Spherical Inward Propagating Flame of Type Ia Supernova

1. Introduction

Supernova represent the catastrophic explosions that mark the end of the life of some stars. The ejected mass is of order 1 to 10 solar masses with bulk velocities ranging from a few thousand to a few tens of thousands of km/s.[^1] The traditional single Chandrasekhar mass C–O White Dwarf burning is still considered to be responsible for a large population of type Ia supernova (SN Ia). Specifically, one of the key issues in its modeling is related to the flame acceleration and deflagration-detonation transition (DDT), with flame front instabilities being considered as a possible mechanism in driving the acceleration. The perspective of this proposal is to give a set of solutions of this problem. The milestones of this project are planed to be:

(a) Complete a set of code that can solve the simplest reacting flow in SN Ia conditions.

(b) Try to observe spherical flame acceleration with large Lewis number curvature effect.

(c) Try to observe deflagration-detonation transition (DDT) in (b).

2. Basic Equations

- Control equations of 1D, spherical coordinates:
  - Continuity Equation:

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{\partial(\hat{\rho}u)}{\partial \hat{r}} + \frac{2(\hat{\rho}\hat{u})}{\hat{r}} = 0$$

  - Momentum Equation:

$$\frac{\partial(\hat{\rho}\hat{u})}{\partial \hat{t}} + \frac{\partial(\hat{\rho}\hat{u}^2 + \hat{P})}{\partial \hat{r}} + \frac{2(\hat{\rho}\hat{u}^2)}{\hat{r}} = 0$$

  - Energy Equation:

$$\frac{\partial(\hat{\rho}\hat{E}_s)}{\partial \hat{t}} + \frac{\partial(\hat{\rho}\hat{u}\hat{E}_s + \hat{u}\hat{P})}{\partial \hat{r}} + \frac{2(\hat{\rho}\hat{u}\hat{E}_s + \hat{u}\hat{P})}{\hat{r}} = \lambda\frac{\partial^2 \hat{T}}{\partial \hat{r}^2} + \frac{2\lambda}{\hat{r}}\frac{\partial \hat{T}}{\partial \hat{r}}$$

  - Convection Diffusion Equation:

$$\frac{\partial(\hat{\rho}\hat{Y})}{\partial \hat{t}} + \frac{\partial(\hat{\rho}\hat{u}\hat{Y})}{\partial \hat{r}} + \frac{2(\hat{\rho}\hat{u}\hat{Y})}{\hat{r}} = \frac{\partial}{\partial \hat{r}}(\hat{\rho}D\frac{\partial \hat{Y}}{\partial \hat{r}}) + \frac{2\hat{\rho}D}{\hat{r}}\frac{\partial \hat{Y}}{\partial \hat{r}} - \hat{\omega}$$

  - Equation of Reaction:

$$\hat{\omega} = A\hat{\rho}^k\hat{Y}^2\exp(\frac{-\hat{E}_a}{\hat{T}_9^{\frac{1}{3}}})$$

– Equation of State:

$$\hat{E}_{(\rho,T)} = \frac{3}{4\hat{\rho}}(3\pi^2)^{1/3}\hbar c_1(\hat{\rho}N)^{4/3} + \frac{1}{2}N\frac{(3\pi^2)^{2/3}}{3\hbar c_1}(\frac{1}{\hat{\rho}N})^{1/3}(k\hat{T})^2$$

