

# Combustion Cheat Sheet

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# 1 General

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (1)$$

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \frac{1}{\rho} \nabla p = \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau} + \sum_i Y_i \mathbf{f}_i \quad (2)$$

$$= \frac{1}{\rho} \nabla \cdot (\mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]) + (\kappa - \frac{2}{3} \mu) (\nabla \cdot \mathbf{v}) \mathbf{I} + \sum_i Y_i \mathbf{f}_i \quad (3)$$

$$\frac{\partial e}{\partial t} + (\mathbf{v} \cdot \nabla) e + \frac{p}{\rho} \nabla \cdot \mathbf{v} = -\frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi \quad (4)$$

$$\frac{\partial Y_i}{\partial t} + (\mathbf{v} \cdot \nabla) Y_i = \frac{\sigma_i}{\rho} - \frac{1}{\rho} \nabla \cdot \mathbf{j}_i \quad i = 1, 2, \dots, n \quad (5)$$

$$p = \rho R_u T \sum_{i=1}^n \frac{Y_i}{\bar{m}_i} = \rho R T, \quad R_i = \frac{R_u}{\bar{m}_i} \quad (6)$$

$$R = \sum_{i=1}^n R_i Y_i = R_u \sum_{i=1}^n \frac{Y_i}{\bar{m}_i} = \frac{R_u}{\bar{m}}, \quad \bar{m} = \sum_{i=1}^n \bar{m}_i X_i \quad (7)$$

$$e = \sum_{i=1}^n (h_i Y_i) - \frac{p}{\rho} = h - \frac{p}{\rho} = \sum_{i=1}^n (h_i - R_i T) Y_i \quad (8)$$

$$\boldsymbol{\tau} = \mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T] + (\kappa - \frac{2}{3} \mu) (\nabla \cdot \mathbf{v}) \mathbf{I}, \quad (9)$$

$$\Phi = \boldsymbol{\tau} : \nabla \mathbf{v} \quad \text{viscous heating term} \quad (10)$$

$$\mu = \mu(T, Y_i), \quad \lambda = \lambda(T, Y_i), \quad D_i = D_i(p, T, Y_i) \quad (11)$$

$$h_i(T) = \Delta h_i^0 + \int_{T^0}^T c_{p,i}(T) dT \quad i = 1, 2, \dots, n \quad (12)$$

$$\mathbf{q} = -\lambda \nabla T + \sum_{i=1}^n h_i \mathbf{j}_i \quad (13)$$

$$\mathbf{j}_i = \rho Y_i \mathbf{V}_i \quad \text{species flux} \quad (14)$$

$$\mathbf{V}_i \approx -D_i \nabla \ln(X_i) \quad (\text{diffusion velocity, Fick's law}) \quad (15)$$

$$c_p = \sum_{i=1}^n c_{p,i} Y_i, \quad c_v = c_p - R = \sum_{i=1}^n (c_{p,i} - R_i) Y_i, \quad \gamma = \gamma(T, Y_i) = \frac{c_p}{c_v} \quad (16)$$

$$c_v = R/(\gamma - 1) \quad (17)$$

- **Note 1:** the enthalpy appearing here,  $h_i$ , is the **absolute enthalpy**, which includes the energy of formation  $\Delta h_i^0$  at the reference temperature, usually taken as  $T_0 = 298.15$ .
- **Note 2:** The thermodynamic variables  $c_{p,i}(T)$ ,  $h_i(T)$  are assumed to be mass based instead of mole based (to get the mass based version from the mole based version, divide by  $\bar{m}_i$ ).
- **Note 3:** The quantities  $c_p$ ,  $c_v$  and  $\gamma$  are called the frozen specific heats and gas constant (the non-frozen  $c_p$  is  $\partial h / \partial T$ ).

Other forms for the “energy” equation: Here is the temperature equation (derived in more detail in section (5.1))

$$\frac{DT}{Dt} + (\gamma - 1) T \nabla \cdot \mathbf{v} = \frac{1}{\rho c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) \sigma_i + \nabla \cdot (\lambda \nabla T) - T \sum_{i=1}^n R_i \nabla \cdot \mathbf{j}_i - \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + \Phi \right\} \quad (18)$$

Taking  $RT$  times the continuity equation (1) plus  $\rho R$  times the temperature equation (18) gives the pressure equation

(derived in more detail in section (5.2))

$$\frac{Dp}{Dt} + \gamma p \nabla \cdot \mathbf{v} = \sum_{i=1}^n (\gamma R_i T - (\gamma - 1) h_i) \sigma_i + (\gamma - 1) \nabla \cdot (\lambda \nabla T) \quad (19)$$

$$- \gamma T \nabla \cdot \sum_{i=1}^n R_i \mathbf{j}_i - (\gamma - 1) \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + (\gamma - 1) \Phi \quad (20)$$

Another equation that is often used for low mach number is a combination of the Temperature and pressure equations:

$$\frac{DT}{Dt} - \frac{1}{\rho c_p} \frac{Dp}{Dt} = \frac{1}{\rho c_p} \left\{ - \sum_{i=1}^n (h_i \sigma_i) + \nabla \cdot (\lambda \nabla T) - \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + \Phi \right\} \quad (21)$$

## 1.1 Equations in conservation form

The equations in conservation form (see *Numerical Simulation of Reactive Flow* by Oran and Boris) are

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) + \nabla p &= \nabla \cdot \boldsymbol{\tau} + \sum_i \rho_i \mathbf{a}_i \\ \frac{\partial E}{\partial t} + \nabla \cdot ((E + p) \mathbf{v}) &= \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\tau}) - \nabla \cdot (\mathbf{q} + \mathbf{q}_R) + \mathbf{v} \cdot \sum_i m_i \mathbf{a}_i + \sum_i \mathbf{V}_i \cdot m_i \mathbf{a}_i \\ \frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{v}) &= \sigma_i - \nabla \cdot \mathbf{j}_i \quad i = 1, 2, \dots, n \end{aligned}$$

where the energy density  $E$  is

$$E = \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \rho e$$

and the  $\mathbf{a}_i$  are body forces acting on species  $i$ .

