

EXPLORING THE DEFLAGRATION-AUTOIGNITION-DETONATION TRANSITION IN THE CONTEXT OF PRESSURE GAIN COMBUSTION (WORK IN PROGRESS)

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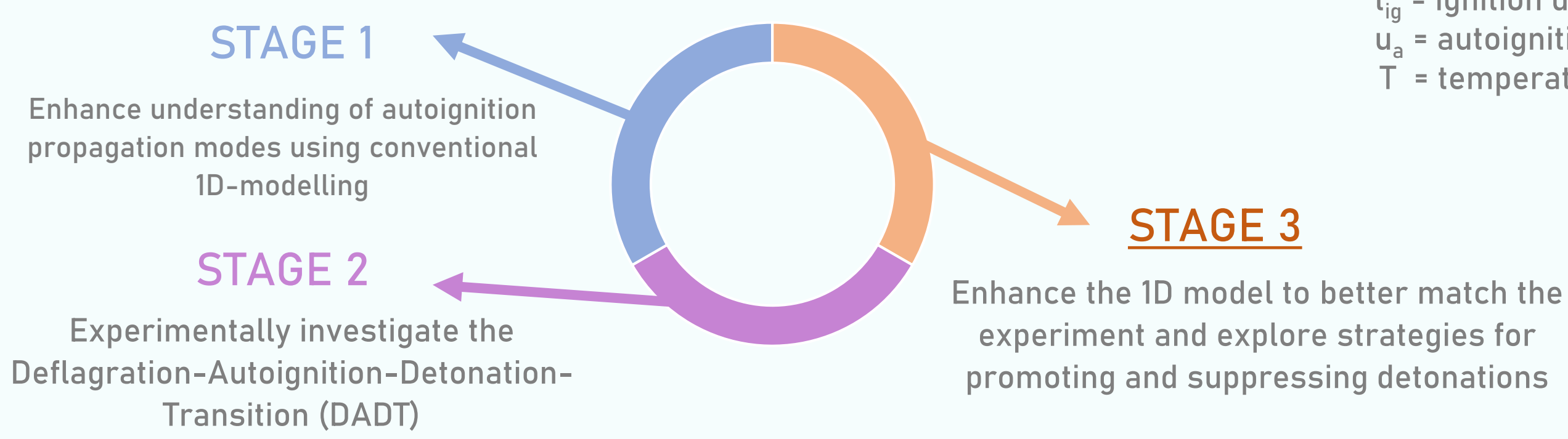
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INTRODUCTION

01 PROJECT MOTIVATION

Autoignition of hot spots can develop into a detonation under certain conditions. Detonations must be suppressed in Constant Volume Combustion and promoted in Rotating Detonation Combustion. Controlling the transition between combustion regimes is key to developing pressure gain combustion.

