Mini-Projet : Complex Chemistry and Entropy as a Lyapounov function

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1 Introduction

In this mini-projet, we will focus on a closed reactor with a reaction mechanism and thermodynamics, such as the one that are used in practical combustion applications, that is potentially involving several tens of species and several hundreds of reactions [1]. The objective of the mini-projet is threefold. First, relying of an axiomatics described in [3, 2] and reproduced in the lecture notes provided [5], there is a theoretical proof that the entropy is a global Lyapounov function, allowing to prove that the dynamics of the system is globally attracted by a single equilibrium state. Second, following the lecture notes, the student is supposed to provide a toy system and integrate it in order to illustrate the theoretical result. Finally, if time is available, we will conduct a simulation of the ignition of a mixture in a reactor using a realistic reaction mechanism.

2 An axiomatic treatment of chemistry and thermodynamics

In this first part, the purpose is to understand and present the structure of thermodynamics and chemistry of a set of species and elementary reactions, so that when such a chemistry is taking place in a closed vessel, we can prove that the entropy of the mixture is decreasing in time and the system is asymptotically converging toward the unique chemical equilibrium of the system, thus leading us to a global Lyapounov function of the dynamical system.

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3 Simulating the dynamics of a toy system

The purpose of this part is to rely on the lecture notes of the Agrégation, in order to build a toy system reproducing the previously studied thermodynamics and chemistry axiomatics and to show, by a numerical integration of the dynamics (using your preferred scheme studied in the course), the system is effectively converging toward the unique equilibrium point.

4 Complex chemistry and ignition of a reacting mixture

We now turn to a realistic chemical mechanism and thermodynamics of a reacting mixture. Relying on a library and on an interpreter (Chemkin [4]), as well as on a dedicated integrator, we can propose a numerical simulation of the ignition of a reacting mixture in a combustion environment.

References

[1] S. Descombes, M. Duarte, T. Dumont, F. Laurent, V. Louvet, and M. Massot. Analysis of operator splitting in the nonasymptotic regime for nonlinear reaction-diffusion equations. Application to the dynamics of premixed flames. *SIAM J. Numer. Anal.*, 52(3):1311–1334, 2014.

[2] V. Giovangigli. *Multicomponent Flow Modeling.* Birkhäuser Boston Inc., Boston, MA, 1999.

[3] Vincent Giovangigli and Marc Massot. Asymptotic stability of equilibrium states for multicomponent reactive flows. *Math. Models Methods Appl. Sci.*, 8(2):251–297, 1998.

[4] R.J. Kee, F.M. Rupley, and J.A. Miller. CHEMKIN-II: A Fortran chemical kinetics package for the analysis of gas-phase chemical kinetics. *Tech. Rep. SAND89-8009, Sandia National Lab., Livermore, CA*, 1980.

[5] M. Massot. *"Cinétique Chimique", Préparation à l'Agrégation de Mathématiques, oral de modélisation.* Université Claude Bernard Lyon 1, 2000.