

SDTOOLBOX

NUMERICAL TOOLS FOR SHOCK AND DETONATION WAVE MODELING

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This document is in a state of continuous development and you are examining a snapshot in time. There are sections on real gas thermodynamics and vibrational-rotational-translational equilibrium but no discussion of the related software which is still under development. This version was published just as V2.5.1 of Cantera was released so there few references to the **YAML** format for the thermochemical database.

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Preface

These notes are a tutorial on the analysis and computation of shock and detonation waves in gases with realistic thermochemistry. A library (`SDToolbox`) of Python and MATLAB routines is described for computations of post-shock conditions and Chapman-Jouguet detonation velocity. Notes and demonstration programs are provided for using this library to compute examples of normal and oblique shocks and detonations, shock and detonation tube operations, expansion waves, nozzle flows, ideal detonation and wave structure, propulsion systems and selected wave interaction problems.

The toolbox modules, demonstration scripts and instructions for installation are available on the SD-Toolbox [website](#). In order to use these scripts, the reader must install the Cantera software and Python or MATLAB. This revision of the document links to programs that are compatible with the most recent release of Cantera, V2.5; MATLAB, R2020; and Python 3.8. The programs were tested on earlier versions (2.3 and 2.4) of Cantera, MATLAB (2017,2018) and Python (3.5,3.6). The documentation and software for Cantera [Goodwin et al. \(2017\)](#) is open source and available at www.cantera.org.

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Chapter 1

Introduction

These notes are a tutorial on the analysis and computation of shock and detonation waves with selected applications to explosion and propulsion. Numerical solution methods are necessary for solving the conservation equations or jump conditions that determine the properties of shock and detonation waves in a multi-component, reacting gas mixture. Only the idealized situations of perfect (constant heat-capacity) gases with fixed chemical energy release can be treated analytically (Appendix A). Although widely used for simple estimates and mathematical analysis, the results of perfect gas models are not suitable for analysis of laboratory experiments and carrying out numerical simulations based on realistic thermochemical properties.

The science of shock and detonation waves began in the 19th century and continues to be an ongoing activity. Technological applications such as chemical propulsion (rockets, gas turbines and gaseous detonation concepts) and high explosives motivated the development of numerical solution methods and software for modeling chemical equilibrium in multi-species and multi-phase mixtures. These efforts began in the 1950s and some of these software packages are still in use today, however there are issues with using the older software including limited availability due to national security or proprietary concerns, lack of support for legacy software, and challenges of integration into modern software environments. In response to this situation, we have developed a library of software tools, the **Shock and Detonation Toolbox**, that we are making openly available for academic research. The Toolbox and associated demonstration programs are based on the **Cantera** software library to evaluate gas thermodynamic and transport properties, chemical reaction rates and carry out chemical equilibrium computations.

This document is divided into four parts. These parts describe the underlying scientific principles, the functionality of the Toolbox, numerical methods, applications to a variety of combustion problems with links to the programs, graphical and tabular results of program outputs.

In Part I, the fundamentals of thermodynamics, the ideal gas mixture formalism, and the concepts underlying chemical equilibrium are presented. In Part II of the report, we describe the algorithms used in the toolbox for the numerical solution of shock and detonation jump conditions in ideal gas mixtures with realistic thermochemical properties. An iterative technique based on a two-variable Newton's method is selected as being the most robust method for both reactive and nonreactive flows. A library of routines is described for Python and MATLAB computations of post-shock conditions and Chapman-Jouguet detonation velocity. Notes and demonstration programs are provided to illustrate how to use these routines to solve a range of problems. In addition to numerical methods for realistic thermochemistry, perfect gas analytical solutions are also provided.

In Part III of the report, we describe steady flows and some simple unsteady flows which not in equilibrium or frozen and chemical reaction must be considered. The steady flows treated are the reaction zones behind shock and detonation waves moving at constant speed, the reaction zone along the stagnation streamline in supersonic blunt body flows, flow through a converging-diverging nozzle and quasi-one dimensional flows with friction and heat transfer modeled as wall functions. The unsteady flows modeled include reaction occurring

under constant temperature, pressure and volume conditions or with prescribed volume or pressure time dependence.

In Part IV, the software components of the Toolbox and the application programs are described.

1.1 Overview and Quickstart

This overview describes situations that are commonly encountered and links to the associated toolbox routines and demonstration programs. For more details on the input and output parameters for these routines, see Chapter 12. For a listing and links to demonstration programs that illustrate various applications of the toolbox, see Chapter 13. In order to use these scripts, the reader must first install the Cantera software and have previously installed Python or MATLAB. The toolbox modules, demonstration scripts and instructions for installation are available on the SDToolbox [website](#).

1. Non-reactive shock wave. If the chemical reactions occur sufficiently slowly compared to translational, rotational, and vibrational equilibrium,¹ then a short distance behind a shock wave flow can be considered to be in thermal equilibrium but chemical nonequilibrium. This is often referred to as a “frozen shock” since the chemical composition is considered to be fixed through the shock wave. Computations of post-shock conditions are used as initial conditions for the subsequent reaction zone and are therefore a necessary part of computing shock or detonation structure. Usually, these computations proceed from specified upstream conditions and shock speed; the aim of the computation is to determine the downstream thermodynamic state and fluid velocity. On occasion, we consider the inverse problem of starting from a specified downstream state and computing the upstream state.