02 PROJECT OBJECTIVES



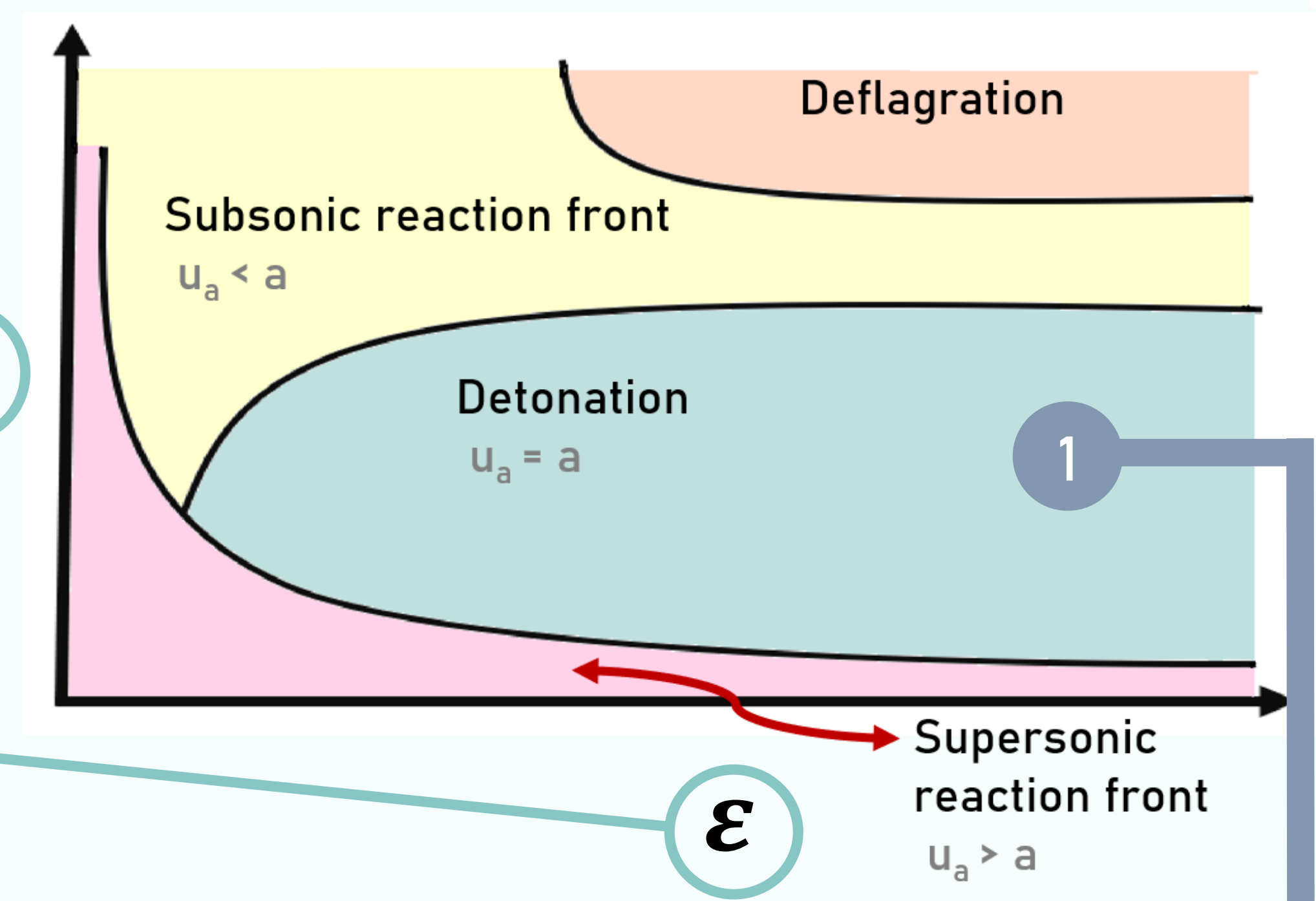
03 REGIME DIAGRAM

The propagation modes of hot spots under different conditions can be represented by a regime diagram. The different hotspot conditions are represented by 2 dimensionless parameters.

a = the local speed of sound
 r = radius
 r_0 = hotspot radius
 t_e = excitation time
 t_{ig} = ignition delay time
 u_a = autoignition wave speed
 T = temperature