## 1.2 Diffusion velocities

In general the diffusion velocities,  $\mathbf{V}_i$ , are determined from the matrix equation

$$\sum_j \left( \frac{X_i X_j}{D_{ij}} \right) (\mathbf{V}_j - \mathbf{V}_i) = \mathbf{G}_i$$

where

$$\mathbf{G}_i = \nabla X_i - (Y_i - X_i) \frac{\nabla p}{p} - \frac{\rho}{p} \sum_j Y_i Y_j (\mathbf{f}_i - \mathbf{f}_j) - \sum_j \left( \frac{X_i X_j}{\rho D_{ij}} \right) \left( \frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i} \right) \frac{\nabla T}{T}$$

## 1.3 Entropy

$$\begin{aligned} \tilde{S} &= \sum_{i=1}^n Y_i (\phi_{0,i}(T) - R_i \ln(X_i)) - R \ln(p) \\ \phi_{0,i}(T) &= \int_{T_0}^T \frac{c_{p,i}(\tau)}{\tau} d\tau \end{aligned}$$

When the flow is frozen ( $Y_i = \text{constant}$ ) and inviscid the entropy will be constant. This can be seen from

$$\begin{aligned} \frac{DS}{Dt} &= \left\{ \sum_{i=1}^n Y_i \frac{c_{p,i}}{T} \frac{DT}{Dt} - R \frac{1}{p} \frac{Dp}{Dt} \right\} \\ &= c_p [ -(\gamma - 1) \nabla \cdot \mathbf{u} ] - R [ -\gamma \nabla \cdot \mathbf{u} ] \\ &= 0 \end{aligned}$$

This is also (supposedly true) in equilibrium flow.

## 1.4 enthalpy

An equation for the enthalpy is obtained by substituting  $e = h - p/\rho$  into the energy equation

$$\frac{Dh}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} + \frac{p}{\rho^2} \frac{D\rho}{Dt} + \frac{p}{\rho} \nabla \cdot \mathbf{v} = -\frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi$$

Use of the continuity equation gives

$$\frac{Dh}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} = -\frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi$$

Replacing  $\mathbf{u} \cdot \nabla p/\rho$  from the momentum equation gives

$$\frac{Dh}{Dt} - \frac{1}{\rho} \frac{\partial p}{\partial t} - \mathbf{v} \cdot [-\mathbf{v}_t - (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla \cdot \boldsymbol{\tau}] = -\frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi$$

or

$$\frac{\partial h}{\partial t} - \frac{1}{\rho} \frac{\partial p}{\partial t} + \frac{1}{2} \frac{\partial(\mathbf{v} \cdot \mathbf{v})}{\partial t} + \mathbf{v} \cdot [\nabla h + (\mathbf{v} \cdot \nabla) \mathbf{v}] = -\frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi + \mathbf{v} \cdot (\nabla \cdot \boldsymbol{\tau}) \quad (22)$$

Thus in steady inviscid 1D flow we have

$$h_x + \frac{1}{2}(u^2)_x = 0 \quad \implies \quad h + \frac{1}{2}u^2 = \text{constant}$$

Another equation for the enthalpy is obtained by substituting  $E = \rho h + \frac{1}{2}\rho v^2 - p$  into the conservative form of the energy equation giving

$$\frac{\partial(\rho h + \frac{1}{2}\rho v^2)}{\partial t} - \frac{\partial p}{\partial t} + \nabla \cdot ((\rho h + \frac{1}{2}\rho v^2) \mathbf{v}) = \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\tau}) - \nabla \cdot (\mathbf{q} + \mathbf{q}_R) + \mathbf{v} \cdot \sum m_i \mathbf{a}_i + \sum_i \mathbf{V}_i \cdot m_i \mathbf{a}_i$$

Thus in steady inviscid flow

$$\begin{aligned} \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \nabla \cdot ((h + \frac{1}{2}v^2) \rho \mathbf{v}) &= 0 \end{aligned}$$

Whence

$$\nabla(h + \frac{1}{2}v^2) \cdot (\rho \mathbf{v}) = 0$$

## 1.5 Reactions:

$$\sum_{i=1}^n \nu'_{ij} A_i \Leftrightarrow \sum_{i=1}^n \nu''_{ij} A_i \quad j = 1, 2, \dots, m$$

$$Y_i = \text{mass fraction} \quad X_i = \text{mole fraction} \quad (23)$$

$$[A] = \text{molar concentration} = \frac{\text{moles}}{\text{volume}} \quad R_u = \text{Universal Gas constant} \quad (24)$$

$$\bar{m}_j = \text{molecular weight} = \frac{\text{grams}}{\text{mole}} \quad \rho = \frac{\text{mass}}{\text{volume}} \quad (25)$$

$$Le = \frac{\lambda}{\rho D c_p} \quad \text{Lewis number} \quad (26)$$

$$Y_i = \frac{[A_i] \bar{m}_i}{\rho} = \frac{\bar{m}_i X_i}{\sum_j \bar{m}_j X_j} = \frac{\bar{m}_i X_i}{\bar{m}} = \frac{\rho_i}{\rho} = \frac{m_i}{m}$$

$$X_j = \frac{(Y_j / \bar{m}_j)}{\sum_{i=1}^n (Y_i / \bar{m}_i)}$$

$$[A_i] = \frac{\rho Y_i}{\bar{m}_i} = \frac{p X_i}{R_u T}$$

## 2 Reaction equations

$$\begin{aligned}
\frac{\partial Y_i}{\partial t} + (\mathbf{v} \cdot \nabla) Y_i &= \frac{1}{\rho} \sigma_i - \frac{1}{\rho} \nabla \cdot \mathbf{j}_i \quad i = 1, 2, \dots, n \\
\sigma_i &\equiv \dot{w}_i = \sigma_i(\rho, T, \mathbf{Y}) \\
\mathbf{j}_i &= \rho Y_i \mathbf{V}_i \quad \text{species flux} \\
\mathbf{V}_i &= -\frac{1}{X_i} D_{im} \mathbf{d}_i - \frac{D_k^T}{\rho Y_i T} \nabla T \quad \text{diffusion velocity} \\
\mathbf{d}_i &= \nabla X_i + (X_i - Y_i) \frac{1}{p} \nabla p \\
D_{im} &= \text{mixture diffusion coefficient} \quad D_k^T = \text{thermal diffusion coefficient}
\end{aligned}$$

