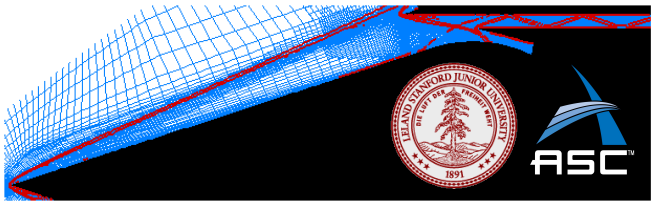
Heat release modeling

FPVA-based model

V. Terrapon and H. Pitsch

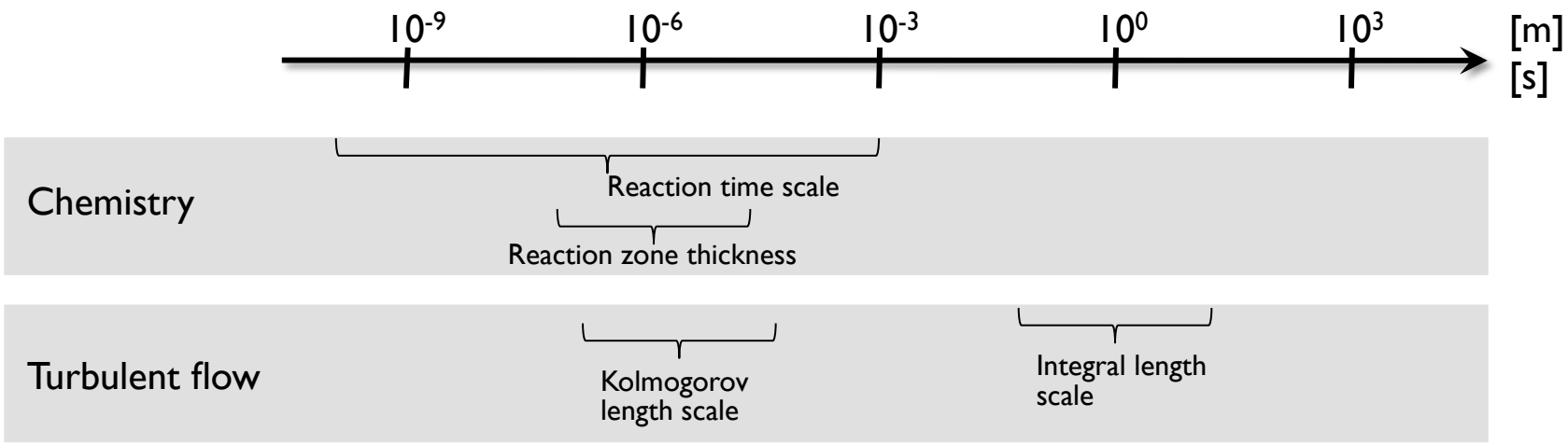


Why is turbulent combustion challenging?

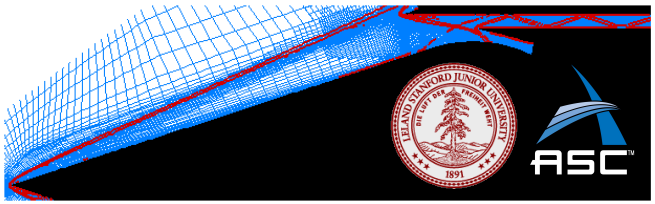
QUALITATIVE

A large range of scales is involved!