$$\xi = a / \left(\frac{dr}{dT} * \frac{dT}{dt_{ig}} \right)$$

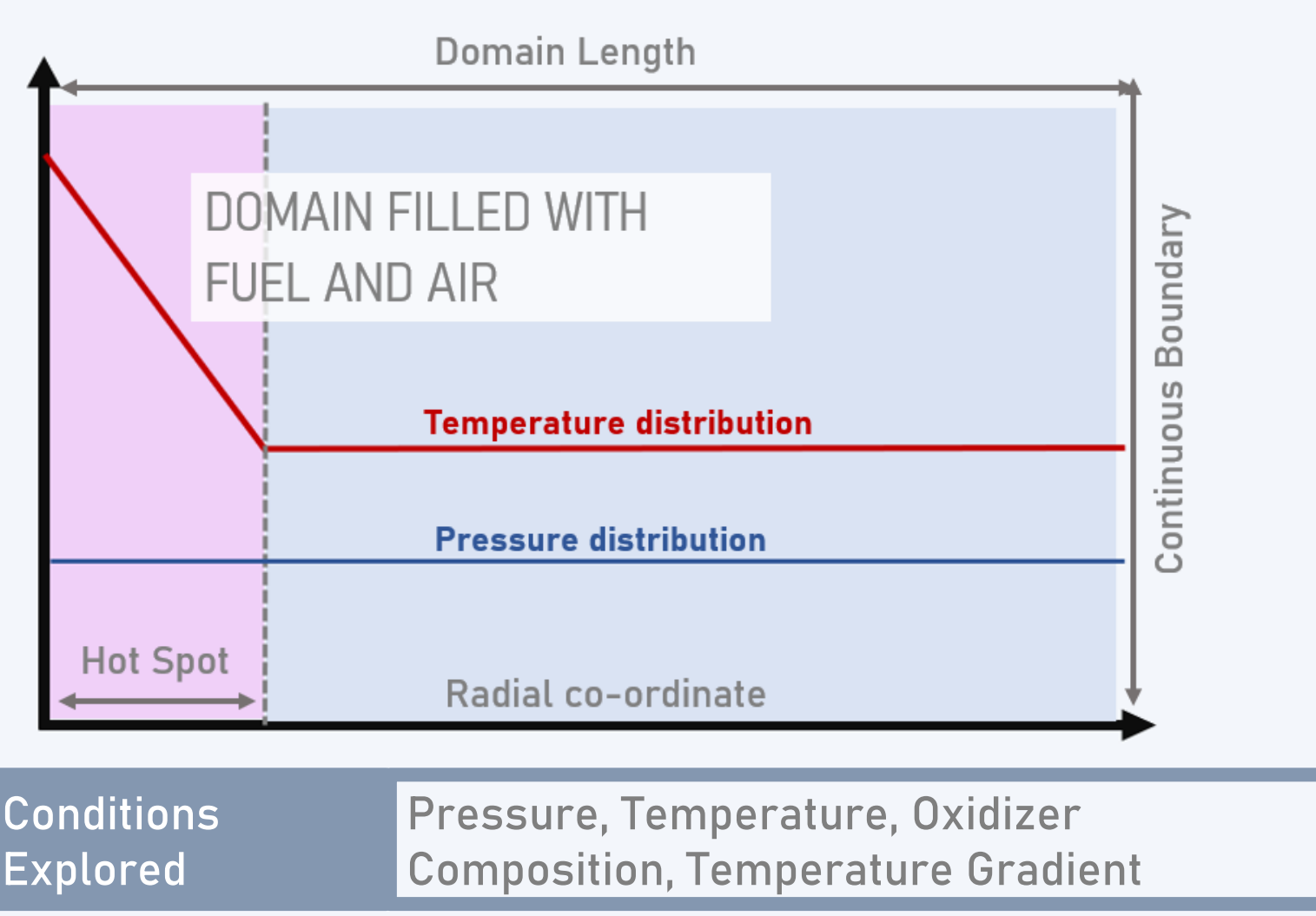
$$\varepsilon = (r_0 / a) / t_e$$



STAGE 1 METHODOLOGY

04 MODEL USED

The diagram below shows the Initial conditions and set-up for a 1-D spherical hotspot simulation.



05 CODE USED

- INSFLA CODE
- Provided by the Karlsruhe Institute of Technology
- Provides time and space solutions for 1-D reacting flows with multi-step chemistry and multi-species transport
- Solves mass, energy, momentum and species conservation equations
- Compressible Navier-Stokes equations, implicit time integration method, finite difference method
- Fixed number of grid points, Grid points move so there is a finer mesh around propagating waves and detonations zones

06 POST PROCESSING

A code was written in Python to track the reaction wave through tracking the maximum concentration gradient of radicals associated with the reaction.