For the species flux we make the approximations

$$\begin{aligned}
\mathbf{V}_i &\approx -\frac{1}{X_i} D_{im} \mathbf{d}_i \quad (\text{the rest is expensive to compute}) \\
\mathbf{d}_i &\approx \nabla X_i \quad (\text{valid for low Mach numbers}) \\
\text{which gives } \mathbf{j}_i &\approx -\rho \frac{Y_i}{X_i} D_{im} \nabla X_i
\end{aligned}$$

and thus the diffusion term on the right hand side of the species equation is

$$\begin{aligned}
-\frac{1}{\rho} \nabla \cdot \mathbf{j}_i &\approx \frac{1}{\rho} \nabla \cdot \left( \rho \frac{Y_i}{X_i} D_{im} \nabla X_i \right) \\
&= \frac{1}{\rho} \nabla \cdot \left( \rho D_{im} \nabla Y_i + \rho D_{im} Y_i \frac{\nabla \bar{m}}{\bar{m}_i} \right)
\end{aligned}$$

The species source terms

$$\sigma_i = \bar{m}_i \sum_{j=1}^m \frac{d}{dt} [A_i]_j \quad (27)$$

$$= \bar{m}_i \sum_{j=1}^m \Delta \nu_{ij} G_j \quad (28)$$

$$G_i = K_{fi}(T) \prod_{k=1}^m [A_k]^{\nu'_{ki}} - K_{bi}(T) \prod_{k=1}^m [A_k]^{\nu''_{ki}} \quad (29)$$

$$= K_{fi}(T) \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu'_{ki}} - K_{bi}(T) \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu''_{ki}} \quad (30)$$

Reaction rate constants,

$$K_{fj}(T) = B_{fj} T^{\alpha_{fj}} \exp\left(\frac{-E_{fj}}{R_u T}\right) \quad (31)$$

$$K_{bj}(T) = B_{bj} T^{\alpha_{bj}} \exp\left(\frac{-E_{bj}}{R_u T}\right) \quad (32)$$

$$\frac{K_f(T)}{K_b(T)} = K_p(T) (R_u T)^{-\Delta \nu} \quad (33)$$

This next Jacobian depends on which dependent variables we use:

$$\frac{\partial G_i}{\partial Y_j} = K_{fi}(T) \frac{\nu'_{j,i}}{Y_j} \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu'_{ki}} - K_{bi}(T) \frac{\nu''_{j,i}}{Y_j} \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu''_{ki}} \quad (34)$$

### 3 Scaling

We nondimensionalize the equations using the scales  $L_0$ ,  $u_0$ ,  $\rho_0$ , and  $T_0$ ,

$$\begin{aligned} t_0 &:= \frac{L_0}{U_0} & \tilde{\mathbf{v}} &:= \frac{\mathbf{v}}{U_0}, & a &= b & \tilde{t} &= \frac{t}{t_0} \\ \tilde{x} &= \frac{x}{L_0} & \tilde{T} &= \frac{T}{T_0} & \tilde{\rho} &= \frac{\rho}{\rho_0} & \tilde{\mathbf{v}} &= \frac{\mathbf{v}}{u_0} \\ \tilde{\mu} &:= \frac{\mu}{\rho_0 U_0 L_0} & p_0 &:= \rho_0 u_0^2, & R_0 &:= \frac{P_0 p_0}{\rho_0 T_0} & \tilde{t} &= \frac{t}{t_0} \\ \tilde{p} &= \frac{p}{p_0} - P_0 & \tilde{R}_i &= \frac{R_i}{R_0} & \tilde{\sigma} &= \frac{\sigma}{\rho_0 U_0 / L_0} & \tilde{h}_i &= \frac{h_i}{R_0 T_0} \\ \tilde{\lambda} &= \frac{\lambda}{\rho_0 U_0 L_0 R_0} & \tilde{D}_i &= \frac{D_i}{L_0 U_0} & \tilde{c}_{p,i} &= \frac{c_{p,i}}{R_0} & \tilde{c}_v &= \frac{c_v}{R_0} = \frac{\tilde{R}}{\gamma - 1} \end{aligned}$$

We have scaled the pressure using a scale for the static pressure and a scale for the dynamic pressure:

$$p = [P_0 + \tilde{p}]p_0, \quad P_{static} = P_0 p_0$$

In general the spatially constant static pressure may vary with time,  $P_0 = P_0(t)$ . Note that  $P_0$  is proportional to one over the square of the Mach number

$$P_0 = \frac{\rho_0 R_0 T_0}{\rho U_0^2} = \frac{1}{\gamma} \frac{\gamma R_0 T_0}{U_0^2} = \frac{1}{\gamma M_0^2} \quad \text{where } M_0 = \frac{U_0}{\sqrt{\gamma R_0 T_0}} = \frac{U_0}{a_0}.$$

Here are the scaled equations

$$\begin{aligned} \frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \tilde{\nabla} \cdot (\tilde{\rho} \tilde{\mathbf{v}}) &= 0 \\ \frac{\partial \tilde{\mathbf{v}}}{\partial \tilde{t}} + (\tilde{\mathbf{v}} \cdot \tilde{\nabla}) \tilde{\mathbf{v}} + \frac{1}{\tilde{\rho}} \tilde{\nabla} \tilde{p} &= \frac{1}{\tilde{\rho}} \tilde{\nabla} \cdot (\tilde{\mu} [\tilde{\nabla} \tilde{\mathbf{v}} + (\tilde{\nabla} \tilde{\mathbf{v}})^T]) - \frac{2}{3} \tilde{\mu} (\tilde{\nabla} \cdot \tilde{\mathbf{v}}) \mathbf{I} \\ \frac{\partial Y_i}{\partial \tilde{t}} + (\tilde{\mathbf{v}} \cdot \tilde{\nabla}) Y_i &= \frac{\tilde{\sigma}_i}{\tilde{\rho}} + \frac{1}{\tilde{\rho}} \tilde{\nabla} \cdot (\tilde{\rho} \tilde{D}_i \nabla Y_i) \quad i = 1, 2, \dots, n \end{aligned}$$