Typical engineering application



→ Equations are very stiff
→ DNS is usually not possible (LES/RANS)



Closure is required

Source term is highly non-linear

Average species transport equation:

$$\frac{\partial \bar{\rho}\tilde{Y}_i}{\partial t} + \nabla\left(\overline{\rho \mathbf{u} Y_i}\right) = \nabla\left(\overline{\rho D_i \nabla Y_i}\right) + \bar{\dot{m}}_i$$

The source term:

$$\dot{m}_i = \sum_{j=1}^{N_{reac}} W_i \nu_{ij} \left(K_{fj} \prod_{k=1}^{N_{sp}} [X_k]^{\nu'_{kj}} - K_{rj} \prod_{k=1}^{N_{sp}} [X_k]^{\nu''_{kj}} \right)$$

with

$$K_{fj} = A_{fj} T^{\beta_j} \exp\left(-\frac{E_j}{RT}\right)$$

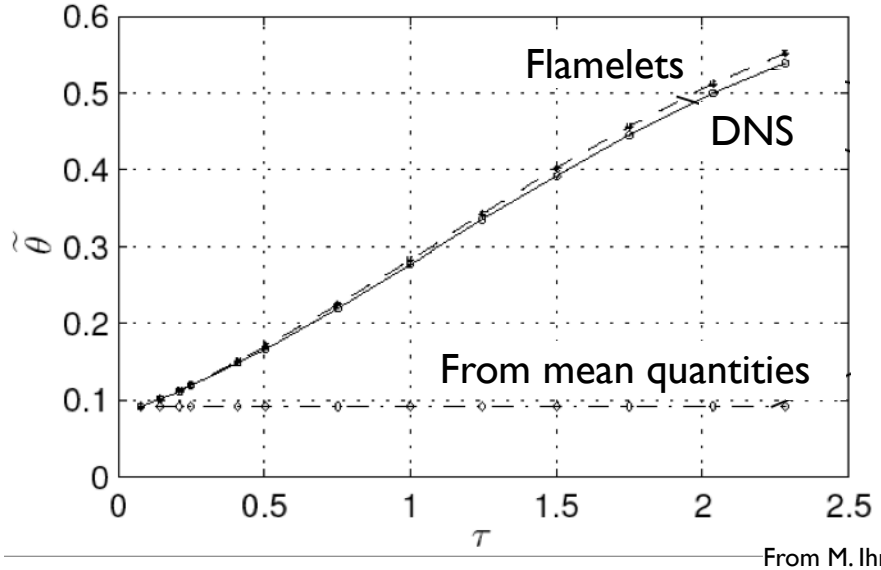
Diffusive and convective terms can usually be treated like for the NS equations

Decaying isotropic turbulence

Average species transport equation simplifies:

$$\frac{\partial \bar{\rho}\tilde{Y}_i}{\partial t} = \bar{\dot{m}}_i$$

Species mass fraction



From M. Ihme

Tabulated chemistry as a potential solution

Transformation and asymptotic approximation leads to equations for the **flame micro-structure** similar to the flamelet equations

$$\frac{\partial \phi}{\partial \tau} = \frac{\rho\chi}{2}\frac{\partial^2 \phi}{\partial Z^2} + \dot{m}_\phi$$