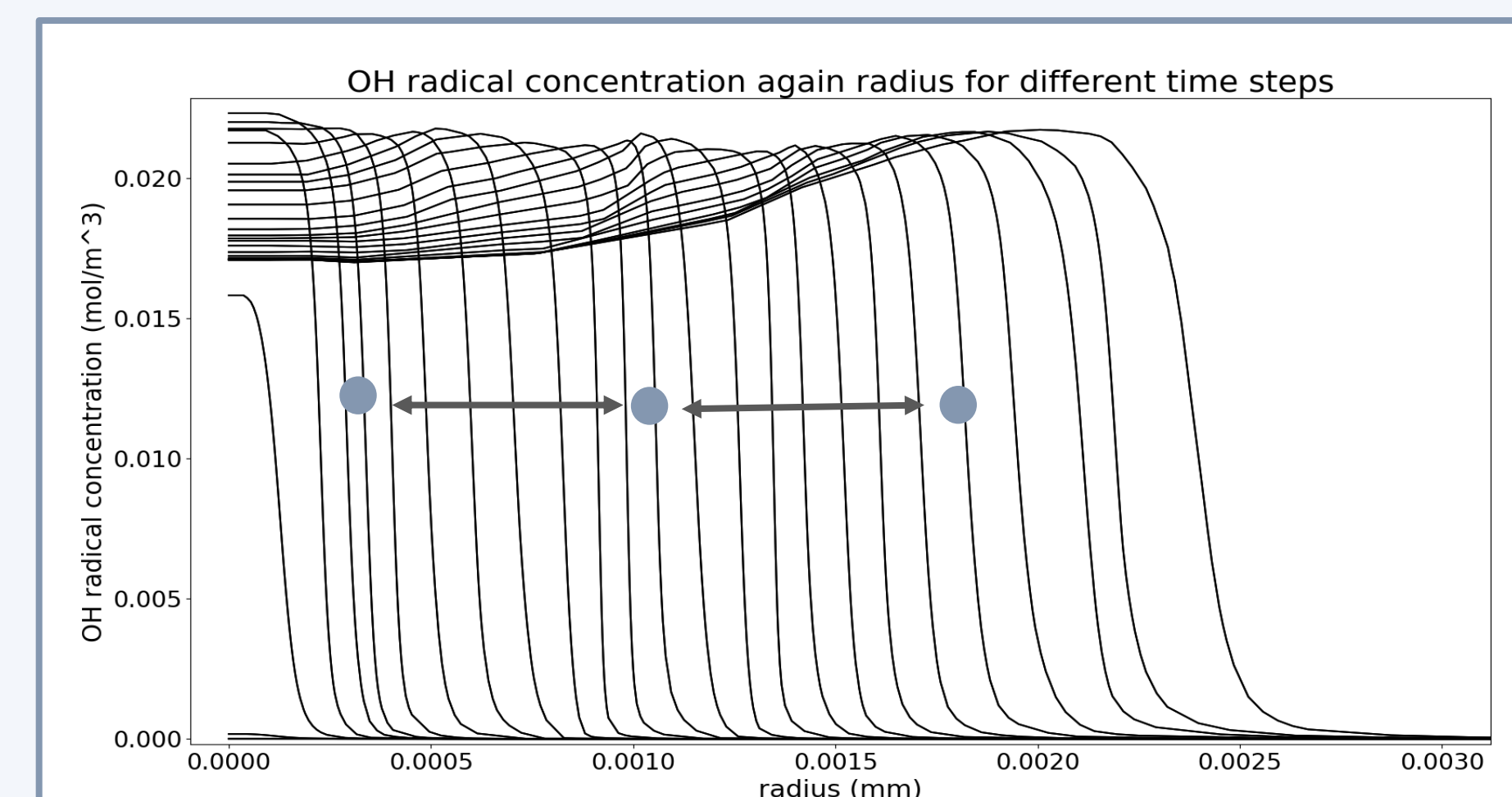


Figure 1: Graph of OH concentration. Each line is a different time profile. The position of maximum OH concentration is used to track the reaction wave and therefore calculate the reaction wave speed.

07 DETONATION IDENTIFICATION

- The reaction front propagation speed reaches at least 90% of the Chapman Jouguet (C-J) detonation speed
- The maximum pressure is at least 2 times the constant volume adiabatic equilibrium pressure (PE)

Figure 2 shows the temperature and pressure profiles for a detonation. Each of the lines represents a different time profile. The sharp pressure spikes associated with detonations can be observed