$$\hat{E}_s = \hat{E}_{(\rho,T)} + \frac{1}{2}\hat{u}^2 + q\hat{Y}$$

$$\hat{P} = \frac{\hat{\rho}\hat{E}_{(\rho,T)}}{3}$$

3. Dimensionless Equations

Dimensionless variables	Reference values
$\rho = \frac{\hat{\rho}}{\hat{\rho_0}}$	$\hat{\rho_0} = 3.5 * 10^{10} kg/m^3$
$u = \frac{\hat{u}}{\hat{u_0}}$	$\hat{u_0} = C_t S_c, S_c = 466 m/s$ (laminar flame speed)
$t = \frac{\hat{t}}{\hat{t_0}}$	$\hat{t_0} = \frac{\delta_f}{\hat{u}_0}, \frac{\delta_f}{S_c} = 1.93{*}10^{-6} s$
$E = \frac{\hat{E}}{\hat{E}(\hat{T}_b, \hat{\rho_0})}$	$\hat{E}(\hat{T}_b, \hat{\rho_0}) = \frac{3}{4\hat{\rho_0}}(3\pi^2)^{1/3}\hat{h}c_1(N\hat{\rho_0})^{4/3} + \frac{1}{2}N\frac{(3\pi^2)^{2/3}}{3\hat{h}c_1}(\frac{1}{\hat{\rho_0}N}$
$T = \frac{\hat{T} - \hat{T_0}}{\hat{T}_{ad} - \hat{T_0}}$	$\hat{T_0} = 1{*}10^8 K; \hat{T_{ad}} = 3.2{*}10^9 K$
$Y = \frac{\hat{Y}}{\hat{Y_0}}$	$\hat{Y_0} = 1$

Dimensionless variables	Reference values
$r = \frac{\hat{r}}{\hat{r_0}}$	$\hat{r_0} = \delta_f = \frac{\lambda}{\rho_0 C_p S_c} = 9{*}10^{-4} m$
$\omega = \frac{\hat{\omega}}{\hat{\omega_0}}$	$\hat{\omega_0} = \frac{\hat{\rho_0}\hat{Y_0} S_c}{\delta_f} = \hat{\omega}(\hat{Y_0}, \hat{T_0}, \hat{\rho_0})$
$P = \frac{\hat{P}}{\hat{P_0}}$	$\hat{P_0} = \frac{\hat{\rho_0}\hat{E}(\hat{T_b}, \hat{\rho_0})}{3}$

Consider velocity dimensionless with sound speed

$$A_1 = \hat{E}(\hat{\rho_0}, \hat{T_b})/\hat{u}_0^2 = 1$$

Enthalpy per unit is

$$\text{qcon} = \frac{\lambda(\hat{T_b} - \hat{T_0})}{\hat{\rho_0} S_c \delta_f \hat{E}(\hat{\rho_0}, \hat{T_b})} = \frac{E(\hat{\rho_0}, \hat{T_b}) - E(\hat{\rho_0}, \hat{T_0})}{E(\hat{\rho_0}, \hat{T_b})} = 0.21811$$

Another constant

$$A_2 = \text{qcon} \times S_c/\hat{u}_0 = 1.460 \times 10^{-5}$$

- Governing Equations:
  - Continuity Equation:
$$\frac{\partial \rho}{\partial t} + (\frac{\partial}{\partial r} + \frac{2}{r})(\rho u) = 0$$
  - Momentum Equation:
$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial r}(\rho u^2 + \frac{A_1 P}{3}) + \frac{2\rho u^2}{r} = 0$$
  - Energy Equation:
$$\frac{\partial(\rho E_s)}{\partial t} + (\frac{\partial}{\partial r} + \frac{2}{r})(\rho u E_s + \frac{uP}{3}) = (\frac{\partial}{\partial r} + \frac{2}{r})(A_2 \frac{\partial T}{\partial r})$$

– Convection Diffusion Equation:

$$\frac{\partial(\rho Y)}{\partial t} + (\frac{\partial}{\partial r} + \frac{2}{r})(\rho u Y) = (\frac{\partial}{\partial r} + \frac{2}{r})(\frac{\rho}{Le_0 C_t}\frac{\partial Y}{\partial r}) - \frac{1}{C_t}\omega$$

– Equation of Reaction:

$$\omega = \rho Y exp(\frac{-Ea}{T_9^{\frac{1}{3}}} - \frac{-Ea}{{T_b}_9^{\frac{1}{3}}})$$

– Equation of State:

$$P = \rho E_{(\rho,T)}$$

$$E_s = E_{(\rho,T)} + \frac{1}{2}u^2 + qY = \frac{E(\hat{\rho},\hat{T})}{E(\hat{\rho_0},\hat{T_b})} + \frac{1}{2A_1}u^2 + qconY$$

