

# Nonlinear Acoustic Wave Effects on Lower Thermosphere Composition

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## Abstract

Small-scale dynamical models for the diffusive and stratified lower thermosphere commonly use single gas approximations with height-dependent physical properties (e.g. mean molecular weight, specific heats) that do not vary with time (fixed composition). This approximation is useful as it is simpler and less computationally expensive than a true multi-constituent fluid model, and still captures the important physical transitions between molecular and atomic gases in the lower thermosphere.

This paper presents a one-dimensional nonlinear mass fraction approach to multi-constituent gas modelling to achieve a less computationally intensive model than a full binary-gas model. The approach uses the finite volume method of Bale et al. implemented in CLAWPACK with a Riemann Solver to solve the Euler Equations including multiple species, defined by their mass fractions, as they undergo advection. Various tests are conducted including, shock tube for two species gas, vertically propagating acoustic waves with oscillations near the cut-off frequency, and propagating nonlinear acoustic waves with steep or pseudo-shock character. The limits of applicability are also investigated.

## Introduction

Wave motion in a diffusively separated atmosphere with height-dependent composition can lead to significant perturbations to constituent density, namely [O], [O<sub>2</sub>], and [N<sub>2</sub>]. The fluctuations are typically modeled through single or binary gas approximation and the addition of more species, in any nonlinear model, creates a more complex system. Thus, investigating single-fluid models as alternatives to multi-fluids has been an active area of research (e.g. Walterscheid and Hickey, 2001, 2012). These investigations seek to simplify computationally-intensive models by assuming all species are well coupled where perturbations to composition affect the equation of state via changes to the ratio of specific heats.

## Governing Equations

This paper considers the one-dimensional Euler Equations, while simultaneously advecting the mass fraction of the dominant species in the atmosphere, with a finite volume method using a Riemann Solver. The numerical solutions were obtained through use of CLAWPACK (Leveque, 2002). The one-dimensional Euler Equations are:

$$\begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix}_t + \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(E + P) \end{bmatrix}_x = \begin{bmatrix} 0 \\ -\rho g \\ -\rho g u \end{bmatrix} \quad (1)$$

$$E = \rho e + \frac{1}{2} \rho u^2 \quad (2)$$

Where the subscripts  $t$  and  $x$  denote temporal and spatial derivatives  $\partial/\partial t$  and  $\partial/\partial x$  respectively. The equations are closed with the equation of state

$$p = \rho e(\gamma - 1) \quad (3)$$

The non-conservative mass fraction approach adds two equations to 1 which take the form

$$\frac{\partial Y_s}{\partial t} + u \frac{\partial Y_s}{\partial x} = 0 \quad (4)$$

Where  $Y_s$  represents the mass fraction of the dominant species.

## Sod Shock Tube

A common test for evaluating the validity of a Riemann Solver is the Sod Shock Tube (Sod, 1978). Its role is to test a code's ability to capture shocks and contact discontinuities with a small number of cells and to produce the correct profile in a rarefaction (Leveque, 2002). The well known solution is shown below (Ketcheson and LeVeque)

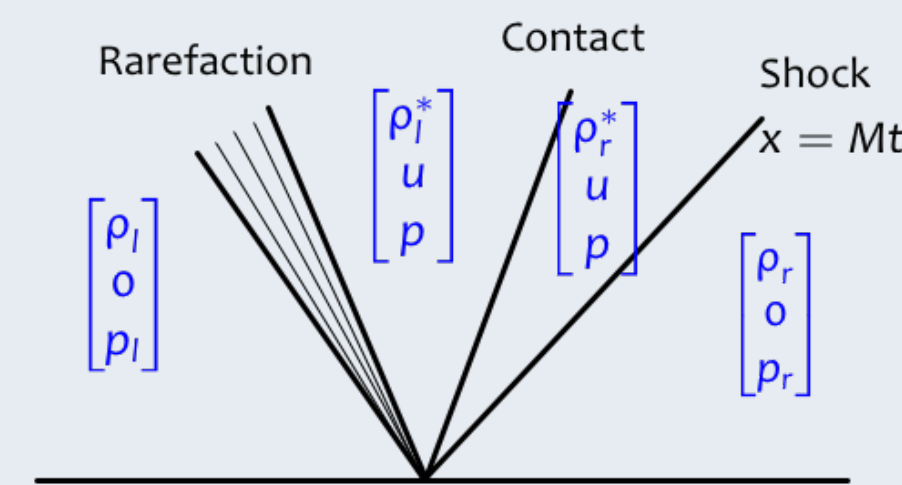


Figure 1: Riemann problem solution

The contact and shock slopes are well known to be  $u$ , and  $u + c$  (depending on the initial conditions).