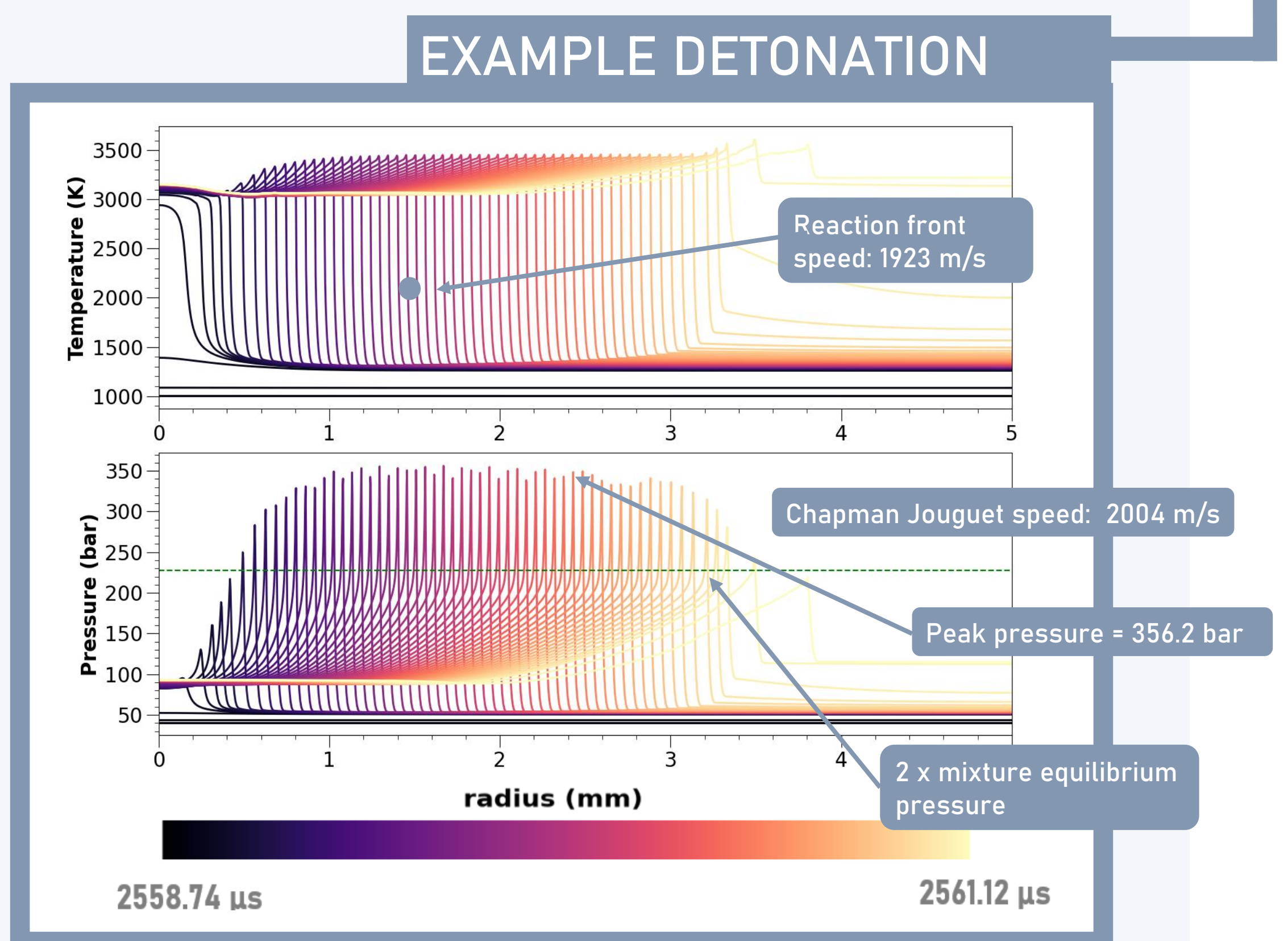


Figure 2: Stoichiometric hydrogen in air, 1000 K, 40.53 bar, 5 cm domain length, 1 mm hotspot radius, temperature gradient of 150 K/m, planar configuration.

STAGE 1 RESULTS AND PERSPECTIVES

The autoignition of hotspots of different radii and temperature gradients were simulated. This was done for both a stoichiometric hydrogen in air mixture and a rich hydrogen in air mixture. For each hotspot, the resulting propagation modes were observed and the dimensionless parameters were calculated. Each hotspot was plotted in the peninsula shown in figure 3.