Mixture fraction

Diffusion flame regime

$$0 = \frac{\rho\chi}{2}\frac{\partial^2 \phi}{\partial Z^2} + \dot{m}_\phi$$

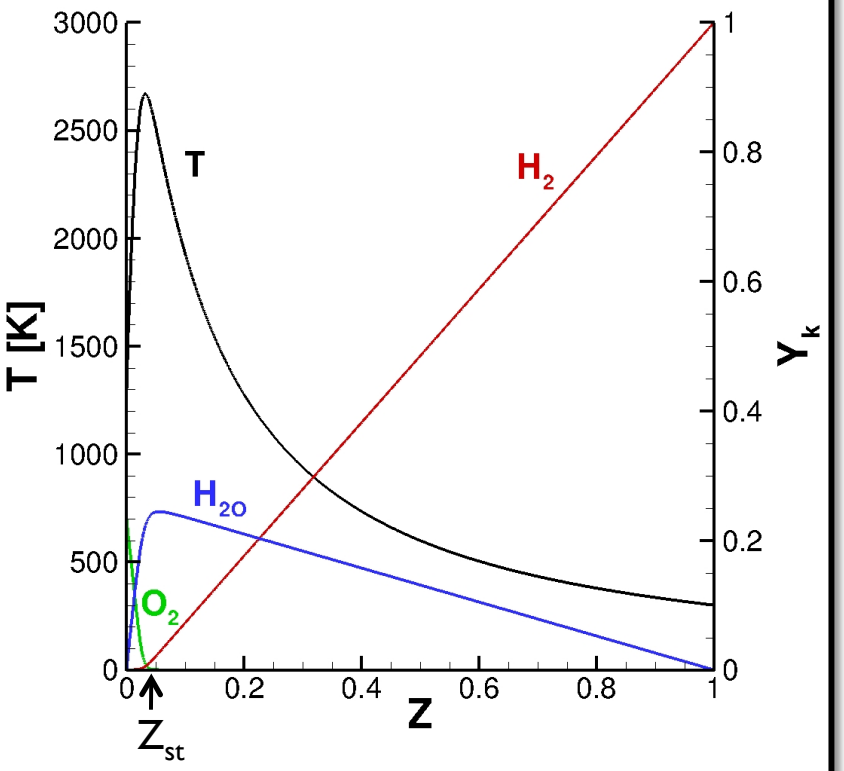
Auto-ignition regime

$$\frac{\partial \phi}{\partial \tau} = \dot{m}_\phi$$

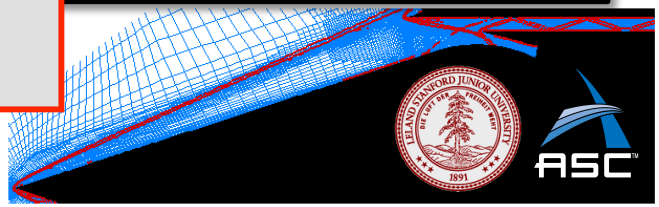
Flame strain is measured by the scalar dissipation rate

$$\chi = 2D\left(\frac{\partial Z}{\partial x}\right)^2$$

Steady diffusion flame solution for H_2/air flame at $\chi_{st} = 1$



Scale separation allows us to pre-compute and tabulate chemistry as function of Z and χ



Combustion model for high-speed flows based on tabulated chemistry

Assumptions

- Species mass fractions independent of compressibility effects
- Flame micro-structure

Current combustion model

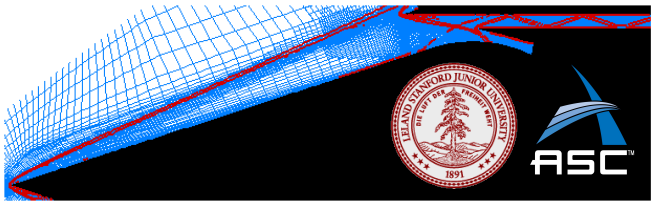
- Based on Flamelet Progress Variable Approach (FPVA)*
- Tabulated chemistry
- Temperature computed from species mass fractions and energy (not from chemistry table)
- 3 additional transport equations for the mean and variance of the mixture fraction and for the progress variable

Pros

+
- Complex chemistry mechanism
- Only few additional scalars to solve
- Turbulence – chemistry interaction