## Simulation Parameters

### Sod Shock Tube

Parameter	Symbol	Value
Density	$\rho_L, \rho_R$	3,1
Pressure	$p_L, p_R$	3,1
[O <sub>2</sub> ] Mass Fraction	$Z_L, Z_R$	0,0
[O] Mass Fraction*	$Y_L, Y_R$	(1,0), (0,1)
Ratio of Specific Heat*	$\gamma_L, \gamma_R$	(5/3, 7/5), (7/5, 5/3)

\* A second simulation was ran with these values in reverse.

### Wave Simulations

Parameter	Lg. Amp. Wave	Tohoku
Source	S. Gaussian**	S. Heavise**
Amplitude	50 cm/s	3.49 cm/s
Resolution	100m	(100m,1km)
Max Alt.	400km	600km
Angular Freq.	0.104 rad/s	0.035 rad/s

\*\* S. - Sinusoidal.

## Initial Atmospheric Profile

A large amplitude wave and a wave similar to the Zettergren et al, 2017 of the 2011 Tohoku Earthquake (see *Simulation Parameters*) were simulated to explore the models behavior during an extreme case, and apply it to a real phenomena, respectively. For these two simulations, viscosity terms (not shown in Equation 1), are included. Both cases included atmospheric profiles derived from NRLMSISE00 [Picone et al., 2002]. The figures below show the resulting atmospheric parameters

