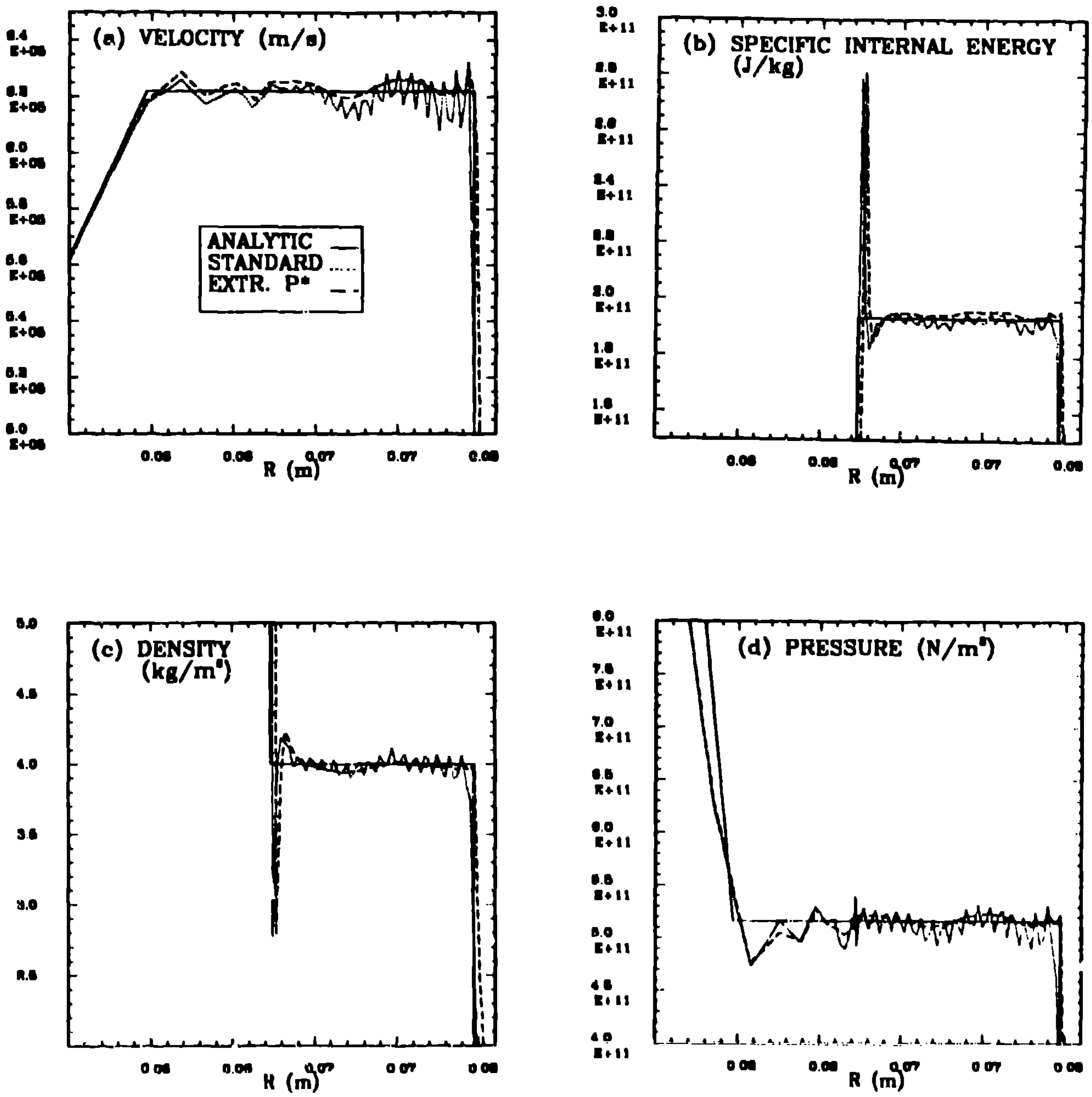

Fig. 8. Planar Strong Shock Tube problem for (a) velocity, (b) specific internal energy, (c) density, and (d) pressure, at time = 6.0 seconds.