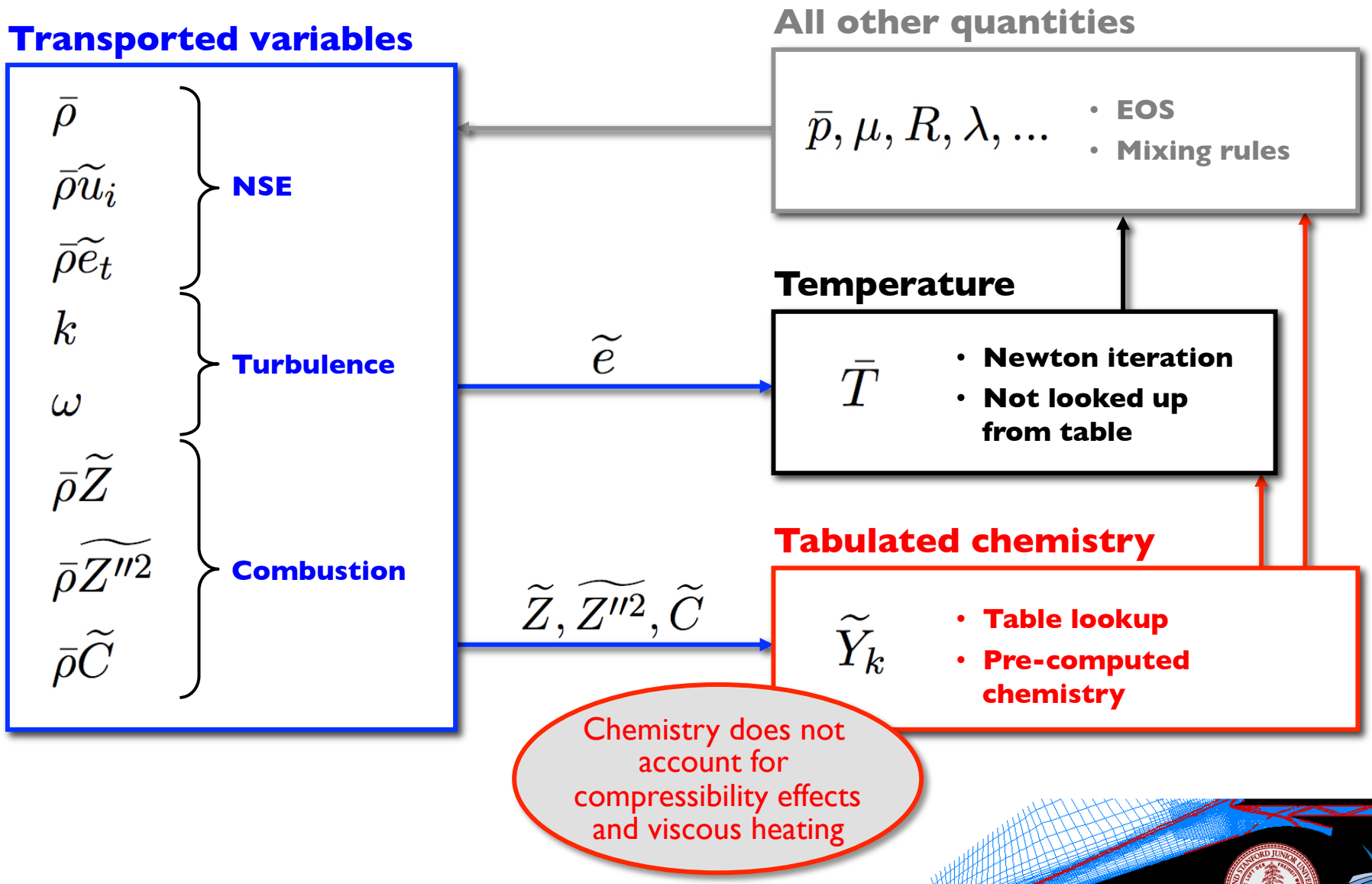
Cons

-
- Compressibility effects on chemistry not accounted for
- Accuracy of ignition dynamics