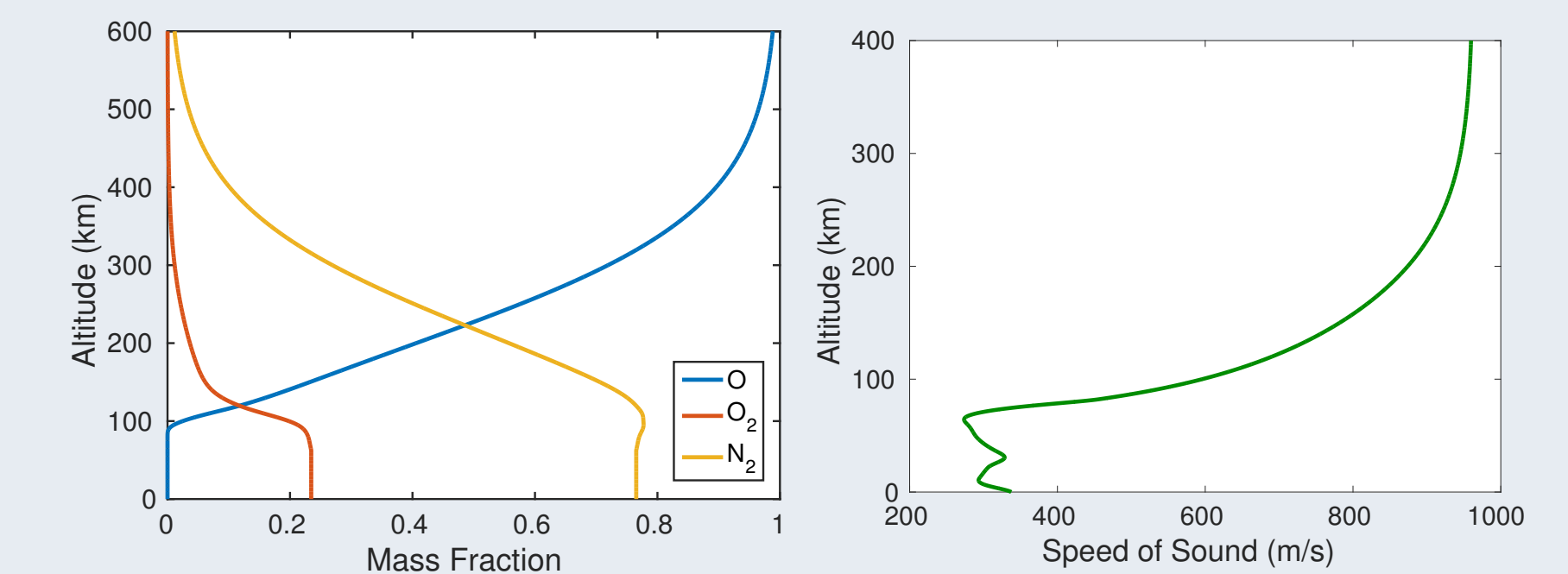


Figure 5: Initial mass density fraction profiles (left) and speed of sound (right) for the atmosphere's major constituents based on NRLMSISE00 data. The speed of sound profile is similar to the atmosphere's temperature profile.

## Results

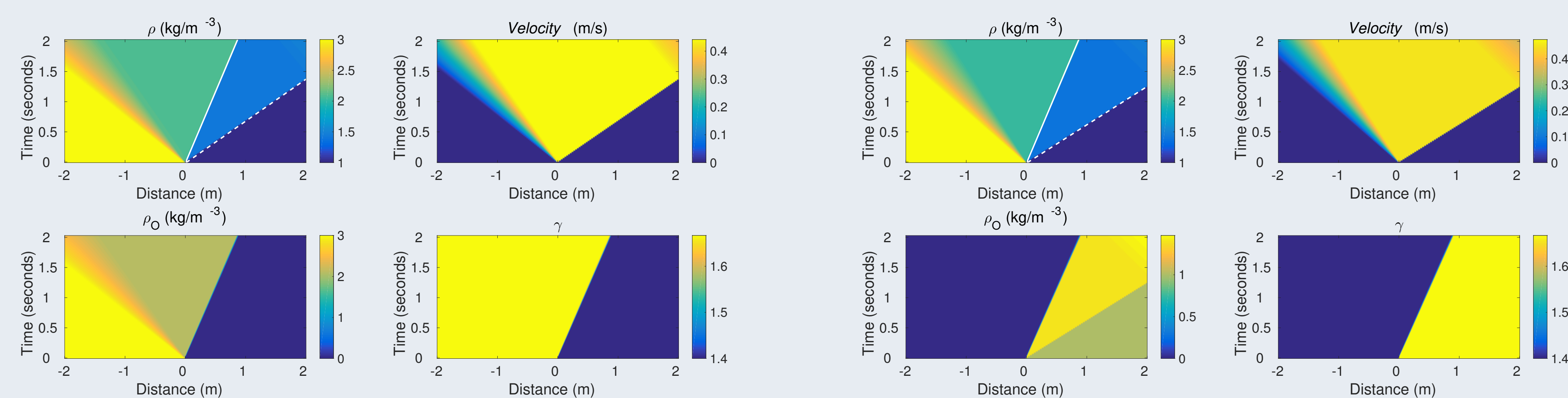


Figure 2: Atomic Oxygen begins on the left (shown by the figure on the left initially at rest). Once the membrane is ruptured, the gas expands and three primary features are produced as a result of the expansion, rarefaction, contact, and shock. The contact and shock are indicated by the solid white line and dashed line respectively. This validates the model since the slope matches with the predicted gas velocity  $u$  and  $u + c$

