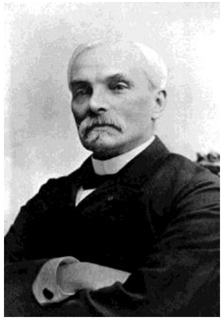
Onsager Relationships and the Chapman-Jouguet Deflagration

Eran Sher, Irena Moshkovich, Beni Cukurel
Faculty of Aerospace Engineering
The Technion - Israel Institute of Technology, Haifa, Israel

Mallard and Le-Chatelier 1886



François Ernest Mallard 1833-1894

Henry Louis Le Chatelier 1850-1936

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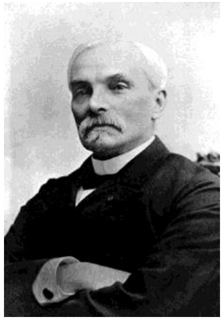

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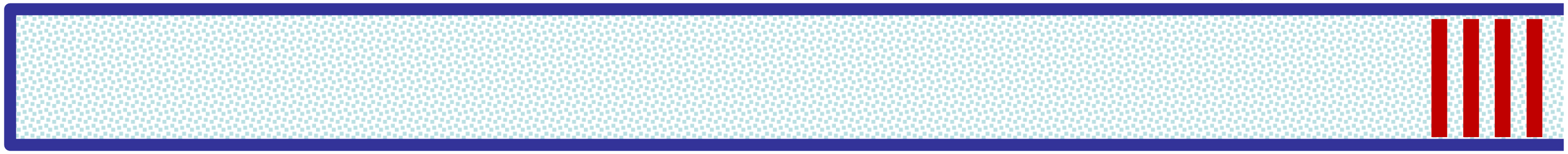

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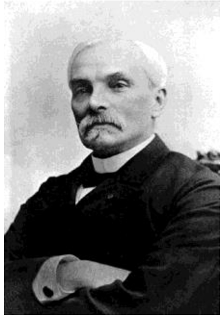

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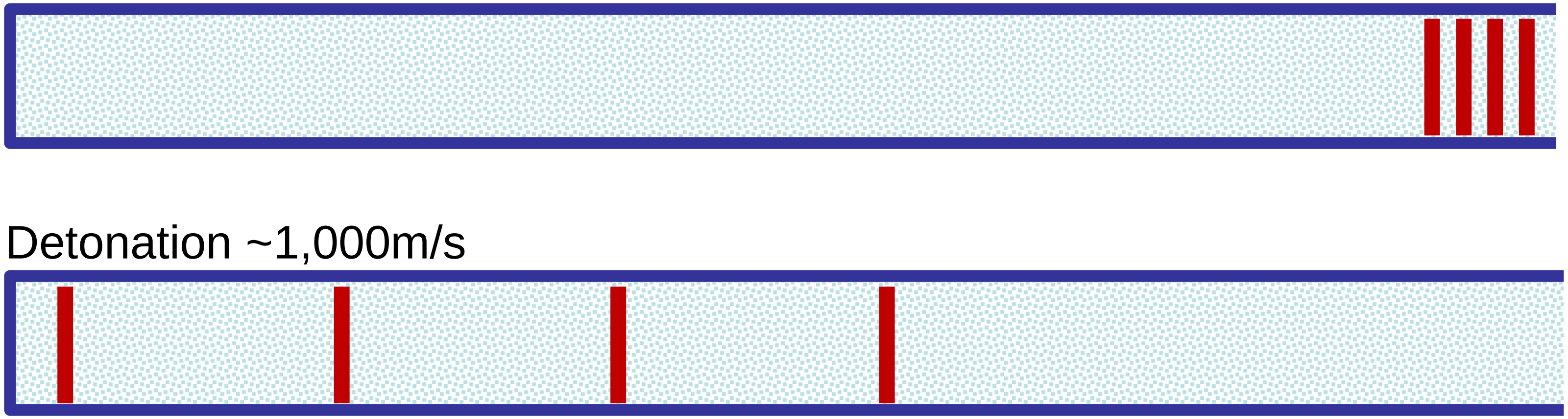
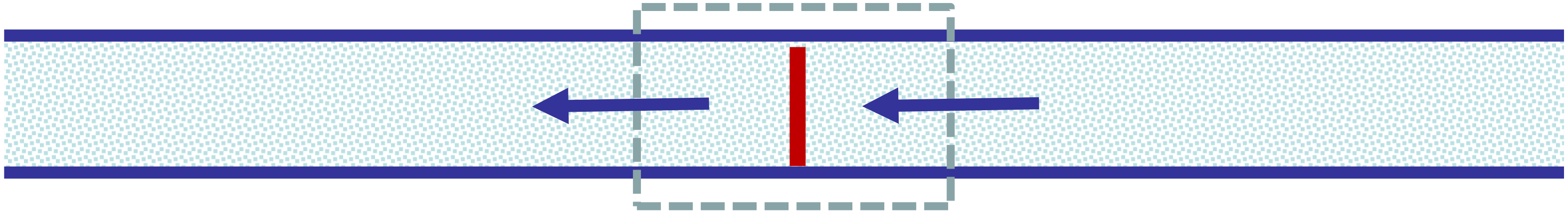
Ignition