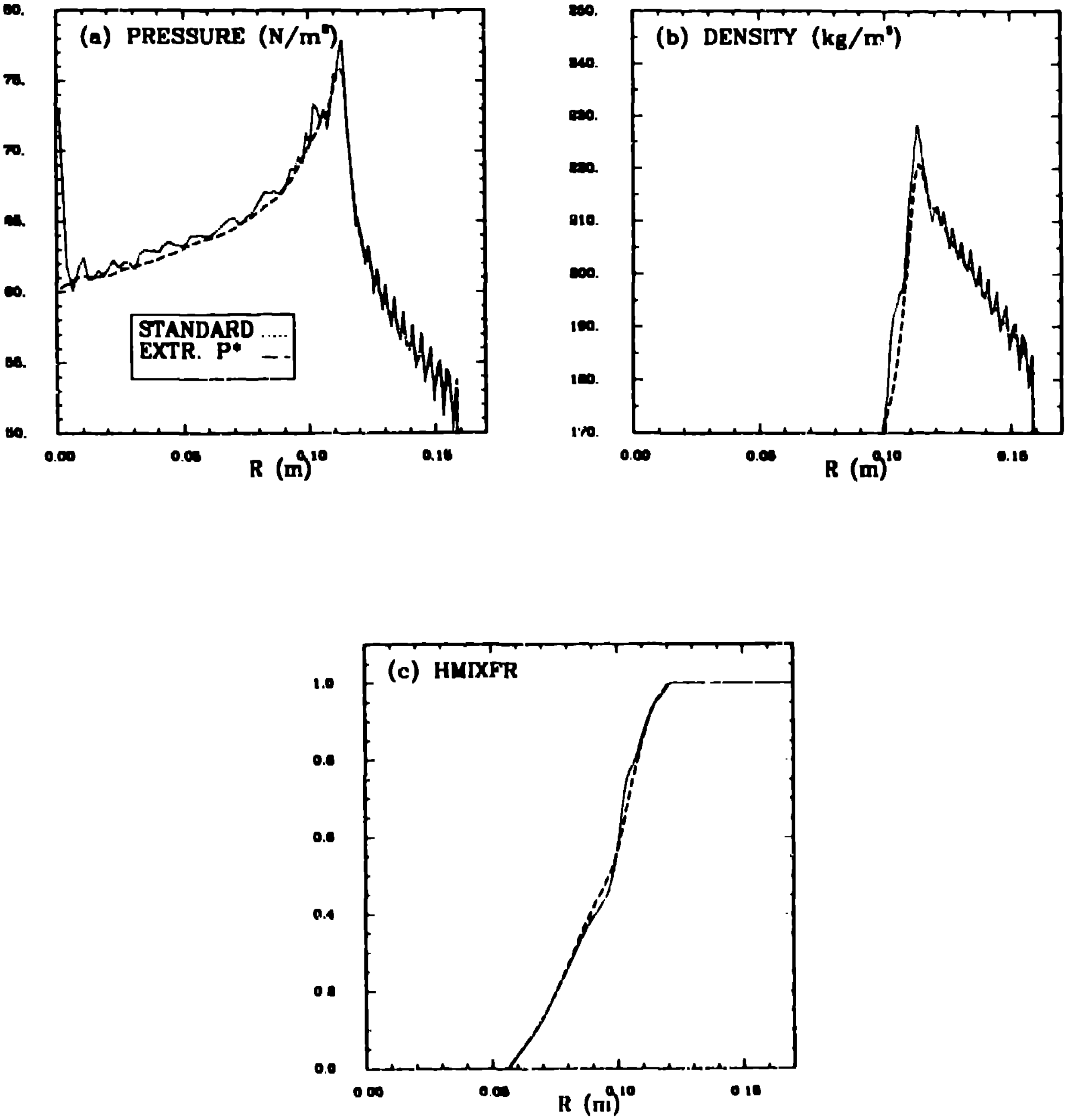

Fig. 9. Modified Noh problem, dynamical mixing, for (a) pressure, (b) density, and (c) hmixfr (fraction of zone mass that is the heavier material), at time = 0.6 second.