Function `PostShock_fr`: Demos - MATLAB: `demo_PSfr.m` Python: `demo_PSfr.py`

2. Reactive shock wave. The region sufficiently far downstream from the shock wave is considered in thermodynamic equilibrium. Thermodynamics can be used to determine the chemical composition, but this is coupled to the conservation equation solutions since the entropy and enthalpy of each species is a function of temperature. As a consequence, the solution of the conservation equations and chemical equilibrium must be self-consistent, requiring an iterative solution for the general case. In the case of endothermic reactions (i.e., dissociation of air behind the bow shock on re-entry vehicle), there are no limits on the specified shock velocity and the computation of the downstream state for specified upstream conditions is straightforward. For exothermic reactions, solutions are possible only for a range of wave speeds separated by a forbidden region. The admissible solutions are detonation (high velocity, i.e., supersonic) and deflagration (low velocity, i.e., subsonic) waves, and there are usually two solutions possible for each case.

Function `PostShock_eq`: Demos - MATLAB: `demo_PSeq.m` Python: `demo_PSeq.py`

3. Chapman-Jouguet (CJ) detonation. This is the limiting case of the minimum wave speed for the supersonic solutions to the jump conditions with exothermic reactions. The Chapman-Jouguet solution is often used to approximate the properties of an ideal steady detonation wave. In particular, detonation waves are often observed to propagate at speeds within 5-10% of their theoretical CJ speeds in experimental situations where the waves are far from failure.

Function `CJSpeed`: Demos - MATLAB: `demo_CJ.m` Python: `demo_CJ.py`

4. Reflected shock wave. When a detonation or shock wave is incident on a hard surface, the flow behind the incident wave is suddenly stopped, creating a reflected shock wave that propagates in the opposite direction of the original wave. If we approximate the reflecting surface as rigid, then we can compute the speed of the reflected shock wave given the incident shock strength. This computation is frequently carried out in connection with estimating structural loads from shock or detonation waves.

Function `reflected_eq` and `reflected_fr`:

Demos - MATLAB: `demo_reflected_eq.m` and `demo_reflected_fr.m`

Python: `demo_reflected_eq.py` and `demo_reflected_fr.py`

¹The structure of shock waves with vibration non-equilibrium is discussed at length by [Clarke and McChesney \(1964\)](#) and [Vincenti and Kruger \(1965\)](#)

5. ZND Model Detonation Structure Computation. The idealized reaction zone behind a steady shock or detonation wave is one-dimensional reactive flow. The model equations and properties were first explored by Zel'dovich (1940), von Neumann (1942), and Doering (1943). The solution method used in the toolbox is to convert the differential-algebraic equations representing the conservation of mass, momentum, energy and species evolution to a fully differential system of ODE and integrate these with a method suitable for stiff equations.

Function **ZND**:

Demos - MATLAB: `demo.ZNDCJ.m`, `demo.ZNDshk.m` and `demo.ZND_CJ.cell.m`

Python: `demo.ZNDCJ.py`, `demo.ZNDshk.py` and `demo.ZND_CJ.cell.py`

6. CV Model Explosion Structure Computation. The time-evolution of a mass of fluid reacting at constant volume is frequently used as a surrogate for the reaction process behind incident and reflected shock waves, as well as detonations. The model equations are based on the first law of thermodynamics for an adiabatic, constant-volume system. The ordinary differential equations for energy conservation and species evolution are integrated with a stiff ODE solver.

Function **CV**:

Demos - MATLAB: `demo.cv.m`, `demo.cv_comp.m`, `demo_cvCJ.m`, `demo_cvshk.m`

Python: `demo_cvCJ.py`, `demo_cvshk.py`

DRAFT

Part I

Thermodynamics

Shock waves and detonation computations for reacting gases are based on the fundamental concepts of combining pure species properties to obtain mixture properties and the methods of chemical equilibrium to compute composition. This part of the notes presents the essential background and a brief introduction to chemical equilibrium computations.

Chapter 2

Fundamentals

Thermodynamics is fundamental to all the computations and analysis in this version of the SDT. The principles can be found in many textbooks, for example, [Kondepudi and Prigogine \(1998\)](#). Classical references with a emphasis on chemical reactions and chemical equilibrium include [Denbigh \(1981\)](#) and [Smith and Missen \(1991\)](#). This chapter focuses on the definitions and relationships between properties that are essential in the reacting flows of gases.

2.1 General Principles

A fluid substance such as a gas can be subdivided into elements or volumes that are transported and deformed during motion but retain their identity as a fixed quantity of material if we neglect diffusive transport. The elements can be considered as thermodynamic systems with an internal energy E , temperature T , pressure P , and volume V . The internal energy¹ changes dE of the element are determined by the First Law of Thermodynamics

$$dE = dQ + dW \quad (2.1)$$

and the energy added in the form of heat dQ , and the mechanical work dW . For *reversible changes*, we can define an entropy function S related to the heat interaction

$$dS = \frac{dQ}{T} \quad (2.2)$$

and the work interaction can be defined in terms of pressure and volume changes

$$dW = -PdV \quad (2.3)$$

The evolution of an isolated (no heat or work interactions, fixed quantity of material) system is determined by the Second Law of Thermodynamics

$$dS \geq 0 \quad (2.4)$$

If the element is made up of K distinct molecular species each in amounts N_1, N_2, \dots, N_K that can react with each other, the internal energy can be written as

$$E = E(S, V, N_1, N_2, \dots, N_K) \quad (2.5)$$

and the changes in energy for a fixed mass of reacting material can be computed as

$$dE = TdS - PdV + \sum_{i=1}^K \mu_i dN_i \quad (2.6)$$

¹The internal energy is the thermodynamic contribution to the total energy of a moving parcel of fluid and is usually denoted with the symbol U . Because we often use U for velocity in fluid mechanics, we use the symbol E instead. Equation (2.1) only applies in the frame of reference of the moving fluid and in the absence of any external forces. In general, the left-hand side should be the total energy of the system, U + kinetic energy + potential energy + ...