Deflagration ~40cm/s

Detonation ~1,000m/s

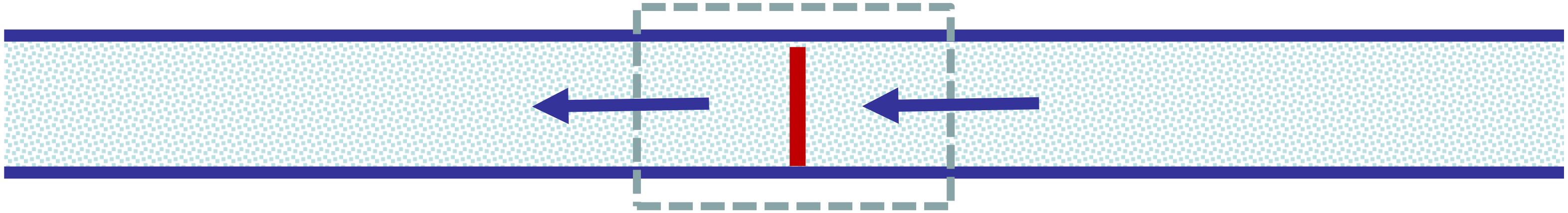


Classical Analysis - Assumptions



- SSSF
- Adiabatic duct
- The fluid inviscid $(\mu = 0)$
- The thermal conductivity is negligible $(k = 0)$
- The particles diffusivity is negligible
- The mixture behaves as ideal gas
- $C_P = const$

Classical Analysis - Equations



$T_P\ , P_P\ , \rho_P\ , u_P$ $\qquad$ $T_R\ , P_R\ , \rho_R , u_R$

Continuity: $\rho_R u_R = \rho_P u_P$

Momentum: $\rho_R u_R^2 + P_R = \rho_P u_P^2 + P_P$

Energy: $\dfrac{u_R^2}{2} + h_R = \dfrac{u_P^2}{2} + h_P$

Ideal gases: $Pv = RT$

Rayleigh-Hugoniot Equations

Lord Baron Rayleigh 1842-1919
Received the Nobel Prize 1904 in Physics

Rayleigh equation:

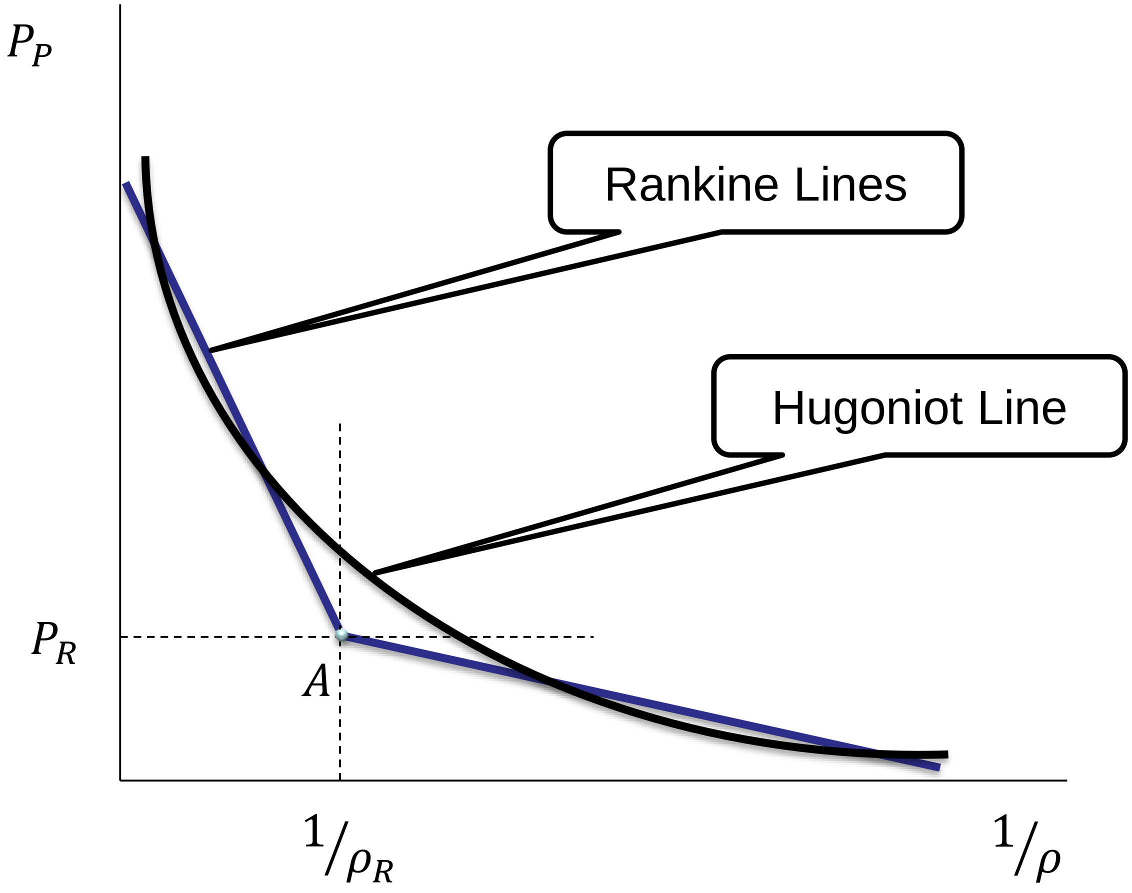
$$P_P = P_R - \left(\frac{1}{\rho_P} - \frac{1}{\rho_R}\right)\rho_R^2 u_R^2$$

