Universität der Bundeswehr München

A computational study of the influence of real-gas effects in underexpanded hydrogen and methane jets

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02. December 2016

Outline

- Motivation
- Numerical Models
  - Fluid Flow
  - Thermodynamics
- Generic Test Case & Setup
- Results
  - Validation Case
  - Computational Study
- Conclusion

High-Pressure Gas Injections

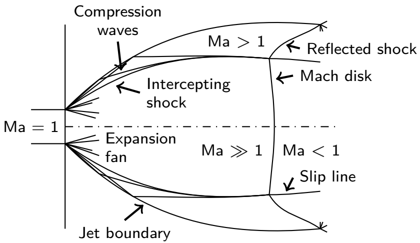
Gaseous fuels?

- Better mixture formation
- Higher compression ratio
- Lean burning capabilities
- Lower fuel costs
- Higher durability of engine lubricant

⇒ Better performance
⇒ Higher efficieny
⇒ Less pollutant emission

Characteristics

- Near-nozzle flow structure
- Jet penetration Z_{tip}
- Fuel-air mixing



Challenges

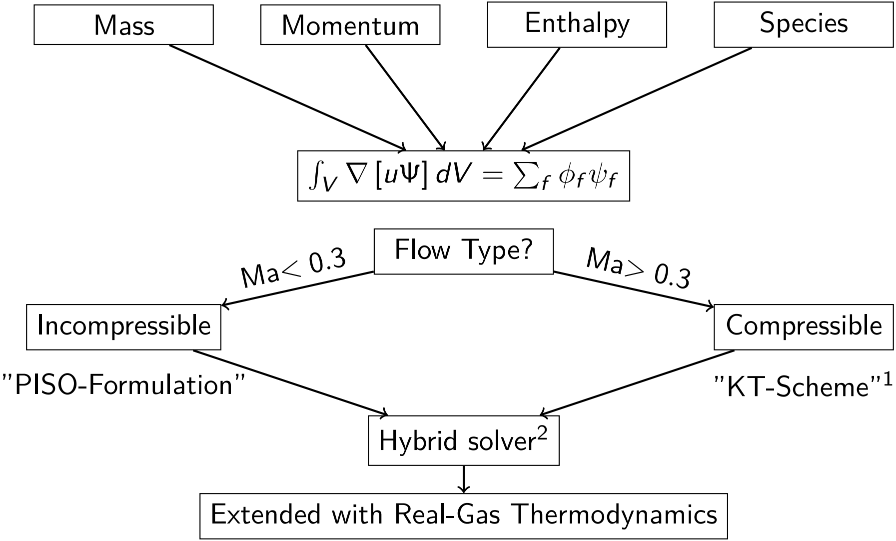
Operating points

- Total pressures up to $p_{tot} = 50\,\text{MPa}$
- Back pressures at around $p_{stat} = 2.5\,\text{MPa} - 20\,\text{MPa}$
- Total temperatures at around $T_{tot} = 250\,\text{K} - 350\,\text{K}$
- Combustion chamber temperatures at around $T_{stat} = 750\,\text{K} - 1100\,\text{K}$

Numerical Aspects

- Assumption of ideal gas law not valid, supercritical fluid
  $\Rightarrow$ real-gas thermodynamics
- High nozzle pressure ratios (NPR)
  $\Rightarrow$ sub-, trans- and supersonic flowfield
  $\Rightarrow$ large range of Mach numbers
  $\Rightarrow$ quickly changing fluid properties

Fluid Flow

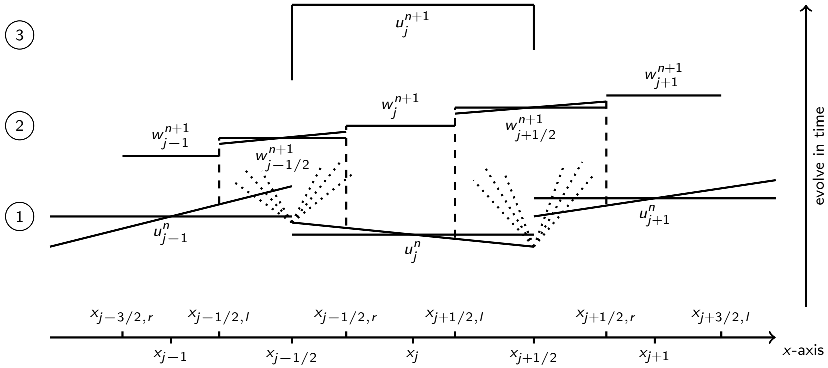


[1] Kurganov and Tadmor 2000.