$$\frac{D\tilde{T}}{D\tilde{t}} + (\gamma - 1) \tilde{T} \tilde{\nabla} \cdot \tilde{\mathbf{v}} = \frac{1}{\tilde{\rho} \tilde{c}_v} \left\{ \sum_{i=1}^n (\tilde{R}_i \tilde{T} - \tilde{h}_i) \tilde{\sigma}_i + \tilde{\nabla} \cdot (\tilde{\lambda} \tilde{\nabla} \tilde{T}) - \tilde{T} \sum_{i=1}^n \tilde{R}_i \tilde{\nabla} \cdot \tilde{\mathbf{j}}_i - \tilde{\nabla} \tilde{T} \cdot \sum_{i=1}^n \tilde{c}_{p,i} \tilde{\mathbf{j}}_i + \frac{1}{P_0} \tilde{\Phi} \right\}$$

or the alternative form

$$\frac{D\tilde{T}}{D\tilde{t}} - \frac{1}{P_0} \frac{1}{\tilde{\rho} \tilde{c}_p} \frac{D\tilde{p}}{D\tilde{t}} = \frac{1}{\tilde{\rho} \tilde{c}_p} \left\{ - \sum_{i=1}^n (\tilde{h}_i \tilde{\sigma}_i) + \tilde{\nabla} \cdot (\tilde{\lambda} \tilde{\nabla} \tilde{T}) - \tilde{\nabla} \tilde{T} \cdot \sum_{i=1}^n \tilde{c}_{p,i} \tilde{\mathbf{j}}_i + \frac{1}{P_0} \tilde{\Phi} \right\}$$

$$\begin{aligned} \frac{D\tilde{p}}{D\tilde{t}} + \frac{\partial P_0}{\partial \tilde{t}} + \gamma (P_0 + \tilde{p}) \tilde{\nabla} \cdot \tilde{\mathbf{v}} &= P_0 \left\{ \sum_{i=1}^n (\gamma \tilde{R}_i \tilde{T} - (\gamma - 1) \tilde{h}_i) \tilde{\sigma}_i + (\gamma - 1) \tilde{\nabla} \cdot (\tilde{\lambda} \tilde{\nabla} \tilde{T}) \right. \\ &\quad \left. - \gamma \tilde{T} \tilde{\nabla} \cdot \left( \sum_{i=1}^n \tilde{R}_i \tilde{\mathbf{j}}_i \right) - (\gamma - 1) \tilde{\nabla} \tilde{T} \cdot \sum_{i=1}^n \tilde{c}_{p,i} \tilde{\mathbf{j}}_i + \frac{1}{P_0} (\gamma - 1) \tilde{\Phi} \right\} \end{aligned}$$

where

$$\begin{aligned} R_e &= \frac{1}{\tilde{\mu}} = \frac{\rho_0 U_0 L_0}{\mu} & \text{Reynolds number} \\ P_r &= \text{Prandtl number} \\ Le &= \frac{\lambda}{\rho D c_p} & \text{Lewis number} \end{aligned}$$

## 4 Solution of the Reaction equations

The temperature and reactions equations

$$\begin{aligned} \frac{DT}{Dt} &= \frac{1}{\rho c_p} \left\{ - \sum_{i=1}^n h_i \sigma_i + \nabla \cdot (\lambda \nabla T) - \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + \Phi \right\} \\ \frac{\partial Y_i}{\partial t} + (\mathbf{v} \cdot \nabla) Y_i &= \frac{1}{\rho} \sigma_i(\rho, T, Y_k) - \frac{1}{\rho} \nabla \cdot \mathbf{j}_i \quad i = 1, 2, \dots, n \end{aligned}$$

are solved with a Backward Euler scheme (here we assume that we are given  $p^{n+1}$  and we must solve for  $\rho^{n+1}$ ,  $T^{n+1}$  and  $Y_i^{n+1}$ )

$$\begin{aligned} p^{n+1} &= \rho^{n+1} R^{n+1} T^{n+1} \\ \frac{T^{n+1} - T^n}{\Delta t} - \frac{1}{\rho^{n+1} c_p(\mathbf{Y}^{n+1}, T^{n+1})} - \sum_{i=1}^n h_i \sigma_i(\mathbf{Y}^{n+1}, T) &= \text{stuff} \\ \frac{\mathbf{Y}^{n+1} - \mathbf{Y}^n}{\Delta t} - \frac{1}{\rho^{n+1}} \boldsymbol{\sigma}(\mathbf{Y}^{n+1}, T) &= \left\{ -\mathbf{v} \cdot \nabla \mathbf{Y} - \frac{1}{\rho} \nabla \cdot \mathbf{j}_i \right\}^{n+\frac{1}{2}} \end{aligned}$$

or

$$\begin{aligned} p^{n+1} &= \rho^{n+1} R^{n+1} T^{n+1} \\ T_{n+1} - \frac{\Delta t}{\rho^{n+1} c_p(\mathbf{Y}^{n+1}, T^{n+1})} - \sum_{i=1}^n h_i \sigma_i(\mathbf{Y}^{n+1}, T) &= T^n + \Delta t \{ \text{stuff} \} \\ \mathbf{Y}^{n+1} - \frac{\Delta t}{\rho^{n+1}} \boldsymbol{\sigma}(\mathbf{Y}^{n+1}, T) &= \mathbf{Y}^n + \Delta t \left\{ -\mathbf{v} \cdot \nabla \mathbf{Y} - \frac{1}{\rho} \nabla \cdot \mathbf{j}_i \right\}^{n+\frac{1}{2}} \end{aligned}$$

We solve this nonlinear equation by Newton's method. We write the system of equations for  $T^{n+1}$  and  $\mathbf{Y}^{n+1}$  as

$$\begin{aligned} \mathbf{Z}^{n+1} - \Delta t \mathbf{S}(\mathbf{Z}^{n+1}) &= \mathbf{G} \\ \mathbf{Z}^{n+1} &= \mathbf{Z}^n + \delta \mathbf{Z} \end{aligned}$$

where

$$\mathbf{Z} = \begin{bmatrix} T^{n+1} \\ \mathbf{Y}^{n+1} \end{bmatrix} \quad \mathbf{S} = \begin{bmatrix} -\frac{1}{\rho c_p} \sum h_i \sigma_i \\ \frac{1}{\rho} \boldsymbol{\sigma} \end{bmatrix}$$