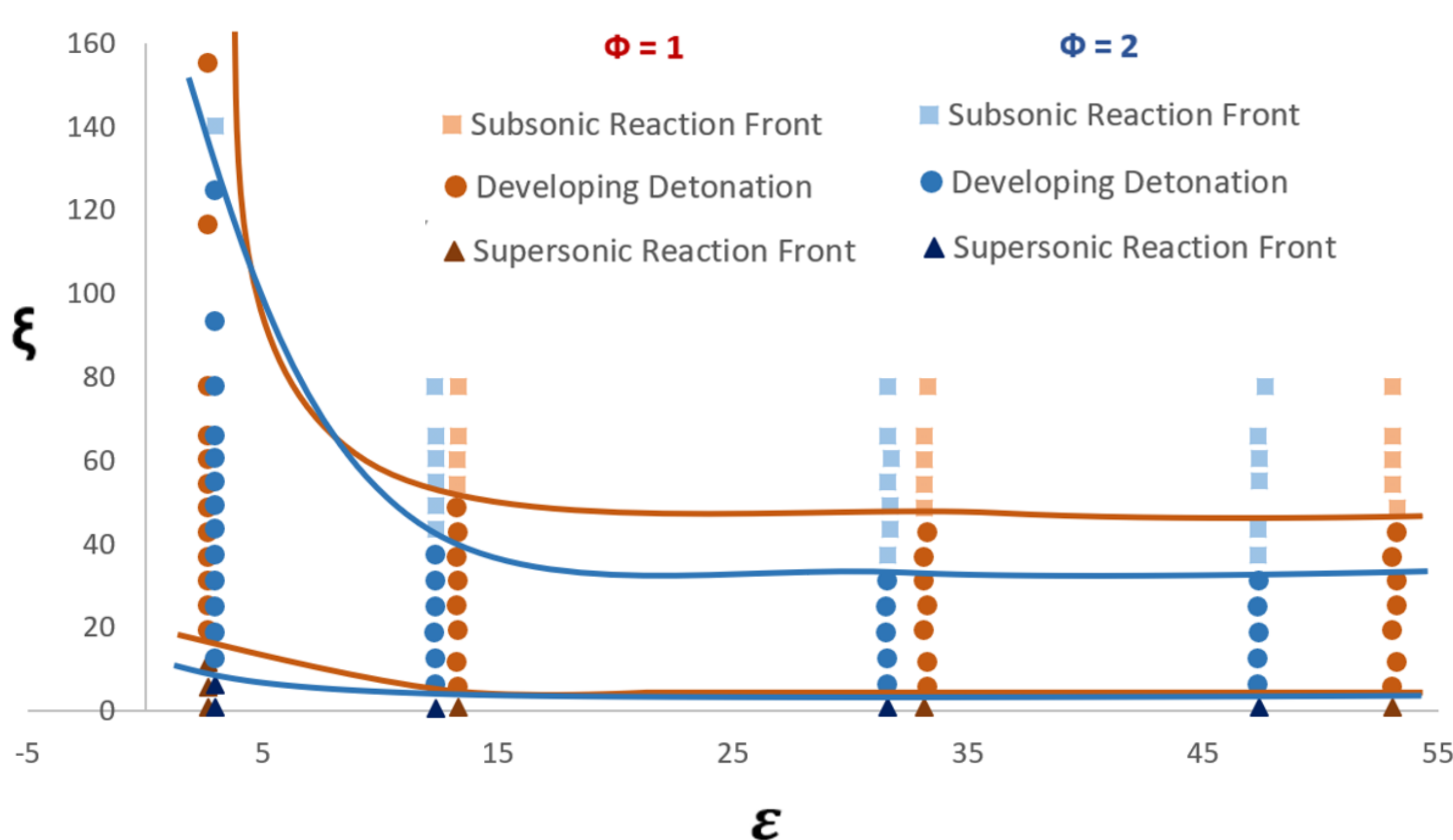


Figure 3: Detonation peninsula for hydrogen in air at 40 atm and 1000 K. The orange points are for the stoichiometric case where $\Phi = 1$ and the blue points are for the rich case where $\Phi = 2$. The lines enclose the boundaries for developing detonations.

To try and understand the trends observed in the results, X-T diagrams were plotted for a case where a detonation developed outside of the hotspot radius. Key observations are displayed in figure 4