[2] Kraposhin, Bovtrikova, and Strijhak 2015.

Fluid Flow

Kurganov-Tadmor Scheme:



Thermodynamics

Equation of State (EoS)

- Ideal Gas (IG):

$$p = \frac{RT}{v_{IG}}$$

- Peng-Robinson (PR)[3]:

$$p = \frac{RT}{v_{PR} - b_m} - \frac{a_m(T)}{v_{PR}^2 + 2b_m v_{PR} - b_m^2}$$

- Soave-Redlich-Kwong (SRK)[4]:

$$p = \frac{RT}{v_{SRK} - b_m} - \frac{a_m(T)}{v_{SRK}^2 + b_m v_{SRK}}$$

- Pressure correction for caloric properties:

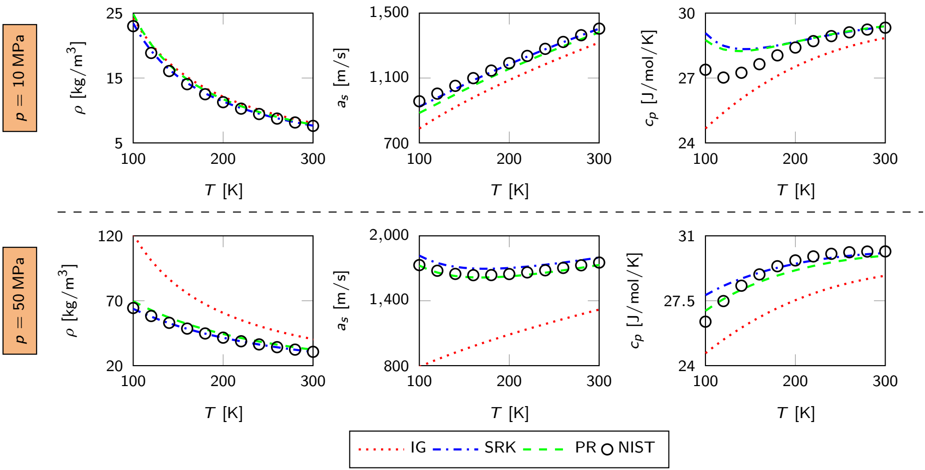
$$h(T,p) = h_0(T) + \int_{p_0}^{p} \left(v - T \left.\frac{\partial v}{\partial T}\right|_p \right) dp$$

[3] Peng and Robinson 1976.

[4] Soave 1972.