Then a Newton step is

$$\left[ I - \Delta t \frac{\partial \mathbf{S}}{\partial \mathbf{Z}}(\mathbf{Z}^n) \right] \delta \mathbf{Z} = -\mathbf{Z}^n + \Delta t \mathbf{S}(\mathbf{Z}^n) + \mathbf{G}$$

## 5 Derivation of Some Equations

### 5.1 Derivation of the Temperature Equation

Differentiating

$$e = \sum_{i=1}^n (h_i - R_i T) Y_i$$

gives

$$\begin{aligned} \frac{De}{Dt} &= \sum_{i=1}^n \left\{ (c_{p,i} - R_i) \frac{DT}{Dt} Y_i + (h_i - R_i T) \frac{DY_i}{Dt} \right\} \\ &= c_v \frac{DT}{Dt} + \sum_{i=1}^n (h_i - R_i T) \frac{DY_i}{Dt} \end{aligned}$$

Substituting this last expression into the energy equation

$$\frac{\partial e}{\partial t} + (\mathbf{v} \cdot \nabla)e + \frac{p}{\rho} \nabla \cdot \mathbf{v} = -\frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi$$

results in

$$c_v \frac{DT}{Dt} + \frac{p}{\rho} \nabla \cdot \mathbf{v} = \sum_{i=1}^n (R_i T - h_i) \frac{DY_i}{Dt} - \frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi$$

and thus

$$\begin{aligned} \frac{DT}{Dt} + \frac{p}{\rho c_v} \nabla \cdot \mathbf{v} &= \frac{1}{\rho c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) (\sigma_i - \nabla \cdot \mathbf{j}_i) - \nabla \cdot \mathbf{q} + \Phi \right\} \\ &= \frac{1}{\rho c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) \sigma_i + \nabla \cdot (\lambda \nabla T) - \sum_{i=1}^n (R_i T - h_i) \nabla \cdot \mathbf{j}_i - \nabla \cdot \left( \sum_{i=1}^n h_i \mathbf{j}_i \right) + \Phi \right\} \\ &= \frac{1}{\rho c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) \sigma_i + \nabla \cdot (\lambda \nabla T) - T \sum_{i=1}^n R_i \nabla \cdot \mathbf{j}_i - \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + \Phi \right\} \end{aligned}$$

whence

$$\frac{DT}{Dt} + (\gamma - 1) T \nabla \cdot \mathbf{v} = \frac{1}{\rho c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) \sigma_i + \nabla \cdot (\lambda \nabla T) - T \sum_{i=1}^n R_i \nabla \cdot \mathbf{j}_i - \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + \Phi \right\}$$

**Note:** An alternative form of the temperature equation retains the pressure as a variable in

$$e = \sum_{i=1}^n (h_i Y_i) - \frac{p}{\rho}$$

Then

$$\begin{aligned} \frac{De}{Dt} &= c_p \frac{DT}{Dt} + \sum_{i=1}^n (h_i \frac{DY_i}{Dt}) + \frac{p}{\rho^2} \frac{D\rho}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} \\ &= c_p \frac{DT}{Dt} + \sum_{i=1}^n (h_i \frac{DY_i}{Dt}) - \frac{p}{\rho} \nabla \cdot \mathbf{v} - \frac{1}{\rho} \frac{Dp}{Dt} \end{aligned}$$

Substituting this last expression into the energy equation gives

$$\frac{DT}{Dt} - \frac{1}{\rho c_p} \frac{Dp}{Dt} = \frac{1}{\rho c_p} \left\{ - \sum_{i=1}^n (h_i \sigma_i) + \nabla \cdot (\lambda \nabla T) - \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + \Phi \right\} \quad (35)$$

This last equation is useful if  $p = \text{constant}$ .

## 5.2 Derivation of the pressure equation

From  $p = \rho R T$  it follows that

$$\frac{Dp}{Dt} = RT \frac{D\rho}{Dt} + \rho R \frac{DT}{Dt} + \rho T \frac{DR}{Dt} \quad (36)$$

and

$$\frac{DR}{Dt} = \sum_{i=1}^n R_i \frac{DY_i}{Dt} \quad (37)$$

whence

$$\frac{Dp}{Dt} + \gamma p \nabla \cdot \mathbf{v} = \frac{R}{c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) (\rho \frac{DY_i}{Dt}) + \nabla \cdot (\lambda \nabla T) + \Phi \right\} + \rho T \sum_{i=1}^n R_i \left( \frac{DY_i}{Dt} \right) \quad (38)$$



or substituting for  $DY_i/Dt$

$$\frac{Dp}{Dt} + \gamma p \nabla \cdot \mathbf{v} = \frac{R}{c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) \sigma_i + \nabla \cdot (\lambda \nabla T) - T \nabla \cdot \left( \sum_{i=1}^n R_i \mathbf{j}_i \right) - \nabla T \cdot \left( \sum_{i=1}^n c_{p,i} \mathbf{j}_i \right) + \Phi \right\} \quad (39)$$

$$+ \rho T \sum_{i=1}^n R_i \left( \frac{\sigma_i}{\rho} - \frac{1}{\rho} \nabla \cdot \mathbf{j}_i \right) \quad (40)$$

giving the pressure equation

$$\frac{Dp}{Dt} + \gamma p \nabla \cdot \mathbf{v} = \sum_{i=1}^n (\gamma R_i T - (\gamma - 1) h_i) \sigma_i + (\gamma - 1) \nabla \cdot (\lambda \nabla T) \quad (41)$$

$$- \gamma T \nabla \cdot \left( \sum_{i=1}^n R_i \mathbf{j}_i \right) - (\gamma - 1) \nabla T \cdot \sum_{i=1}^n c_{p,i} \mathbf{j}_i + (\gamma - 1) \Phi \quad (42)$$

where we have used

$$\frac{R}{c_v} = \gamma - 1 \quad (43)$$

## 6 Frozen Flow

The equations for frozen flow are determined by keeping the mass fractions  $Y_i$  constant in space and time. Then  $DY_i/Dt$  in equations (35) and (38) is zero and thus