Hugoniot equation:

$$\frac{k}{k-1}\left(\frac{P_P}{\rho_P} - \frac{P_R}{\rho_R}\right) - \frac{1}{2}(P_P - P_R)\left(\frac{1}{\rho_R} + \frac{1}{\rho_P}\right) = h_c$$

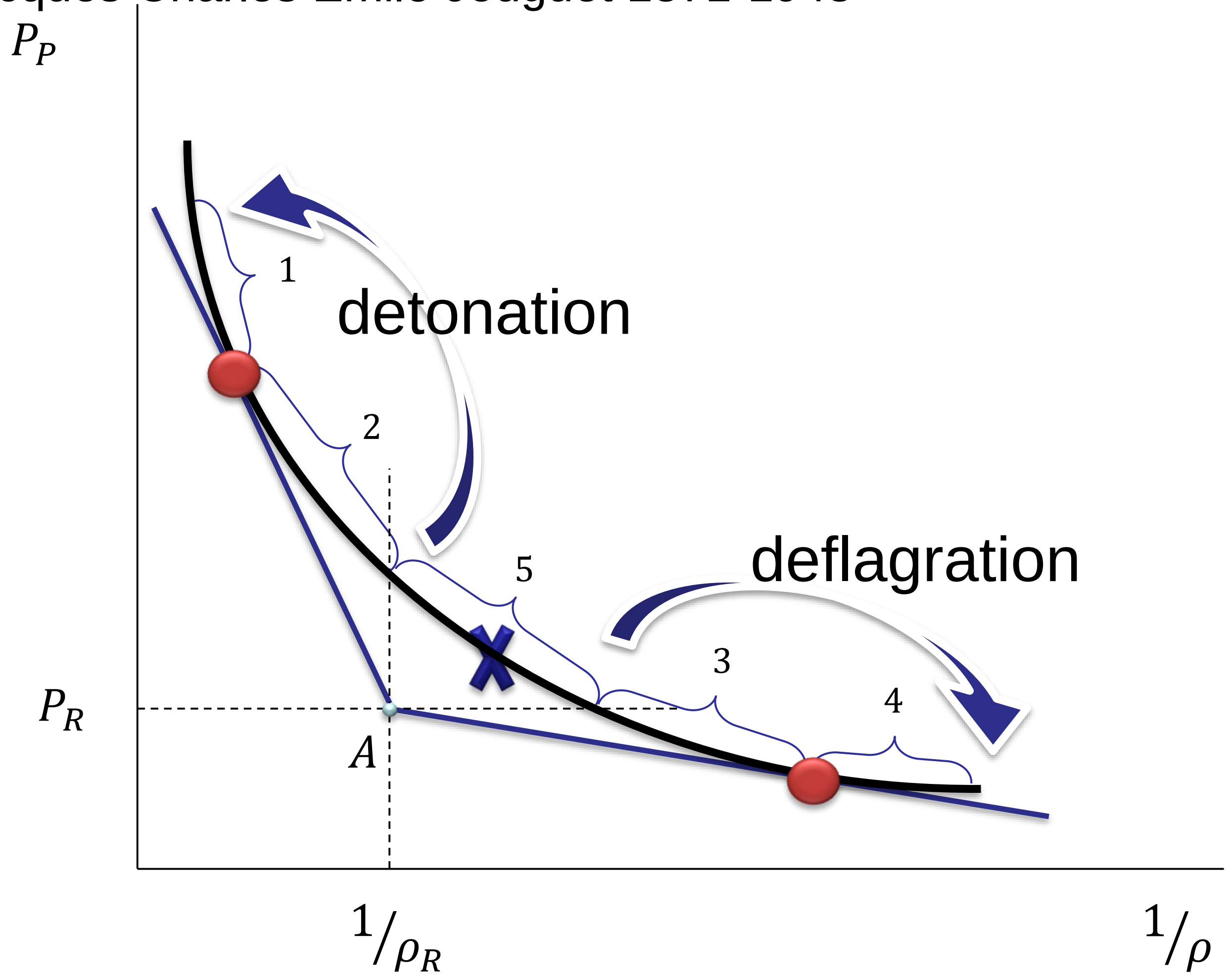
Rankine-Hugoniot Lines

Pierre-Henri Hugoniot 1851-1887
William John Macquorn Rankine 1820-1872

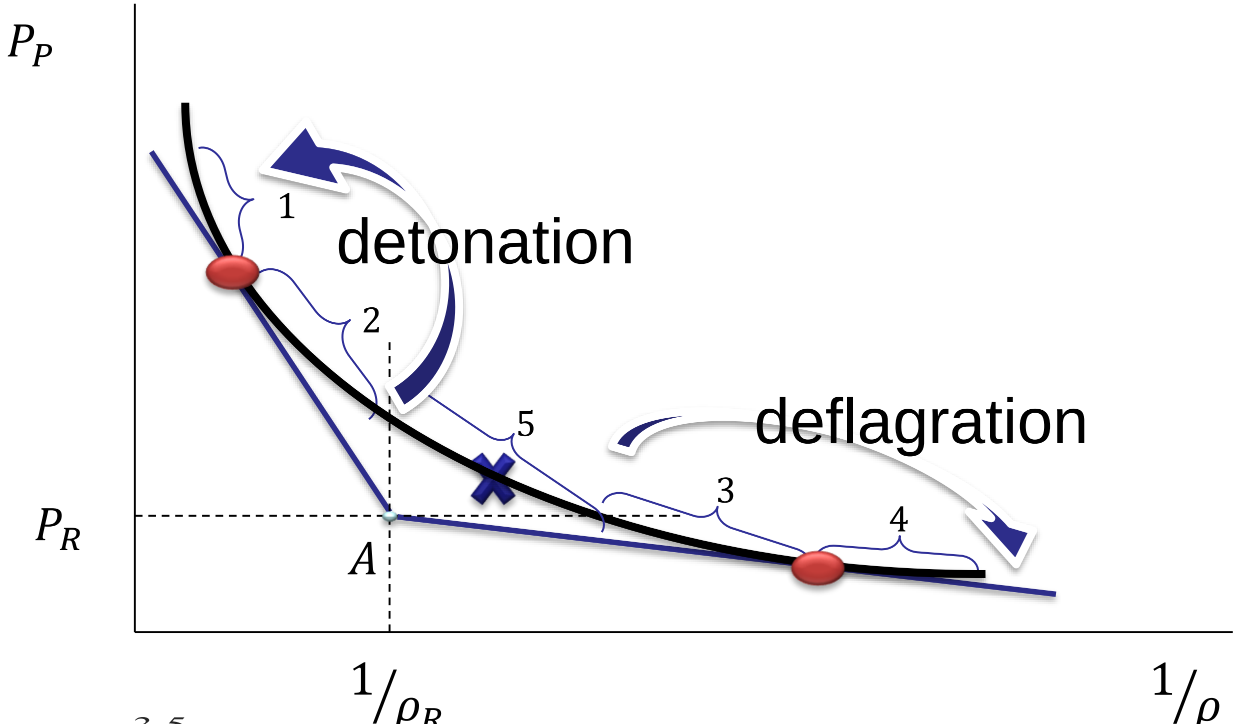


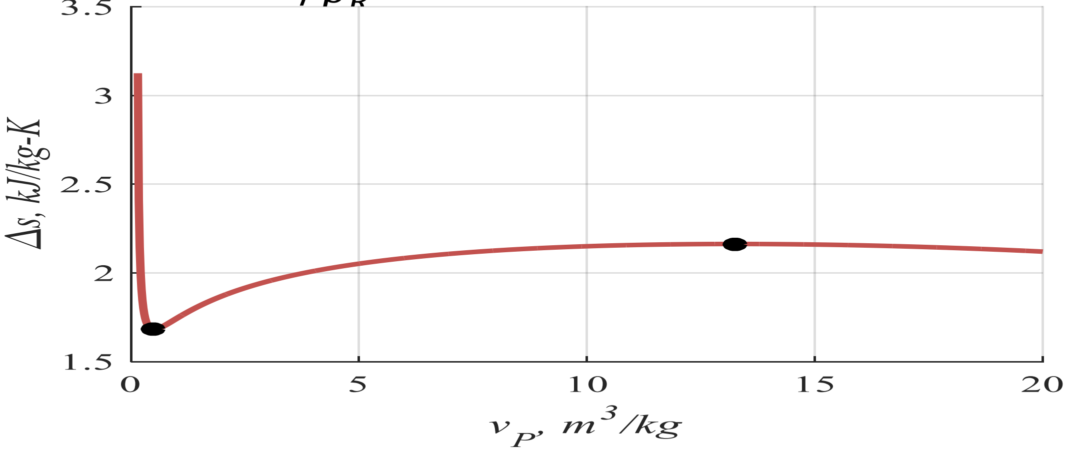
Chapman-Jouguet Points

David Leonard Chapman 1869-1958
Jacques Charles Émile Jouguet 1871-1943

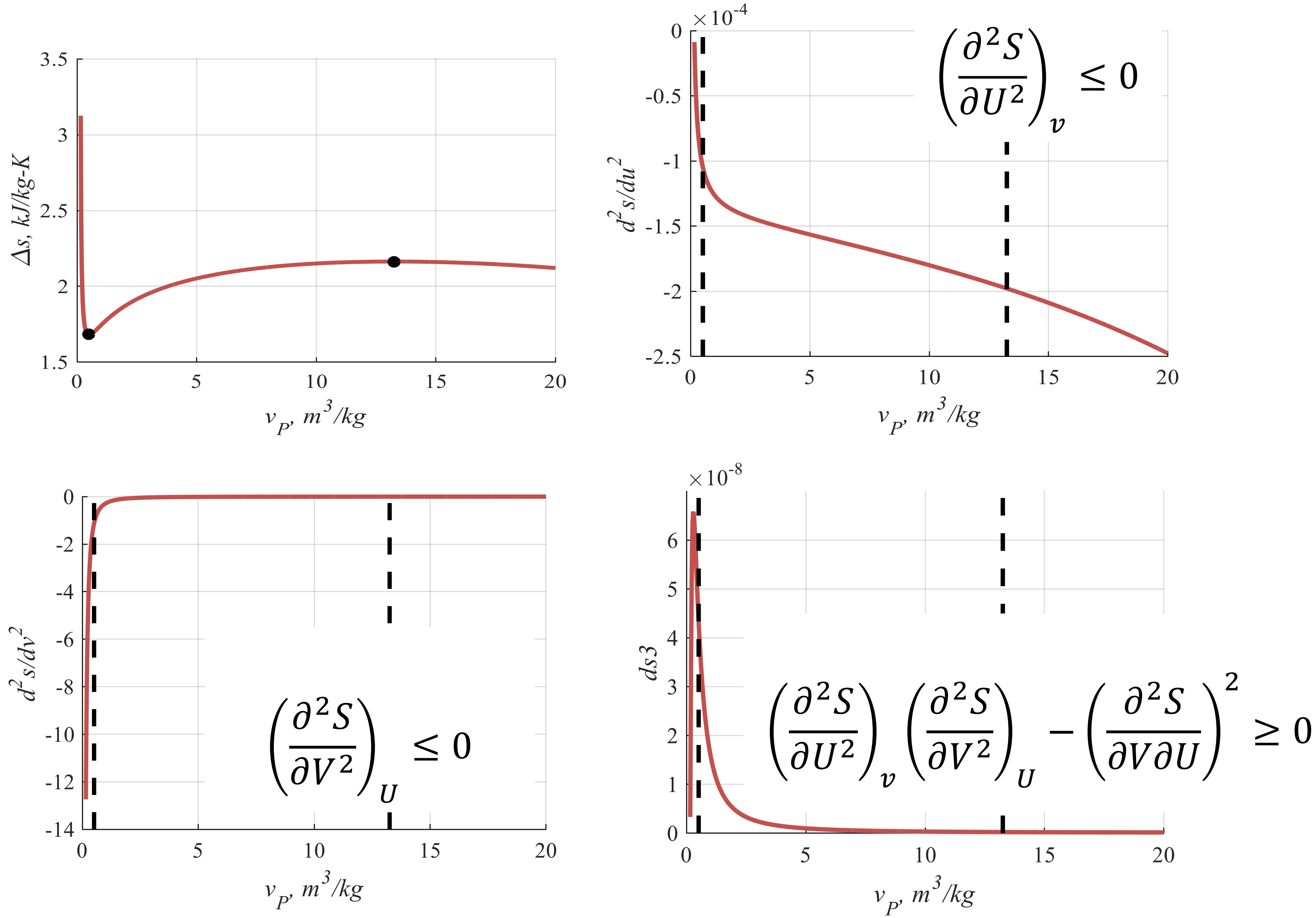


Entropy Change



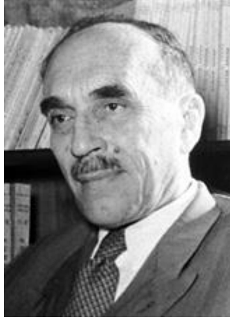


Stability Criteria



The Thermal Theory

Nikolay Semenov (Nobel Prize 1956), David Albertovich Frank-Kamenetskii, Yakov Borisovich Zel'dovich