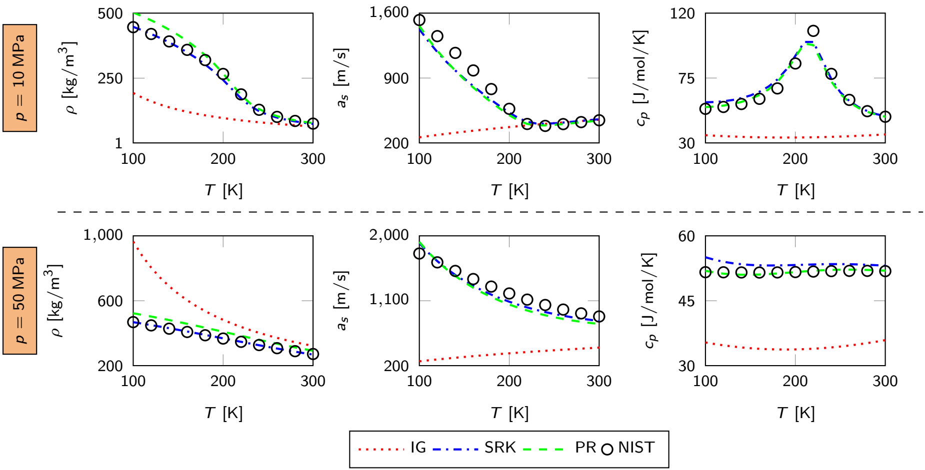
Thermodynamics

EoS Comparison for Hydrogen



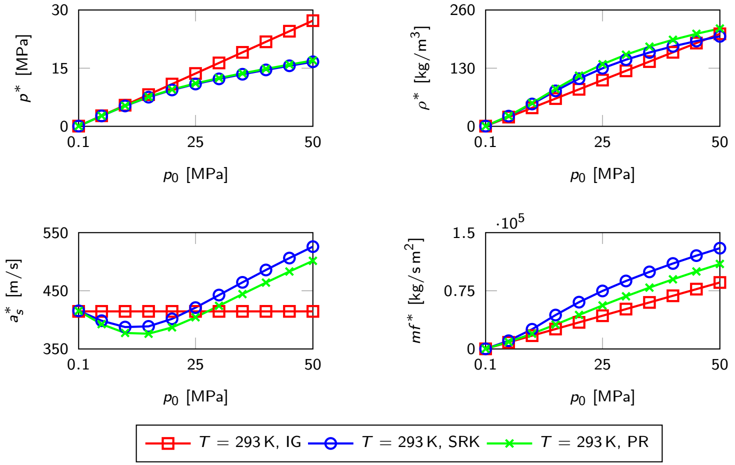
Thermodynamics

EoS Comparison for Methane



Thermodynamics

EoS Comparison for Methane, Critical Values



Thermodynamics

Mixing Rules (EoS: PR)[5]*:*

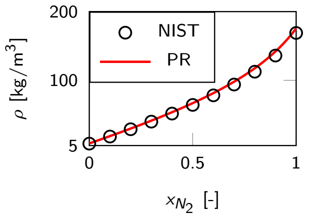
$$p = \frac{RT}{v_{PR} - b_m} - \frac{a_m(T)}{v_{PR}^2 + 2 b_m v_{PR} - b_m^2}$$

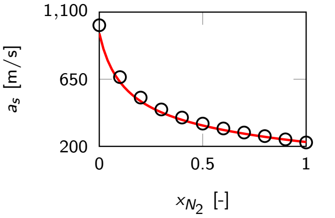
$$a_m = \sum \sum x_i x_j a_{ij}$$

$$a_{ij}(T) = 0.4274 \left(\frac{R^2 T_{c,ij}^2}{p_{c,ij}} \right) \left[1 + k_{ij} \left(1 - \sqrt{\frac{T}{T_{c,ij}}} \right) \right]^2$$

$$b_m = \sum x_i b_i$$

H2/N2, $p = 5\,\mathrm{MPa}$, $T = 150\,\mathrm{K}$

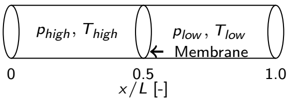


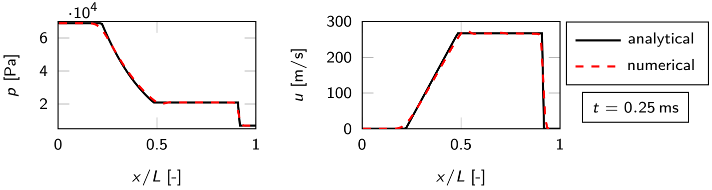


[5] Müller et al. 2015.

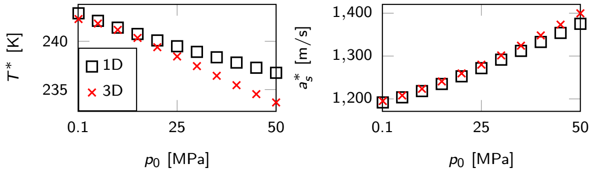
Solver Validation

Fluid Flow: Shock tube problem

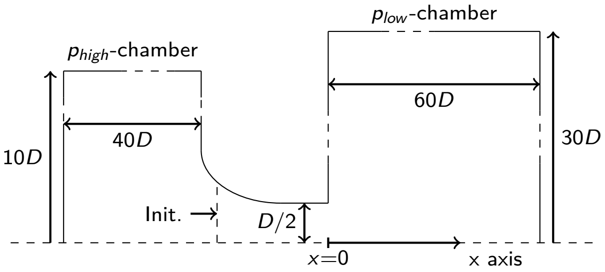




Real-Gas Thermodynamics: Critical values



Geometry



Setup

- axisymmetric nozzle
- $D = 1.5\,\mathrm{mm}$
- Structured mesh
- Refined area: $D/40$
- Mesh size: 150 000 cells

Boundary Conditions

- Total inlet pressure
- Total inlet temperature
- Static outlet pressure
- Init. up to $x = -1.4\,\mathrm{D}$