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \frac{1}{\rho} \nabla p &= \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau} \\ \frac{DT}{Dt} + (\gamma - 1) T \nabla \cdot \mathbf{v} &= \frac{1}{\rho c_v} \{ \nabla \cdot (\lambda \nabla T) + \Phi \} \\ \frac{Dp}{Dt} + \gamma p \nabla \cdot \mathbf{v} &= \nabla \cdot (\lambda \nabla T) + (\gamma - 1) \Phi \\ \frac{\partial Y_i}{\partial t} &= 0 \end{aligned}$$

## 7 Equilibrium Flow

In equilibrium flow the reactions are assumed to proceed infinitely fast so that  $\sigma_i = 0$ . In this case we retain the term  $DY_i/Dt$  in equations (35) and (38) Note that we could not set  $\sigma_i = 0$  in the temperature and pressure equations as this would not conserve energy.

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \frac{1}{\rho} \nabla p &= \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau} \\ \frac{DT}{Dt} + (\gamma - 1) T \nabla \cdot \mathbf{v} &= \frac{1}{\rho c_v} \left\{ \sum_{i=1}^n (R_i T - h_i) \left( \rho \frac{DY_i}{Dt} \right) + \nabla \cdot (\lambda \nabla T) + \Phi \right\} \\ \frac{Dp}{Dt} + \gamma p \nabla \cdot \mathbf{v} &= \sum_{i=1}^n (\gamma R_i T - (\gamma - 1) h_i) \left( \rho \frac{DY_i}{Dt} \right) + (\gamma - 1) \nabla \cdot (\lambda \nabla T) + (\gamma - 1) \Phi \\ \sigma_i(Y_i, T, \rho) &= 0 \end{aligned}$$

## 8 The Bomb problem: constant pressure combustion

A standard test for Chemkin is the constant pressure combustion problem for a gas mixture

The equations that are solved are

$$\begin{aligned}\frac{\partial T}{\partial t} &= -\frac{1}{\rho c_p} \sum_{i=1}^n (h_i \sigma_i) \\ \frac{\partial Y_i}{\partial t} &= \frac{1}{\rho} \sigma_i \quad i = 1, 2, \dots, n \\ p_0 &= \rho R T\end{aligned}$$

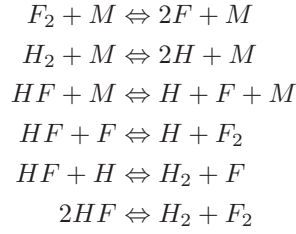
NOTE that since the pressure is constant, the density will vary and thus  $\nabla \cdot (\rho \mathbf{v})$  will not be zero. This would correspond to a reaction in a box that is allowed to expand to keep the pressure constant.

**Note:** that the equation for  $T$  comes from the temperature/pressure equation (21) rather than the temperature equation (18). Use of the latter would result in a different answer!

## 9 H-F reactions

Here is the H-F reaction taken from Zucrow and Hoffaman.

Reaction mechanism:



Source terms:

$$\begin{aligned}\sigma_{H_2} &= \bar{m}_{H_2} [-G_1 + G_4 + G_5] \\ \sigma_{F_2} &= \bar{m}_{F_2} [-G_0 + G_3 + G_5] \\ \sigma_{HF} &= \bar{m}_{HF} [-G_2 - G_3 - G_4 - 2G_5] \\ \sigma_H &= \bar{m}_H [2G_1 + G_2 + G_3 - G_4] \\ \sigma_F &= \bar{m}_F [2G_0 + G_2 - G_3 + G_4]\end{aligned}$$

Reaction step functions:

$$\begin{aligned}G_0 &= K_{f0}(T)[F_2][M] - K_{b0}(T)[F]^2[M] \\ G_1 &= K_{f1}(T)[H_2][M] - K_{b1}(T)[H]^2[M] \\ G_2 &= K_{f2}(T)[HF][M] - K_{b2}(T)[H][F][M] \\ G_3 &= K_{f3}(T)[HF][F] - K_{b3}(T)[H][F_2] \\ G_4 &= K_{f4}(T)[HF][H] - K_{b4}(T)[H_2][F] \\ G_5 &= K_{f5}(T)[HF]^2 - K_{b5}(T)[H_2][F_2]\end{aligned}$$

Reaction rate constants, cm, Mole, K

$$\begin{aligned}
K_{b0} &= 1.10 \times 10^{18} T^{-3/2} \\
K_{b1} &= 7.50 \times 10^{18} T^{-1} \\
K_{b2} &= 7.50 \times 10^{18} T^{-1} \\
K_{b3} &= 5.28 \times 10^{12} T^{1/2} \exp(-4000/T) \\
K_{b4} &= 5.00 \times 10^{12} \exp(-5700/T) \\
K_{b5} &= 1.75 \times 10^{10} T^{1/2} \exp(-19,997/T)
\end{aligned}$$

The forward rates are related to the backward rates through the equilibrium constants,  $K_p$ .

$$\begin{aligned}
K_{f0} &= 1.10 \times 10^{18} T^{-3/2} K_{p,F}^2 (AR_u T)^{-1} \\
K_{f1} &= 7.50 \times 10^{18} T^{-1} K_{p,H}^2 (AR_u T)^{-1} \\
K_{f2} &= 7.50 \times 10^{18} T^{-1} K_{p,H} K_{p,F} / K_{p,HF} (AR_u T)^{-1} \\
K_{f3} &= 5.28 \times 10^{12} T^{1/2} K_{p,H} / (K_{p,HF} K_{p,F}) \exp(-4000/T) \\
K_{f4} &= 5.00 \times 10^{12} K_{p,F} / (K_{p,HF} K_{p,H}) \exp(-5700/T) \\
K_{f5} &= 1.75 \times 10^{10} T^{1/2} 1 / K_{p,HF}^2 \exp(-19,997/T)
\end{aligned}$$

Since the values of  $K_P$  from the JANNAF tables are based on a reference pressure of 1 atmosphere, we need to convert some of the  $K_p$  by the factor  $A = \text{atmospheres}/(Nm^2) = 1./1.01325e5$  if we want to use MKS units.

