Revisions for SHOC-D-19-00046: StanShock: A Gasdynamic Model for Shock Tube Simulations with Non-ideal Effects and Chemical Kinetics

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We thank the referees for the constructive comments to this manuscript submission. The reviewers’ comments asked for clarification of modeling details and asked for expanded discussion of the model’s results. Below, please find a detailed account of revision made the manuscripts and response the questions by the reviewer.

**Reviewer #1:**

The manuscript addresses the lack of computational tools available to successfully model the behavior in shock tubes mainly used for chemical kinetics and ignition studies. The validations show that the boundary layer model developed is successful in capturing the experimental boundary layer effect in the shock tube. It would be of interest to see how well the predictions are when the boundary layer effects are expected to be severe such as in case of shock tubes with extremely small bores. In such tubes the pressure rise in post reflected shock region is very large, as observed experimentally.

The insert optimization algorithm will provide relief from the laborious task of designing the most optimum insert design analytically and will be of great utility to the shock tube community as a whole. The effect of discretized versus continuous insert was often neglected but the results shown in this manuscript would urge investigating the effects of the insert geometry.

In Fig 11(a) the experimental pressure trace shows a slight pressure bump near the end of the residence time which is usually attributed to contact surface effects. The simulation does have very good agreement with the initial boundary layer rise, which continues as a rise over the pressure bump, but does not capture the pressure bump similar to the experiment. A few questions may arise due to this - Are contact surface effects included in the model? Is the contact surface decoupled from the non-ideal boundary layer pressure rise? If it is, can each effect be individually simulated in the absence of the other? The user would greatly benefit by knowing answers to these questions to ensure the simulation is addressing the correct effect observed in the experiment. This would also provide the additional benefit of obtaining tailoring conditions, whose calculations are also equally laborious.

The use of the simulated shock tube performance, as provided at the github location, directly as an input to a chemical kinetic solver like Cantera, Chemkin etc. will provide great benefit in designing the experiments and to draw a base line for expectations from an experiment with acceptable computational time. The answers to the contact surface related questions raised above would be beneficial to the community and the user of the code. Overall the manuscript should be accepted for publication.

*Response: We thank the reviewer for the positive feedback in this work in that the gas dynamic solver developed in this work will be of great benefit to the design of shock tube experiments. As the reviewer mentions, non-ideal gas dynamics in small bore shock tubes are of great interest; correspondingly, we augmented Fig. 9 to include the sensitivity of the model to a reduction in the diameter. With respect to the reviewer’s comments on Fig 11(a), we included clarifying discussion in the text on the modeling of the contact surface.*

­­­**Reviewer #2**

In this manuscript, a new computational tool is presented that can be used to simulate shock tube nonideal effects from the ground up, so to speak. That is, the simulation uses viscous and heat losses to model the boundary-layer effects, which them manifest into pressure waves that disturb the test conditions behind the incident and reflected shock waves in a shock tube. The author show that the model can also be used to design driver insert geometries that will provide flat pressure (and temperature) time histories in the test region behind the reflected shock wave. The paper is well laid out and it suitably describes the model and its validation. Some examples are given. Although the examples are limited, I am not sure if a journal manuscript is the appropriate place to demonstrate the model over an extensive array of test conditions. The paper is appropriate for Shock Waves and presents an advancement in the state of the art of shock tubes for chemical kinetic studies. Some additional comments and edits are provided below.

If I understand the approach correctly, the model does not take any a priori inputs regarding the incident-shock attenuation. That is, the shock attenuation is predicted by the model and is due to the viscous effects at the wall. There seems to be good agreement with the few test data that are used for validation. However, as shown in several past studies on nonideal behavior, the shock attenuation in a real shock tube is only partly due to the BL effects, as predicted by a model such as developed by Mirels. A major contribution to the shock attenuation seems to be due to the nonideal diaphragm rupturing and possible the related nonideal formation of a normal shock wave thereafter. How does the model account for this effect?

*Response: The reviewer is correct that non-ideal diaphragm rupture is a major contributor the shock attenuation. Additional discussion on possible ways to model non-ideal diaphragm rupture has been provided in the discussion of the time-varying area term near Eq. 5 and in the discussion of the non-ideal pressure bump seen in Fig. 11.*

The heat transfer effect on the dp/dt is very interesting and is one of the new things in this paper. It would be appropriate if the authors could comment on why this is the case, beyond just the statement of the fact based on the simple convection model (Eqn. 13) employed. Is the heat loss impacting the bl growth and subsequent wave propagation? Is seems unlikely that there is a significant radial variation in temperature outside of the BL at the time scales of the test, as described in other studies in the literature, but maybe there is, which then affects the speed of propagation of the expansion and compression waves down the driven tube.

*Response: We thank the reviewer for identifying this interesting prediction of the model and asking for additional insight. Correspondingly, we extended the discussion of this in Sec. 3.5.1.*

The citation numbering is out of order. Certainly this must be fixed but would be done so one way or the other at the editorial stage before publication.

Edits:

1) page 12, section 3.5, should be "…increasing the values of the kinetic rate coefficients…" (add the "s" to value and coefficient)

2) page 18, last paragraph, should it be "damps" instead of "dampens", since dampen means to moisten, typically.

3) top of page 20, should be "…driver section are denoted…" (change is to are)

4) page 20, second paragraph, should be "ab initio due to its smoothness…" (add "to")

*Response: We are grateful that the reviewer found the typographical errors upon careful review. We corrected these in the manuscript.*