Operating Points

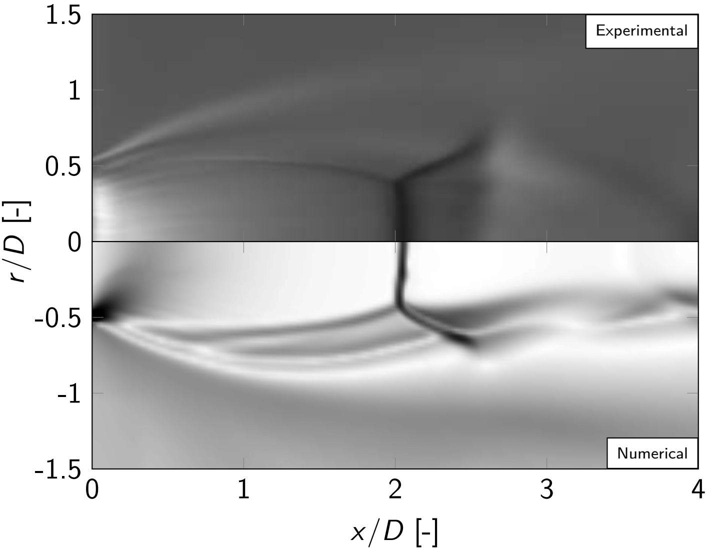
Validation Case:

	p_{high}-chamber	p_{low}-chamber
Fluid [–]	H_2	Air
NPR [–]	10	
Pressure [kPa]	983.70	98.37
Temperature [K]	295.4	296.0
EoS [–]	IG	

Computational Study:

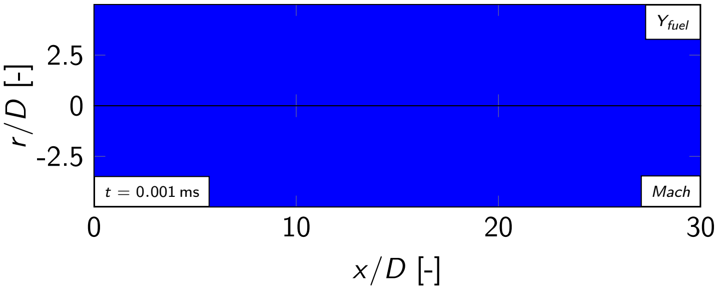
	p_{high}-chamber	p_{low}-chamber
Fluid [–]	H_2 / CH_4	N_2
NPR [–]	10	
Pressure [MPa]	1/10/50	0.1/1/5
Temperature [K]	293.0	
EoS [–]	IG/SRK	