Eigenvalue of the jacobian

$$\begin{aligned}
\frac{\partial G_i}{\partial Y_j} &= K_{fi}(T) \frac{\nu'_{j,i}}{Y_j} \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu'_{ki}} - K_{bi}(T) \frac{\nu''_{j,i}}{Y_j} \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu''_{ki}} \\
&= K_{bi}(T) \left( K_{pi}(T) (R_u T)^{-\Delta \nu_j} \frac{\nu'_{j,i}}{Y_j} \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu'_{ki}} - \frac{\nu''_{j,i}}{Y_j} \prod_{k=1}^m \left( \frac{\rho Y_k}{\bar{m}_k} \right)^{\nu''_{ki}} \right)
\end{aligned}$$

## 10 Coso: Combustion Solver

Coso is a program that solves the full time dependent equations with finite difference methods.

Coso can be used to solve one dimensional reacting flow.

Current features, limitations are

- no transport terms yet, i.e. no real viscous, or diffusion terms
- simple artificial viscosity
- Dependent variables can be  $\rho, u, p, Y_i$  or  $\rho, u, T, Y_i$ .
- Species equations are integrated with backward Euler.
- Chemistry comes Chemkin or an H-F reaction from from Zucrow and Hoffman
- The class Reactions encapsulates the chemistry – number of species, reaction mechanism etc. This allows the reactions to be changed with no changes to Coso.

### 10.1 Flow in a variable area channel

The equations of motion for flow in a channel with cross section  $A(x)$  are

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho u \\ \rho E \\ \rho Y \end{bmatrix} + \frac{1}{A} \frac{\partial}{\partial x} \begin{bmatrix} \rho u A \\ (\rho u^2 + p) A \\ (\rho E u + p u) A \\ \rho u Y A \end{bmatrix} = \begin{bmatrix} 0 \\ \mu \Delta u + \dots \\ -q_x \\ \sigma + \dots \end{bmatrix} \quad (44)$$

or

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho u \\ \rho E \\ \rho Y \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho E u + p u \\ \rho u Y \end{bmatrix} + \frac{u}{A(x)} \frac{dA(x)}{dx} \begin{bmatrix} \rho \\ \rho u + p \\ \rho E + p \\ \rho Y \end{bmatrix} = \begin{bmatrix} 0 \\ \mu \Delta u + \dots \\ -q_x \\ \sigma + \dots \end{bmatrix} \quad (45)$$

or

$$\rho_t + (\rho u)_x + \rho u \frac{A'}{A} = 0 \quad \text{or} \quad \rho_t + (\rho u A)_x / A = 0 \quad (46)$$

$$u_t + u u_x + \frac{1}{\rho} p_x = \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau} \quad (47)$$

$$e_t + u e_x + \frac{p}{\rho} (u_x + u \frac{A'}{A}) = -\frac{1}{\rho} \nabla \cdot \mathbf{q} + \frac{1}{\rho} \Phi \quad (48)$$

$$T_t + u T_x + (\gamma - 1) T (u_x + u \frac{A'}{A}) = \dots \quad (49)$$

$$p_t + u p_x + \gamma p (u_x + u \frac{A'}{A}) = \dots \quad (50)$$

$$Y_t + u Y_x = \frac{\sigma_i}{\rho} + \frac{1}{\rho} \nabla \cdot (\rho D_i \nabla Y_i) \quad (51)$$

## 11 Numerical Experiments

### 11.1 Flow in a De Laval Nozzle with an H-F reaction

Here we attempt to reproduce the results from the Zucrow and Hoffman.

We have two solution techniques. The first technique follows the method proposed in the book, using significant analytical simplifications for steady flow. The results for frozen and equilibrium flow in a nozzle are shown in figures 1 to 3.

The second solution technique is el brute force, solving the full time dependent equations (program Coso, CCombustion Solver). The results for frozen, equilibrium and non-equilibrium flow are shown in figures 4 - 12. In these figures we solve the pressure equation and get the temperature from the equation of state.

In figure 12 the eigenvalues of the scaled species jacobian matrix,

$$\frac{1}{\rho} \frac{\partial \sigma_i}{\partial Y_j} \frac{L_0}{U_0}$$

are shown. The eigenvalues are all real and less than or equal to zero. These values are indicative of the stiffness of the chemistry.