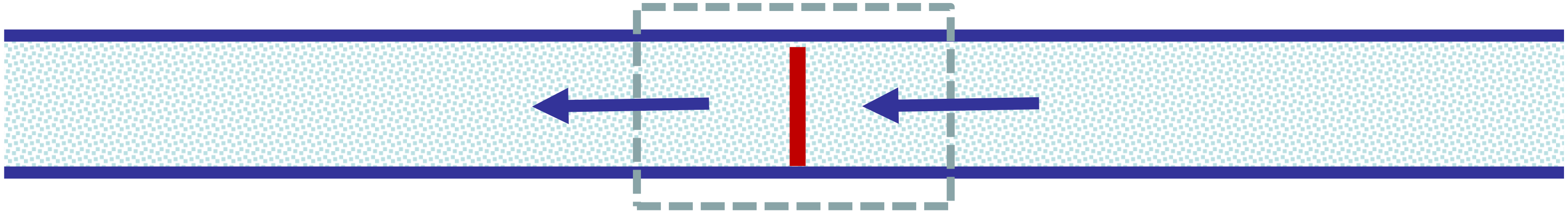
$$\delta_q = \frac{2K}{\rho_R S_L c_{p0}} = \frac{2\alpha}{S_L}$$

$$S_L = \sqrt{\frac{\alpha M_F \frac{d[F]}{dt}}{\rho_R \frac{FA}{1+FA}}}$$

$$\frac{d[F]}{dt} = -k_f [F]^{\nu_F} [O_2]^{\nu_{O_2}} \exp\left(\frac{-\bar{E}_a}{\bar{R} T_{ig}}\right)$$

Jacobus Henricus
Van Hoff, 1884

Classical Analysis - Equations



T_P , P_P , ρ_P , u_P $\quad$ T_R , P_R , ρ_R, u_R

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Ideal gases: $Pv = RT$

Thermodynamics of Irreversible Processes

A system must depart from equilibrium, even if only a slight departure, in order to change from one equilibrium state to another.