Validation Case



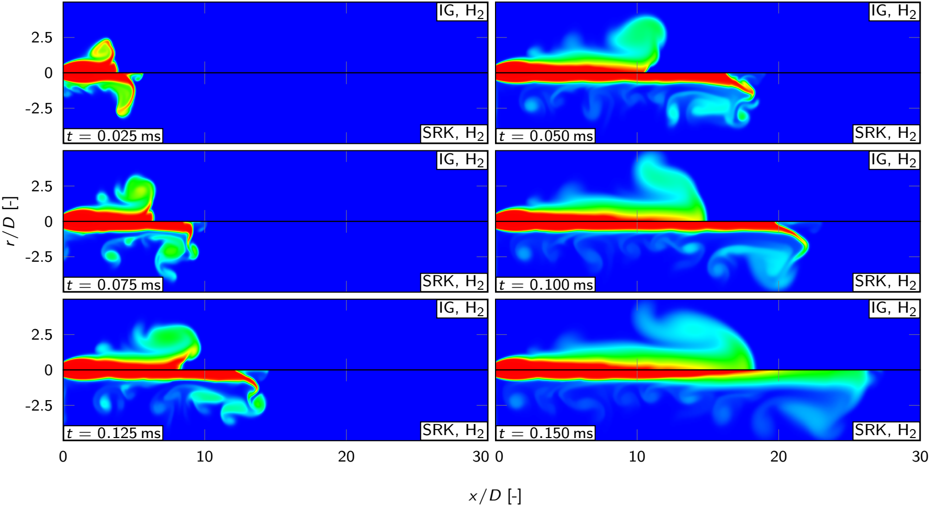
Computational Study

Hydrogen Injection, $p = 10\,\text{MPa}$, *NPR=10, EoS: SRK*



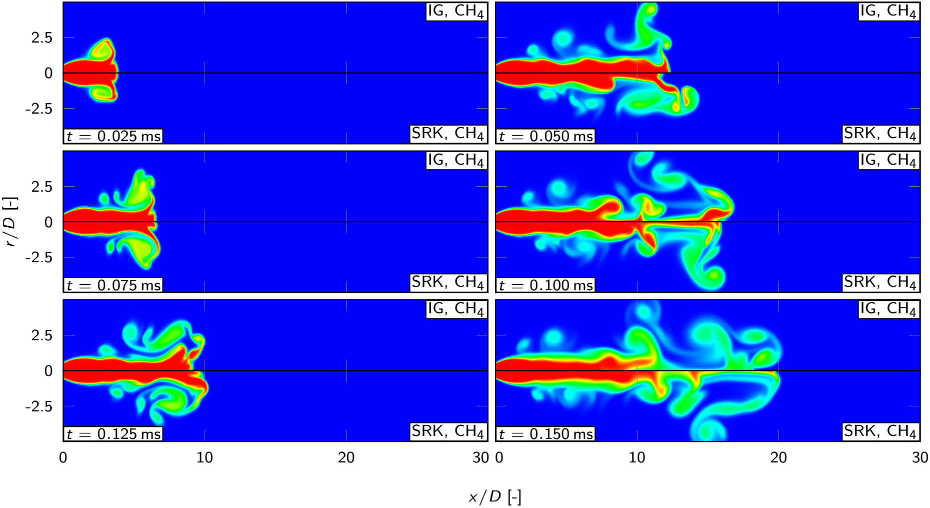
Computational Study

Hydrogen Injection, $p = 10\,\mathrm{MPa}$, NPR=10

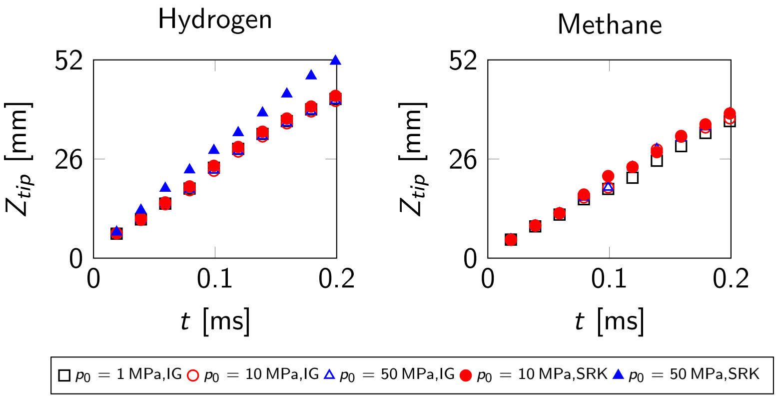


Computational Study

Methane Injection, $p = 10\,\mathrm{MPa}$, NPR=10



Computational Study



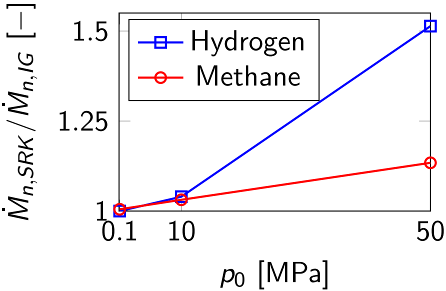
Computational Study

Jet penetration depth[6]:

$$Z_t = \Gamma \left(\frac{\dot{M}_n}{\rho} \right)^{1/4} t^{1/2}$$

Momentum flux at nozzle exit:

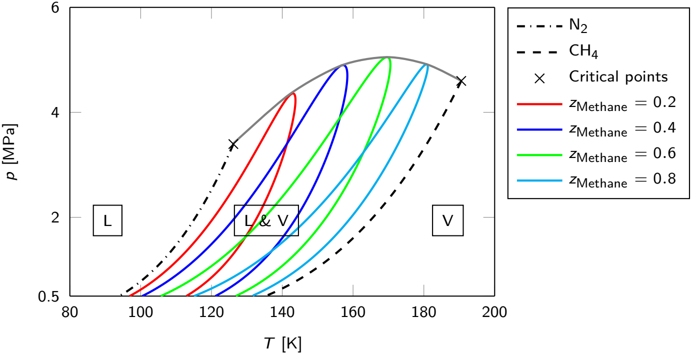
$$\dot{M}_n = U_n^2 \frac{d^2}{4} \pi \rho_n$$



[6] Hill and Ouellette 1999.

Computational Study / Outlook

Methane Injection, $p = 50\,\mathrm{MPa}$, modelled with real-gas thermodynamics?
$\Rightarrow$ Possibility of phase separation.