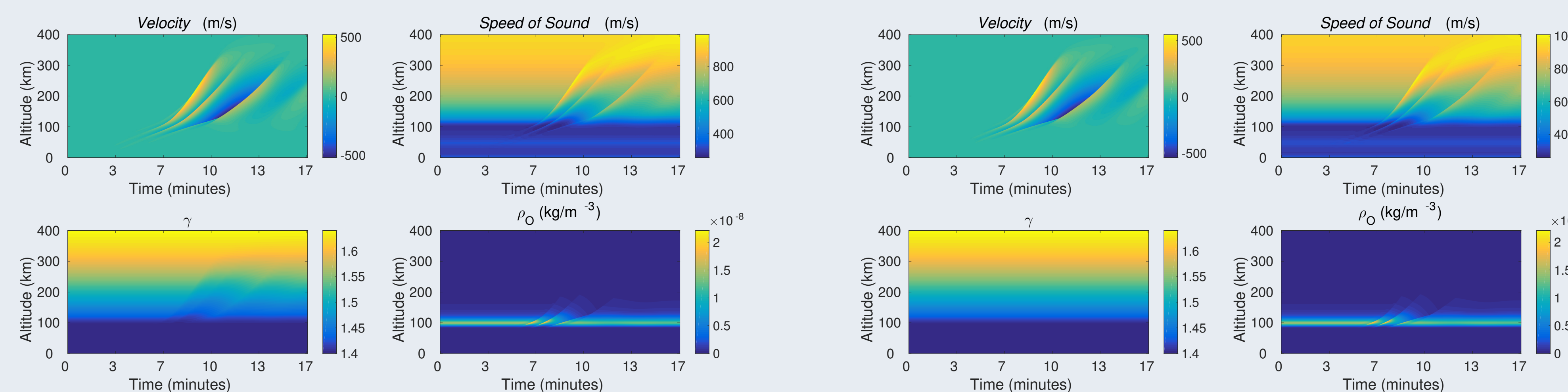


Figure 3: A large amplitude acoustic wave was simulated to evaluate how the model acts when under extreme conditions. The simulation on the left shows a simulation with a mass fraction defined, variable ratio of specific heats while the figure on the right shows the same simulation without specific heat variation. Despite the small variation, the model continues to be stable while retaining the wave modulation of composition.

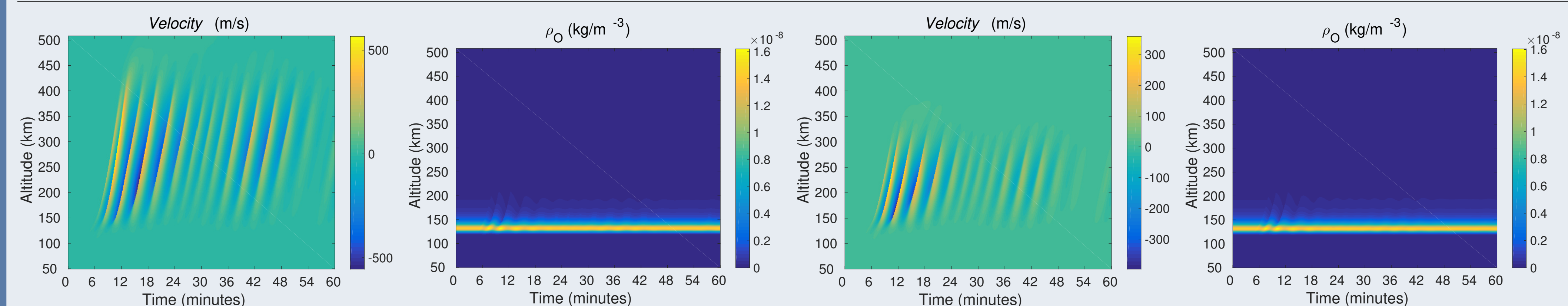


Figure 4: A wave resembling the Zettergren et. al, 2017 simulation of the 2011 Tohoku Earthquake is shown as an application of the model to a real event. The simulations presented have 1km resolution (left 2), and 100m resolution (right 2). The velocities have a noticeable difference in magnitude which is due to the effectiveness of viscosity as resolution is increased.

## Conclusion

- The mass fraction approach showed stability for the cases demonstrated, including the classical shock tube examples and acoustic waves in the atmosphere.
- Results capture the acoustic wave modulation of composition in addition to the ratio of specific heats.
- Results for the Tohoku case further demonstrated the effects of viscosity as a function of the wave scales resolved. The higher the resolution, the more effective the viscosity, due to additional wave steepening.
- An important future step will be to parameterize and validate dissipation for steepened acoustic waves in the atmosphere.
- A new conservative-form version of this model will be investigated, and compared to the results here and to solutions via continuity equations for individual minor species.

## Acknowledgements

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