The energy balance and the principle of increase of entropy predict the overall heat flow and work in various processes, and also the direction of the process, but not **the rate** (the time) at which a change can take place.

Irreversible processes are associated with the transport of heat, mass, momentum and electric charge. Producing this flow (flux) is a **driving force** usually described by the **gradient in some physical property**.

Simplified forms of the Transport Phenomena

Fourier's law (heat flux)	$J_t = -K_t \frac{\partial T}{\partial y}$
Newton's law (momentum flux)	$J_\tau = -\mu \frac{\partial V}{\partial y}$
Fick's law (mass flux)	$J_m = -D \frac{\partial C}{\partial y}$
Ohm's law (charge flux)	$Je = -K_e \frac{\partial E}{\partial y}$

These are not "laws" in the same sense as the 1st and 2nd laws of thermodynamics. They serve as convenient analytical vehicles for describing the physical transport processes.

Onsager Relationships

Lars Onsager 1903-1976.
Received the Nobel Prize 1968 in Chemistry

If more than one driving force is present in the system, there will be more than one flow, **but each flow in such a circumstance is not necessarily a function of a unique driving force.**

When two or more fluxes are present, we say that we have **coupled flows**. In general, under moderate conditions when the system is close to the state of equilibrium, the flows can be expected to be **linear functions of the forces**.

$$J_i = \sum_{j=1}^{n} L_{ij} X_j$$

The coefficients L_{ij} are the **Onsager phenomenological coefficients**.