Solver Capabilities

Numerical Schemes

- Successfully extended hybrid KT scheme for use with real-gas thermodynamics
- Two cubic EoS: Peng-Robinson, Soave-Redlich-Kwong
- Implemented equations for multi-species flow
- Real-Gas Mixing Rules
- Partially validated, more test cases to come

$\Rightarrow$ Solver which is capable of simulation high pressure gas injections using real-gas thermodynamics

Jet Comparison

Ideal-Gas vs. Real-Gas Thermodynamics

With increasing p_0 higher deviations:

- $\text{mass flow}\Big|_{RG} > \text{mass flow}\Big|_{IG}$
- $Z_{tip}\Big|_{RG} > Z_{tip}\Big|_{IG}$
- mixture characteristics
- near-nozzle flow structure, shift of Mach disk position $\uparrow$

$\Rightarrow$ Real-Gas thermodynamics essential for pressures $p_0 > 10\,\text{MPa}$ and/or $T_0 < 273\,\text{K}$

$\Rightarrow$ Differences between IG/RG: Hydrogen-Jets > Methane-Jets

Thank you for your attention.

Governing Equations

Mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(\rho u_i\right)}{\partial x_i} = 0$$

Momentum:

$$\frac{\partial \left(\rho u_i\right)}{\partial t} + \frac{\partial \left(\rho u_j u_i\right)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

Enthalpy:

$$\frac{\partial \left(\rho h\right)}{\partial t} + \frac{\partial \left(\rho h u_i\right)}{\partial x_i} = \frac{\partial p}{\partial t} + \frac{\partial \left(u_i \tau_{ij}\right)}{\partial x_i} - \frac{\partial q_k}{x_i}$$

Species:

$$\frac{\partial \left(\rho Y_k\right)}{\partial t} + \frac{\partial \left(\rho u_i Y_k\right)}{\partial x_i} = -\frac{\partial j_k}{\partial x_i}$$

Governing Equations

Species-Flux:

$$j_k = -\rho D_{k,m} \frac{\partial Y_k}{\partial x_i}$$

Mass diffusivity / Schmidt-Number:

$$Sc_{k,m} = \frac{\mu_m}{(\rho D)_{k,m}} = 1$$

Heat flux:

$$q_k = -\kappa \frac{\partial T}{\partial x_i} + \sum j_k h_k$$

Hybrid Scheme

$$\sum_f \phi_f \Psi_f = \sum_f \left[\alpha_{f+}\phi_{f+}\Psi_{f+} + \alpha_{f-}\phi_{f-}\Psi_{f-} + \omega_f\left(\Psi_{f-} - \Psi_{f+}\right)\right]$$

$$\sum_f \phi_f \Psi_f = \sum_f \left[\Psi_{f+}\left(\alpha f{+}\phi_{f+} + \alpha f{+}\phi_{f-}\right) + \Psi_{f-}\left(\alpha f{-}\phi_{f-} + \alpha f{+}\phi_{f-}\right)\right]$$

Weighting Factor:

$$\alpha_{f+} = \frac{\varphi_{f+}}{\varphi_{f+} + \varphi_{f-}}, \qquad \alpha_{f-} = \frac{\varphi_{f+}}{\varphi_{f+} + \varphi_{f-}}$$

Diffusive volumetric flux:

$$\omega_f = \alpha_{f+}\varphi_{f-}$$

Volumetric flux associated with local speeds of propagation:

$$\varphi_{f+} = \max\left(c_{f+}|S_f| + \phi_{f+}, c_{f-}|S_f| + \phi_{f-}, 0\right)$$
$$\varphi_{f-} = \max\left(c_{f+}|S_f| - \phi_{f+}, c_{f-}|S_f| - \phi_{f-}, 0\right)$$

Hybrid Scheme

Speed of sound:

$$c = \sqrt{\frac{M_w}{\rho} \frac{c_p}{c_v} \left(\frac{\partial p}{\partial v} \right) \Big|_T}$$

Kappa-function:

$$\kappa = \min \left(\frac{M_f}{\mathsf{CFL}}, 1 \right)$$

Mass flux:

$$\begin{aligned} q_f^P &= \kappa_f \rho_f^P \left(\alpha_{f+} \phi_{f+} + \alpha_{f+} \phi_{f-} \right) \\ q_f^N &= \left(1 - \kappa_f \right) \rho_f^P \left(\alpha_{f+} \phi_{f+} + \alpha_{f+} \phi_{f-} \right) + \rho_f^N \left(\alpha_{f-} \phi_{f-} + \alpha_{f+} \phi_{f-} \right) \end{aligned}$$