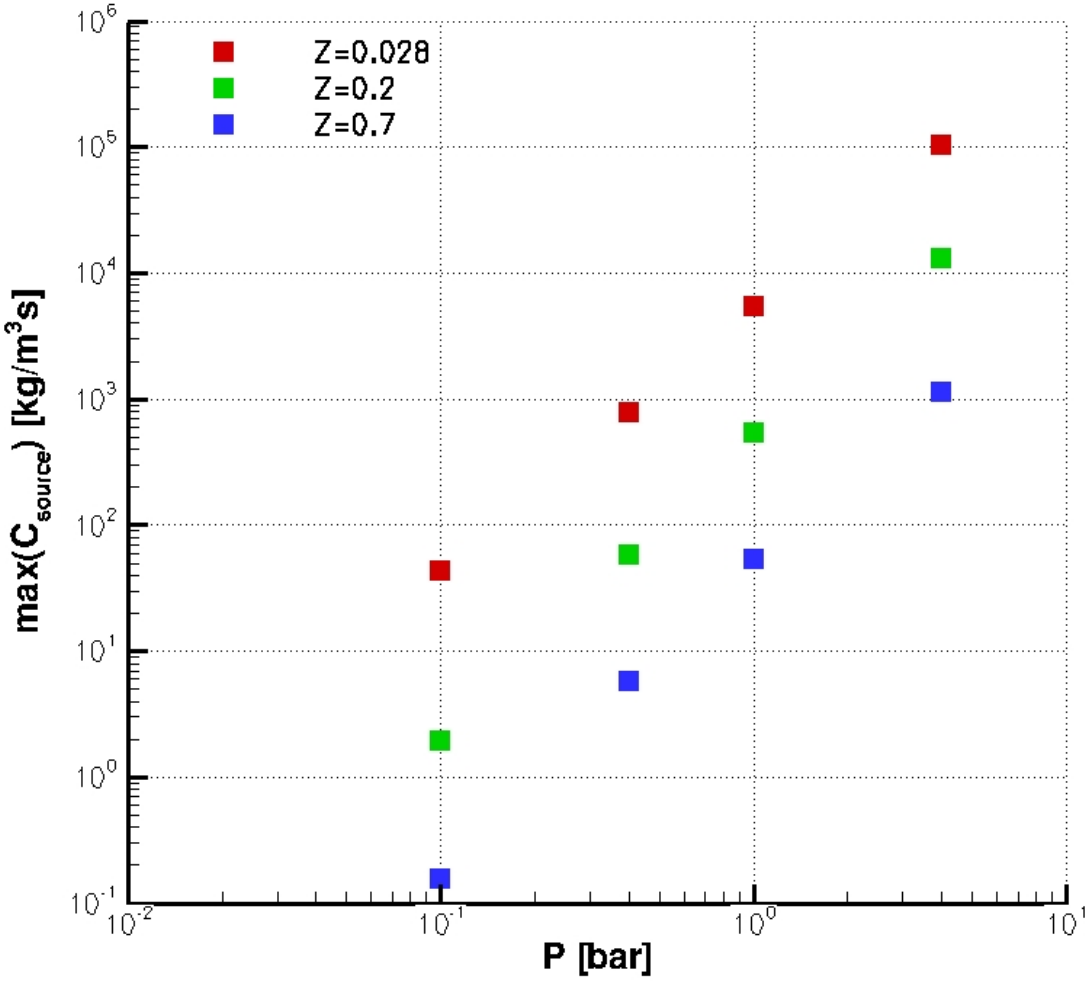


* Pierce & Moin, 2004; Ihme et al., 2005

Model algorithm

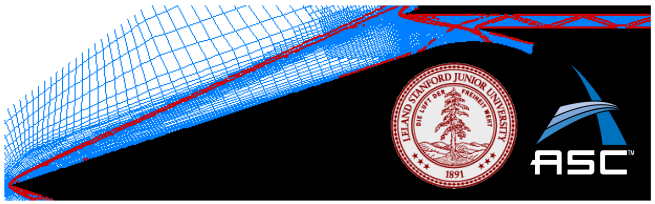


Source term of progress variable C has a strong pressure dependence

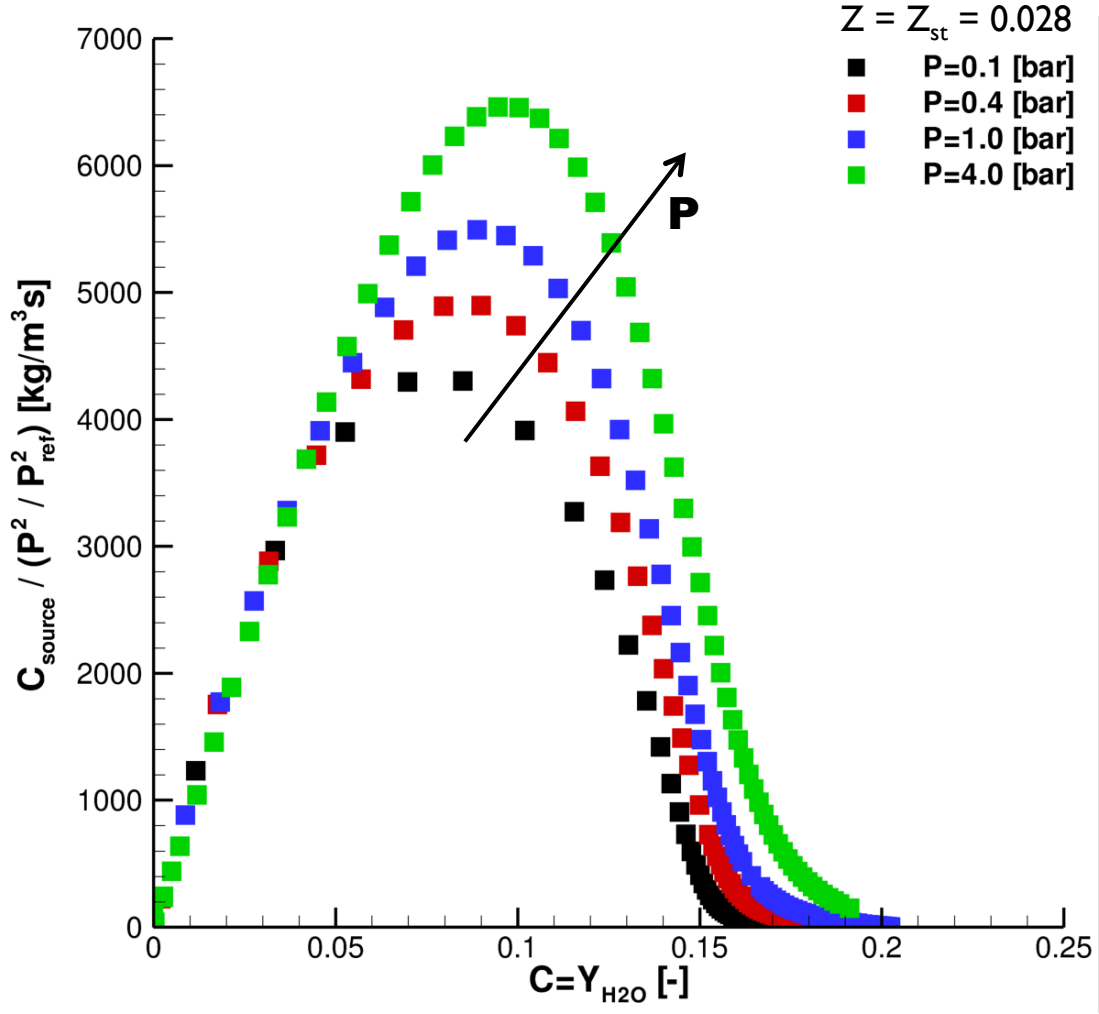


- Dynamics of flame strongly dependent on pressure
- Quadratic dependence (mostly 2 body interactions)
- Rescaling of source term for progress variable

$S_c(P) = S_c(P_{ref})\ P^2/P^2_{ref}$



Rescaled source term as function of the progress variable



- Dynamics of flame strongly dependent on pressure
- Quadratic dependence (mostly 2 body interactions)
- Rescaling of source term for progress variable

$S_c(P) = S_c(P_{ref})\ P^2/P^2_{ref}$