Onsager Relationships

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Based on statistical thermodynamics, Onsager showed that

$$L_{ij} = L_{ji}$$

In order for the reciprocity relation to apply, it is necessary that the total entropy **production per unit time per unit volume resulting from all the irreversible processes be represented as a linear sum of products of forces and fluxes**.

$$\left(\frac{dS}{dt}\right)_{per\ unit\ volume} = \sum_i J_i X_i > 0$$

Introduction of the Onsager Hypothesis

Introduction of the Onsager Hypothesis to the set of conservation equations yields the following closed solution:

$$S_L = \sqrt{\frac{Kb(-B_1)exp\left(\frac{-E_a}{RT_P}\right)M_F(T_P - T_R)^2}{\rho_R^2 c_p B_2}}$$

Where,

$$B_1 = -10^{\alpha} T_P^{\beta} \left(\frac{P_P}{\bar{R}T_P}\right)^n [y_F]^{\epsilon_F} \left[y_{O_2}\right]^{\epsilon_{O2}}$$

$$B_2 = \frac{(T_P - T_R)^2}{T_P T_R \left[ln\left(\frac{T_P}{T_R}\right) - \frac{k-1}{k} ln\left(\frac{P_P}{P_R}\right) - \frac{h_c}{c_p T_P}\right]}$$

Introduction of the Onsager Hypothesis

Introduction of the Onsager Hypothesis to the set of conservation equations yields the following closed solution:

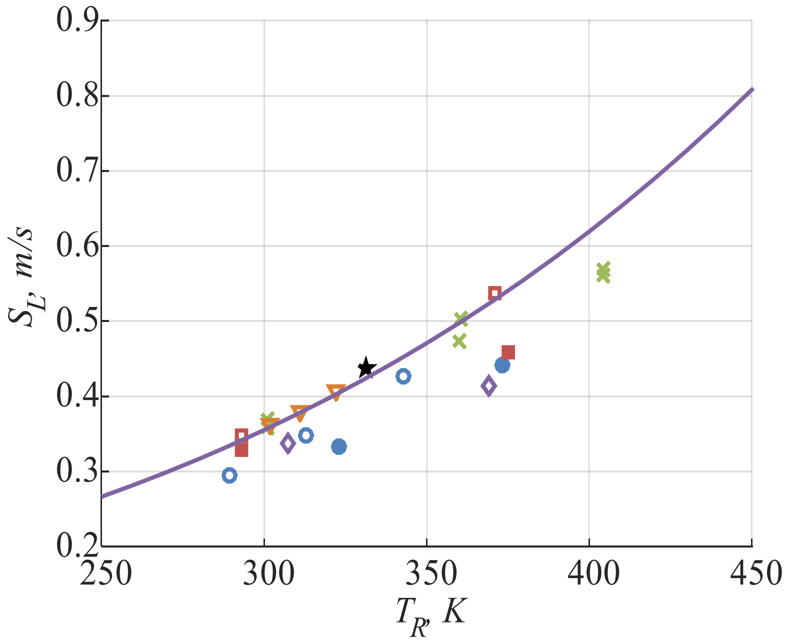
$$S_L = \frac{K}{\rho_R c_p \delta} * \frac{(T_P - T_R)^2}{T_P T_R \left[ln\left(\frac{T_P}{T_R}\right) - \frac{k-1}{k} ln\left(\frac{P_P}{P_R}\right) - \frac{h_c}{c_p T_P} \right]}$$

