

Development of Real Gas Kinetic Chemistry at High Pressure

Shervin Sammak
Research Assistant Professor
Center for Research Computing
E-mail: shervin.sammak@pitt.edu

Motivation

- Lack of real gas models and their application to realistic combustion simulations
- Increase thermal efficiency of combustion
- Lower exhaust pollution
- Reducing fuel consumption

Project Description

- Investigate the effect of high pressure
- Develop kinetic chemistry for those conditions

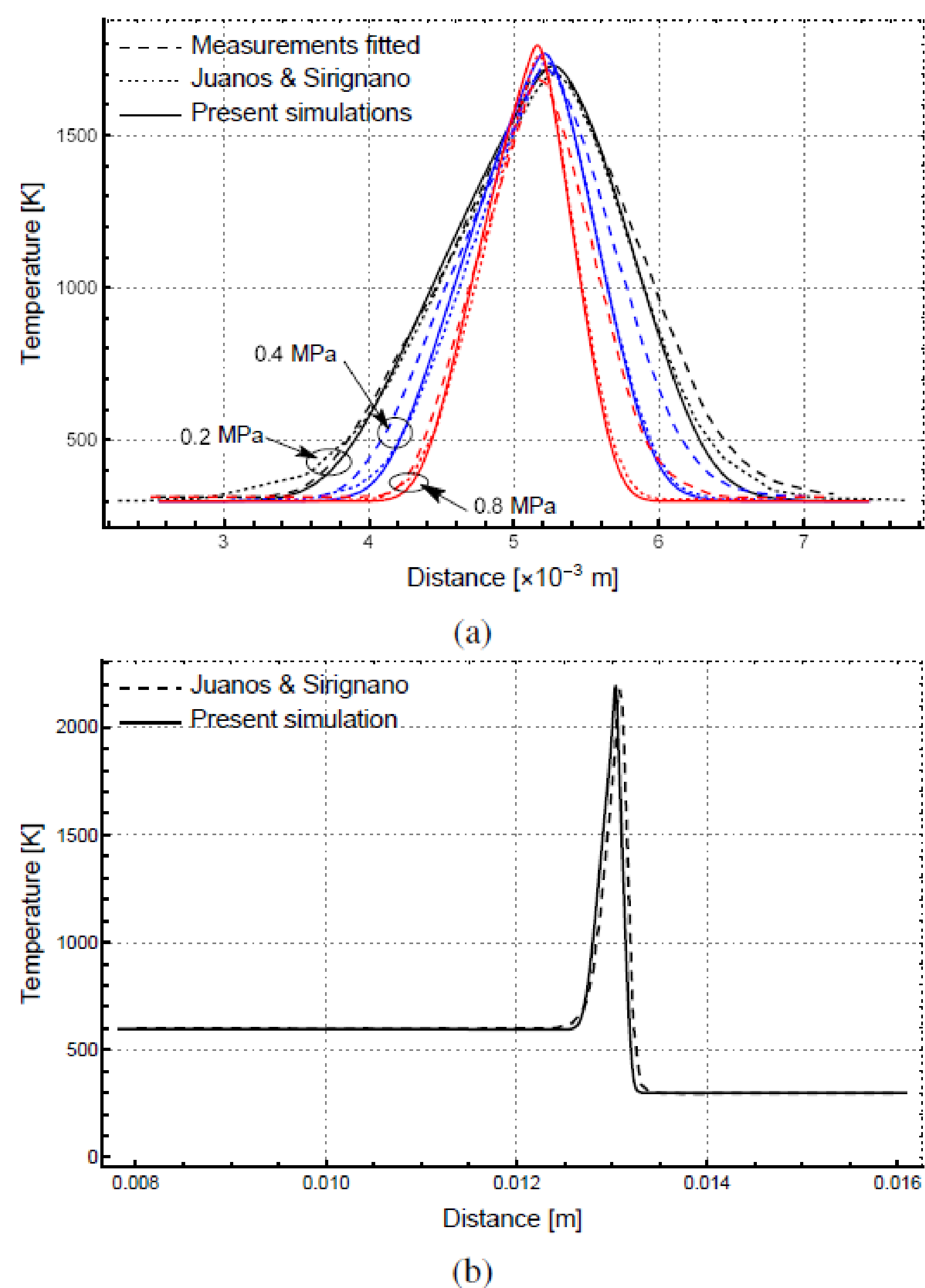


Figure 1: Temperature profile comparisons with experiment data [1] and simulation results [2]. (a) Pressure at 0.2, 0.4 and 0.8 MPa. (b) Pressure at 100 atm.

This encouraging agreement from preliminary results between the previous simulations and experiments with our methodology justifies the present methodology to predict the flammability limit of high pressure water-laden methane/air flame.



Primary project goal

Develop a real gas kinetic chemistry model for high pressure combustion and investigate the physics of the subject under such extreme conditions

Project Deliverables

Short term

- Coupling and assessment of the real gas effects for large scale kinetic reaction
- Implementation of efficient chemistry model for high pressure
- Simulation of laboratory flame mentioned in the previous section for validation and verification

Long term

- Advance the technologies in petroleum-fueled power generation systems
- Produce sufficient preliminary results to serve as the necessary basis for future collaborative proposal

Potential Impact

The significance of this research is also evident from the continuously growing interest of government agencies such as AFRL, DOD, DOE, NASA along with the commercial companies like Honeywell, GE and Boeing. That is due to the impact of this research on important issues such as **combustion efficiency, alternative fuel research and pollution control.**

References and Acknowledgements

[1]- Niemann, U., Seshadri, K., and Williams, F. A., *Combustion and Flame*, 161(1):138–146 (2014).

[2]- Juanos, A. J. and Sirignano, W. A., *Combustion and Flame*, 181:54–70 (2017).

Pitt Research

Center for Research Computing

Mascaro Center
for Sustainable Innovation