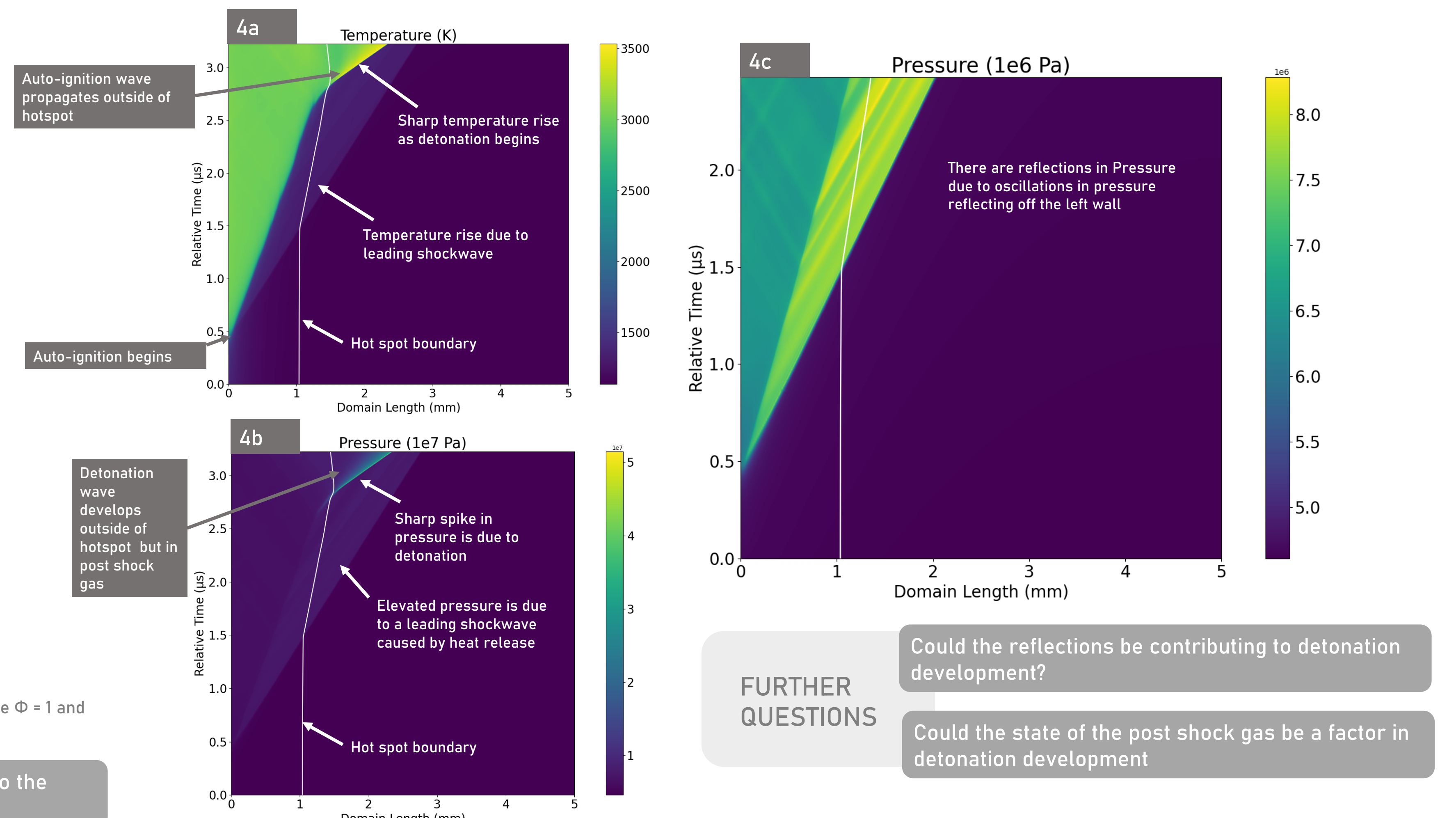


Figure 4: X-T plots of pressure and temperature. Time is measured relative to the time of 2533.471846657967 μs (chosen just before autoignition occurs). Figure 4a shows the temperature profile up until a detonation occurs. Figure 4b is the pressure profile up until a detonation occurs. Figure 4c is the pressure profile before a detonation occurs. This simulation is for a 1 mm hotspot in a 5 mm chamber for a stoichiometric Hydrogen air mixture at 1000 K, 40 Atm and a temperature gradient of 1250 K/m.

OBSERVATIONS

- A richer mixture has a narrower detonation regime when compared to the stoichiometric mixture
- In both cases there is a rhino-horn shape. It appears that the smaller the hotspot, the wider the detonation regime

FURTHER QUESTIONS

- Could the reflections be contributing to detonation development?
- Could the state of the post shock gas be a factor in detonation development