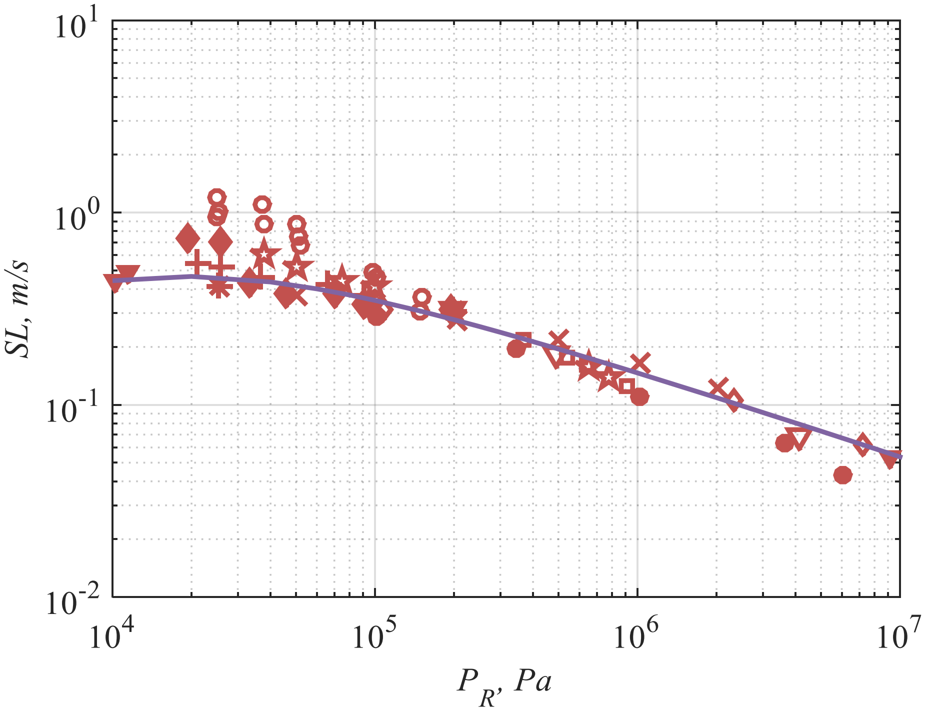
Where,

$$S_L = \frac{K}{\rho_R c_p \delta} B_2 = \frac{\alpha}{\delta} B_2$$

$$B_2 = \frac{(T_P - T_R)^2}{T_P T_R \left[ln\left(\frac{T_P}{T_R}\right) - \frac{k-1}{k} ln\left(\frac{P_P}{P_R}\right) - \frac{h_c}{c_p T_P} \right]}$$

Results





Experimental results for methane/air mixtures of Andrews G.E. and Bradley D., Combustion and Flame 19, 275-288, 1972.

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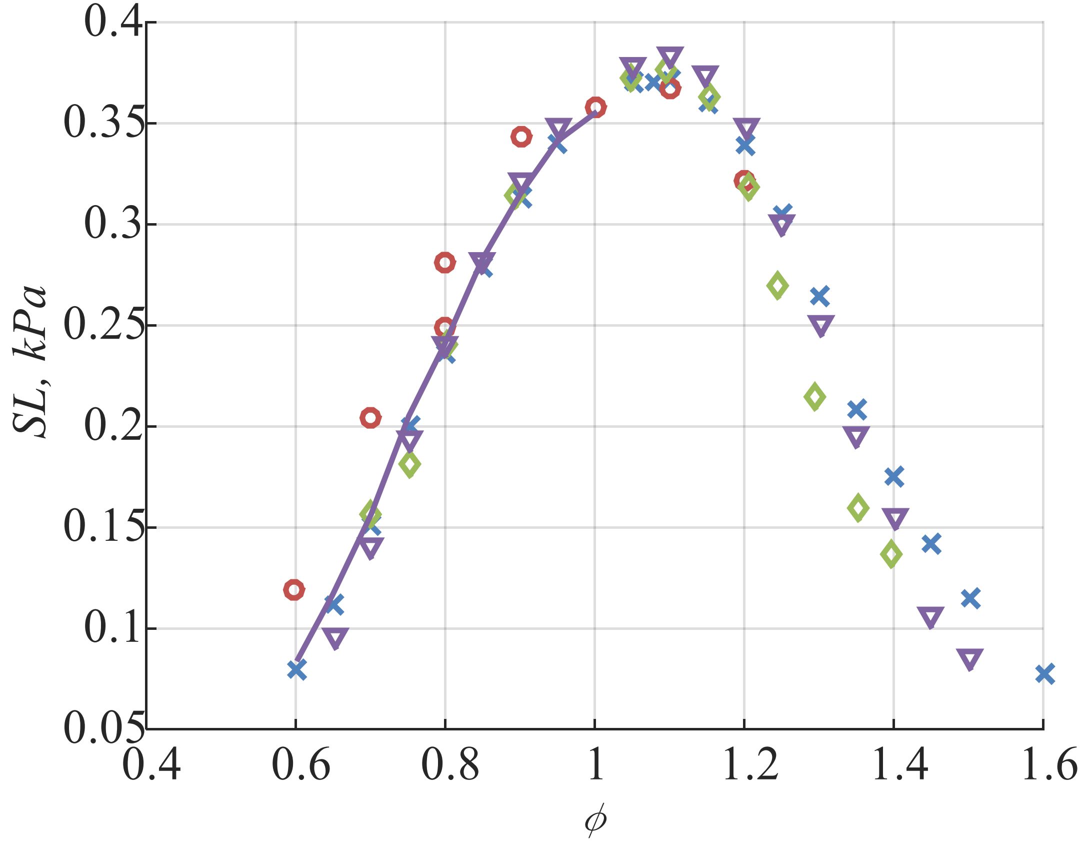

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The End

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