4. Code setting

- Equations for programming:

$$U = (\rho, \rho u, \rho E_s, \rho Y)$$

$$F = (\rho u, \rho u^2 + \frac{A_1 P}{3}, \rho u E_s + \frac{uP}{3}, \rho u Y)$$

$$G = (\rho u, \rho u^2, \rho u E_s + \frac{uP}{3}, \rho u Y)$$

$$D = (0, 0, A_2\frac{\partial T}{\partial r}, \frac{\rho}{Le_0 C_t}\frac{\partial Y}{\partial r})$$

$$S = (0, 0, 0, -\frac{\omega}{C_t})$$

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial r} + \frac{2G}{r} = \frac{\partial D}{\partial r} + \frac{2D}{r} + S$$

- Discrete methods:
  – Time evolution: 3 order TVD `Runge-Kutta`

$$U^{(1)} = U_n + L(U_n)\Delta t$$

$$U^{(2)} = \frac{3}{4}U_n + \frac{1}{4}(U^{(1)} + L(U^{(1)})\Delta t)$$

$$U_{n+1} = \frac{1}{3}U_n + \frac{2}{3}(U^{(2)} + L(U^{(2)})\Delta t)$$

- Convection term:

  `Roe` method: solve convection flux by eigen vector

- Diffusion term: 6 order central difference

  $$\frac{\partial m_i}{\partial x} = \frac{1}{60}m_{i+3} - \frac{9}{60}m_{i+2} + \frac{45}{60}m_{i+1} - \frac{45}{60}m_{i-1} + \frac{9}{60}m_{i-2} - \frac{1}{60}m_{i-3}$$

- Initial conditions:
  - Pressure: whole field the same pressure $\hat{P}(\rho_0, T_0)/\hat{P}_0$
  - Velocity: near zero (can not set zero beacuse of Roe method eigen vector has 1/velocity)
  - Concentration: $Y_0 = 1$
  - Temperature: $T_0 \to T_b$, $\tanh(x)$ profile for about 1 flame thickness area
- Boundary conditions: (cartesian coordinates)
  - Inner boundary conditions:
    * symmetric
  - Outlet boundary conditions
    * symmetric
- Boundary conditions: (spherical coordinates)
  - Inner boundary conditions:
    * conservation ($\int \dot{\rho}_{inner} dV = \int \rho u S dt$)
  - Outer boundary conditions:
    * density: constant
    * velocity: extrapolatation ($m_1 = 2m_0 - m_{-1}$)
    * energy: constant
    * concentration: constant

5. Results

- 1D cartesian coordinates:
  - no reaction acceleration
    * distribution ρ, T, Y, ω of at different time (dimensionless time):
    * flame position and flame velocity (dimensionless time):
  - reaction accelerate ratio = 20
    * distribution ρ, T, Y, ω of at different time:
    * flame position and flame velocity:
  - no reaction acceleration but with wider reaction position

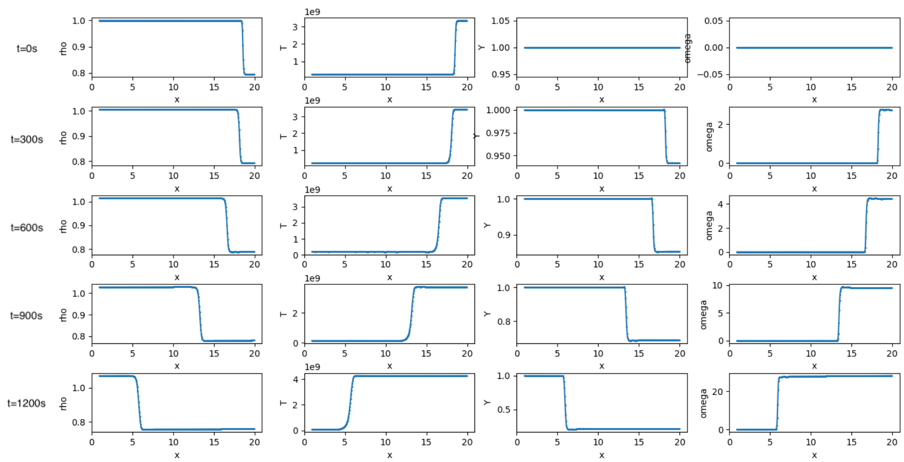

Figure 1: time_eval_no_acc

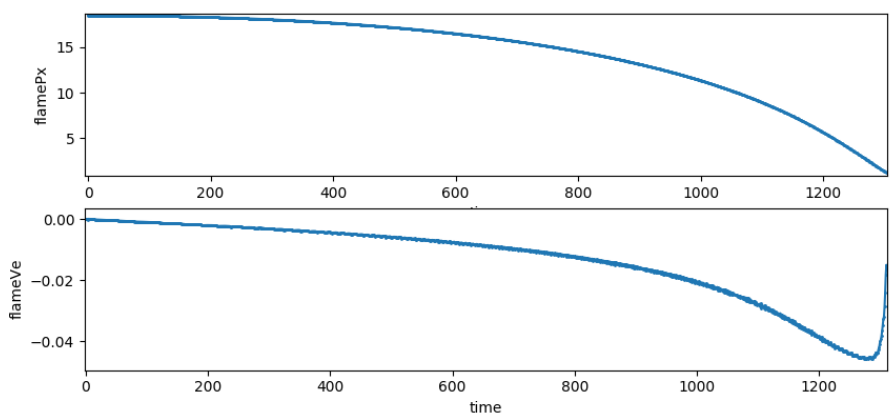

Figure 2: flame_vel_noacc

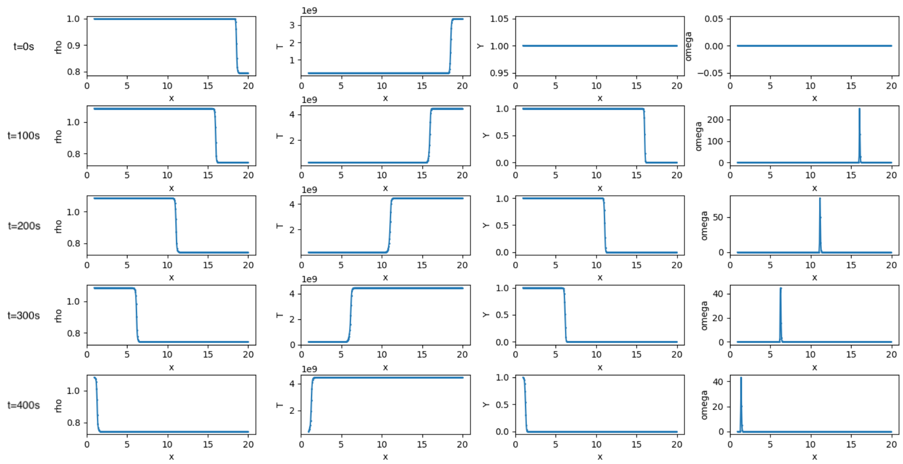

Figure 3: time_eval_acc20

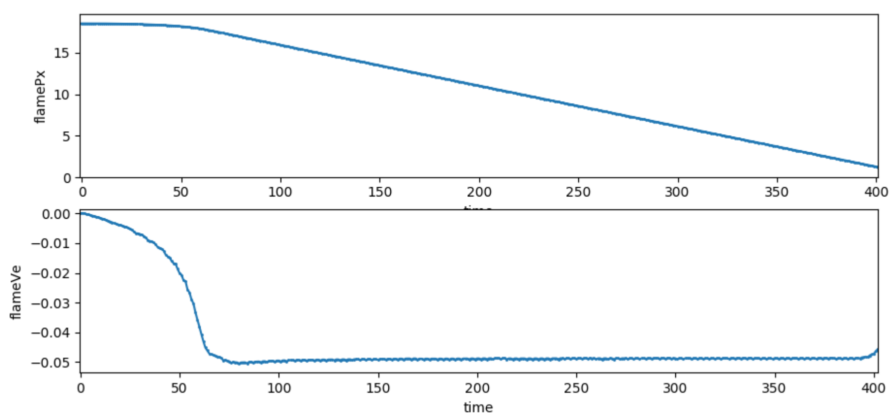

Figure 4: flame_vel_acc=20

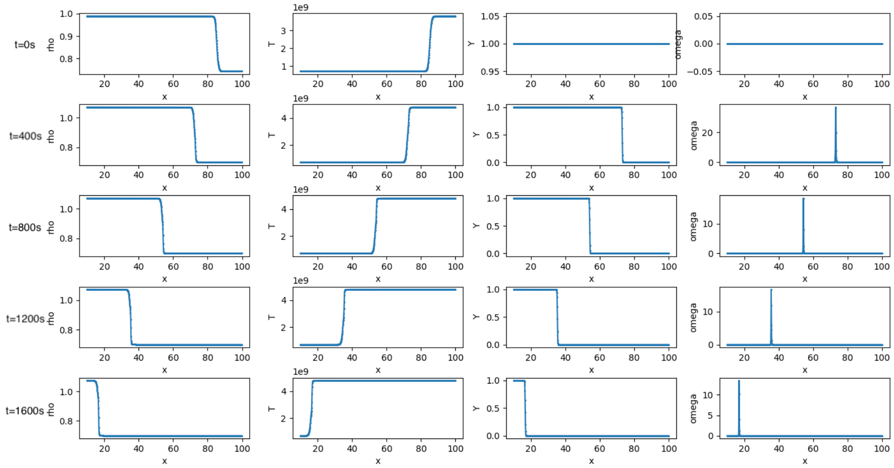

Figure 5: time_eval_acc20

∗ distribution ρ, T, Y, ω of at different time:

∗ flame position and flame velocity:

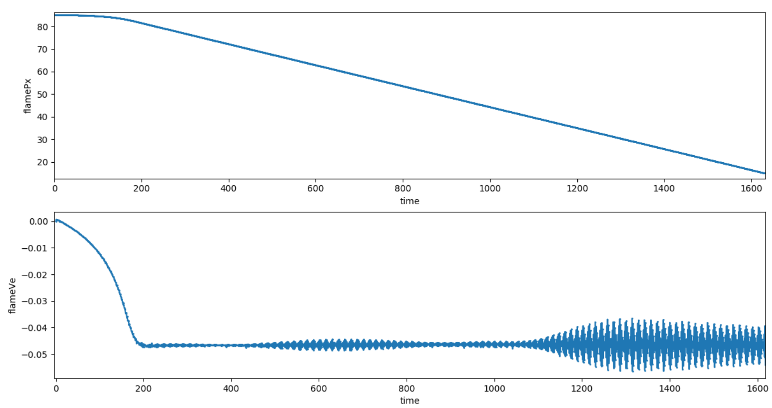

Figure 6: flame_vel_acc

Accelerate as exponential function type and propagates with maximum velocity about 0.05 sound speed

- 1D sphercial coordinates:

6. Appendix

- Calculating ρ from P and $\hat{T}$:
  - Equation of state:

$$\frac{PE_{Tb}}{\rho} = \frac{3}{4}(3\pi^2)^{\frac{1}{3}}\hbar c_1 N^{\frac{3}{4}}\hat{\rho}_0^{\frac{1}{3}}\rho^{\frac{1}{3}} + \frac{1}{2}N^{\frac{2}{3}}(3\pi^2)^{\frac{2}{3}}\frac{k^2}{3\hbar c_1}\hat{T}^2\hat{\rho}_0^{-\frac{1}{3}}\rho^{-\frac{1}{3}}$$

  - Set C_1, C_2 as:
    - $$C_1 = \frac{3}{4}(3\pi^2)^{\frac{1}{3}}\hbar c_1 N^{\frac{4}{3}}\hat{\rho}_0^{\frac{1}{3}}$$
    - $$C_2 = \frac{1}{2}N^{\frac{2}{3}}(3\pi^2)^{\frac{2}{3}}\frac{k^2}{3\hbar c_1}\hat{\rho}_0^{-\frac{1}{3}}$$
  - Set
$$x = \rho^{\frac{2}{3}}$$
  - We have:
$$C_1 x^2 + C_2\hat{T}^2 x = PE_{Tb}$$
  - So:

$$x = \sqrt{\frac{PE_{Tb}}{C_1} + \frac{C_2^2\hat{T}^4}{4C_1^2}} - \frac{C_2\hat{T}^2}{2C_1}$$

$$\rho = (\sqrt{\frac{PE_{Tb}}{C_1} + \frac{C_2^2\hat{T}^4}{4C_1^2}} - \frac{C_2\hat{T}^2}{2C_1})^{\frac{3}{2}}$$

- Calculate $\hat{T}$ from ρ and P:
  - Consider:
$$C_1 x^2 + C_2\hat{T}^2 x = PE_{Tb}$$

$$\hat{T} = \sqrt{\frac{PE_{Tb} - C_1\rho^{\frac{4}{3}}}{C_2\rho^{\frac{2}{3}}}}$$

- Eigen vector for `Roe` method: \$ U = [, u, E_s, Y] = [m_1, m_2, m_3, m_4] \$ \$ F = [u, u^2 + P/3, u E_s + u P/3, u Y] = [m_2, m_2^2/m_1+P/3 (m_3 + P/3) m_2 / m_1, m_4 m_2/m_1] \$
  - Solve by matlab symbol calculation:

```
% definition
syms rho u Es Y real
syms m1 m2 m3 m4 real
syms A1 qcon real

% declaration
P = m3-m2*m2/m1/2-qcon*m4;
Um = [m1 m2 m3 m4];
Fm = [m2; m2*m2/m1+P/3; m3*m2/m1+m2*P/m1/3; m2*m4/m1];

% solve
J = jacobian(Fm,Um);
[RM,RD] = eig(J);
[LM,LD] = eig(J');
```

– Eigenvalue Λ is:

$$\begin{aligned}\Lambda &= diag(m_2/m_1, m_2/m_1, m_2/m_1 + 2^{1/2} * (-m_2^2 + 2 * m_1 * m_3 - 2 * m_1 * m_4 * qcon)^{1/2}/(3 * m_1), m \\ &= diag(u, u, u + c, u - c)\end{aligned}$$

– Sound velocity:

$$\begin{aligned}c &= 2^{1/2} * (-m_2^2 + 2 * m_1 * m_3 - 2 * m_1 * m_4 * qcon)^{1/2}/(3 * m_1) \\ &= \frac{2}{3}\sqrt{-\frac{1}{2}u^2 + E_s - \mathrm{qcon}Y} = \frac{2}{3}\sqrt{P/\rho}\end{aligned}$$

– Right Eigen Matrix RM is:

$$\begin{aligned}RM = &[(2 * m_1^2)/m_2^2, \quad -(2 * m_1^2 * qcon)/m_2^2, m_1/m_4, \\ &[(2 * m_1)/m_2, \quad -(2 * m_1 * qcon)/m_2, (3 * m_2 + 2^{1/2} * (-m_2^2 + 2 * m_1 * m_3 - 2 * m_1 * m_4 * qc \\ &[1, \quad 0, (m_2 * (3 * m_2 + 2^{1/2} * (-m_2^2 + 2 * m_1 * m_3 - 2 * m_1 * m \\ &[0, \quad 1, 1,\end{aligned}$$

7. Reference

[1] Wheeler J C, Harkness R P, Rep. Prog. Phys. 1990, 53:1467-1557[2] https://en.wikipedia.org/wiki/Divergence#Spherical_coordinates[3] Landau L D , Lifshitz E M . Statistical Physics, Part 1[J]. Physics Today, 1980.[4] Woosely. 2011. FLAMES IN TYPE Ia SUPERNOVA: DEFLAGRATION–DETONATION TRANSITION IN THE OXYGEN-BURNING FLAME[5] Fowler, W. A., Caughlan, G. R., & Zimmerman, B. A. 1975, ARA&A, 13, 69