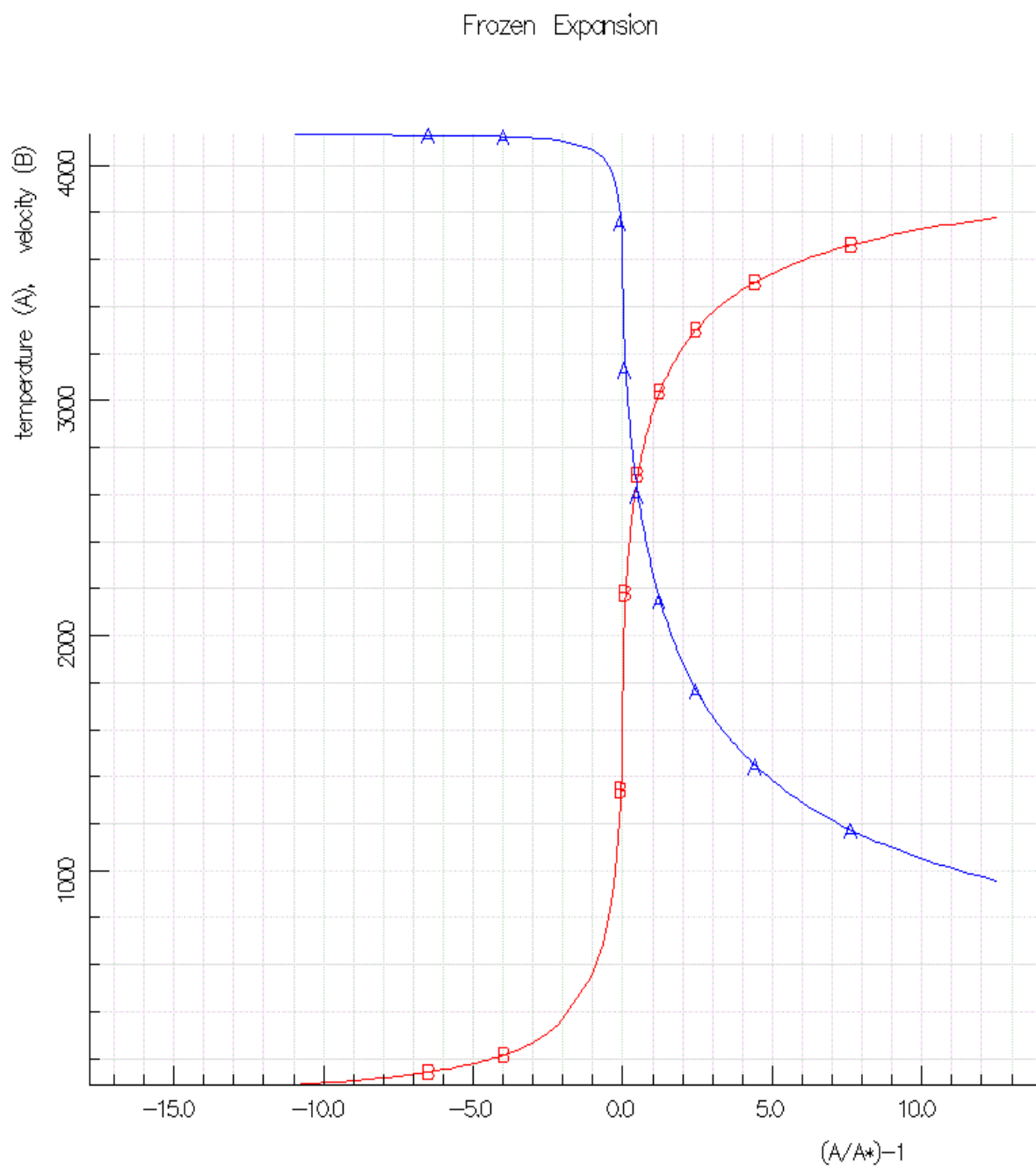


Figure 1: Frozen flow ala Zucrow and Hoffman, temperature and velocity

## Equilibrium Expansion

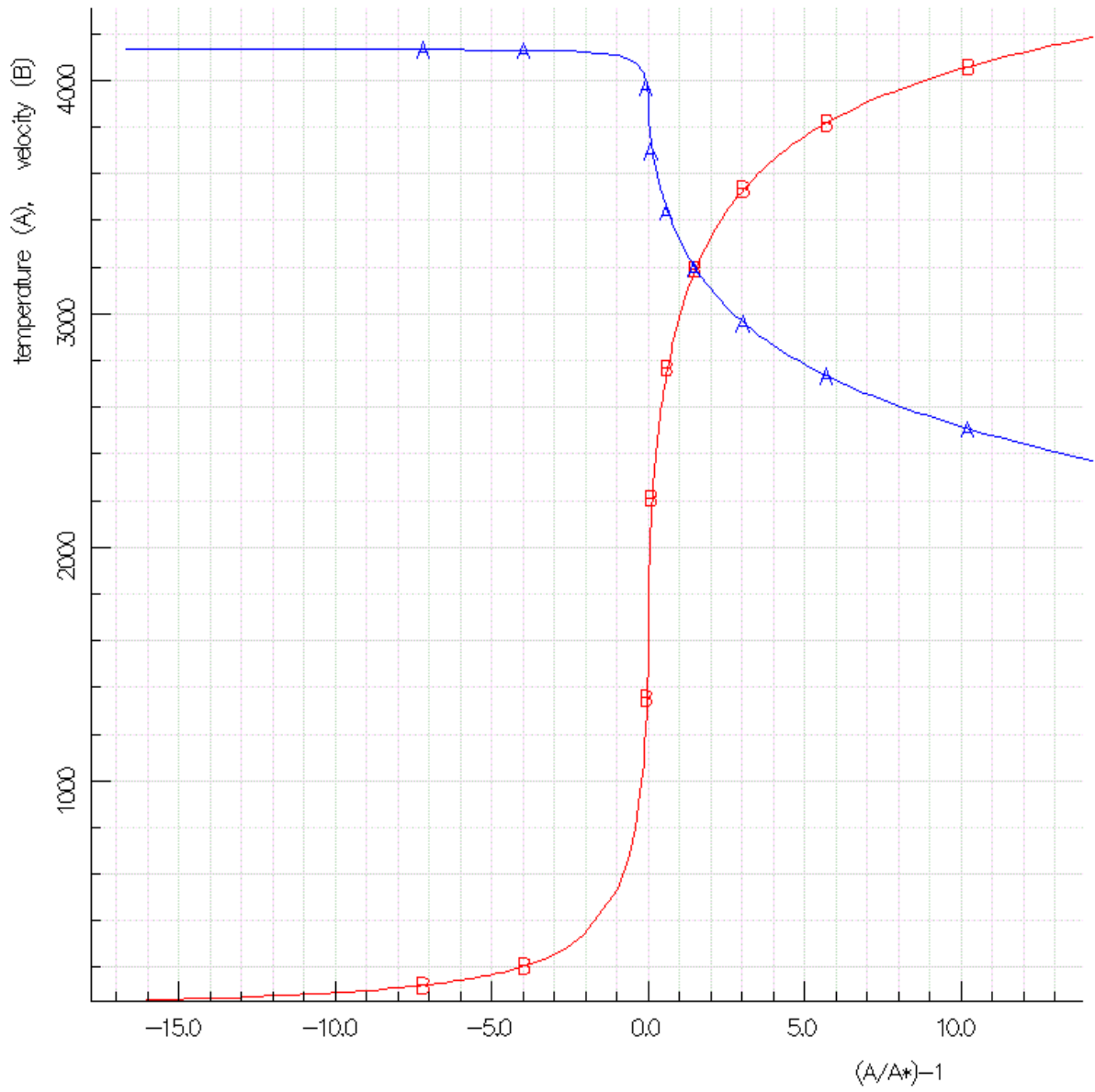


Figure 2: Equilibrium flow ala Zucrow and Hoffman, temperature and velocity

# Equilibrium Expansion

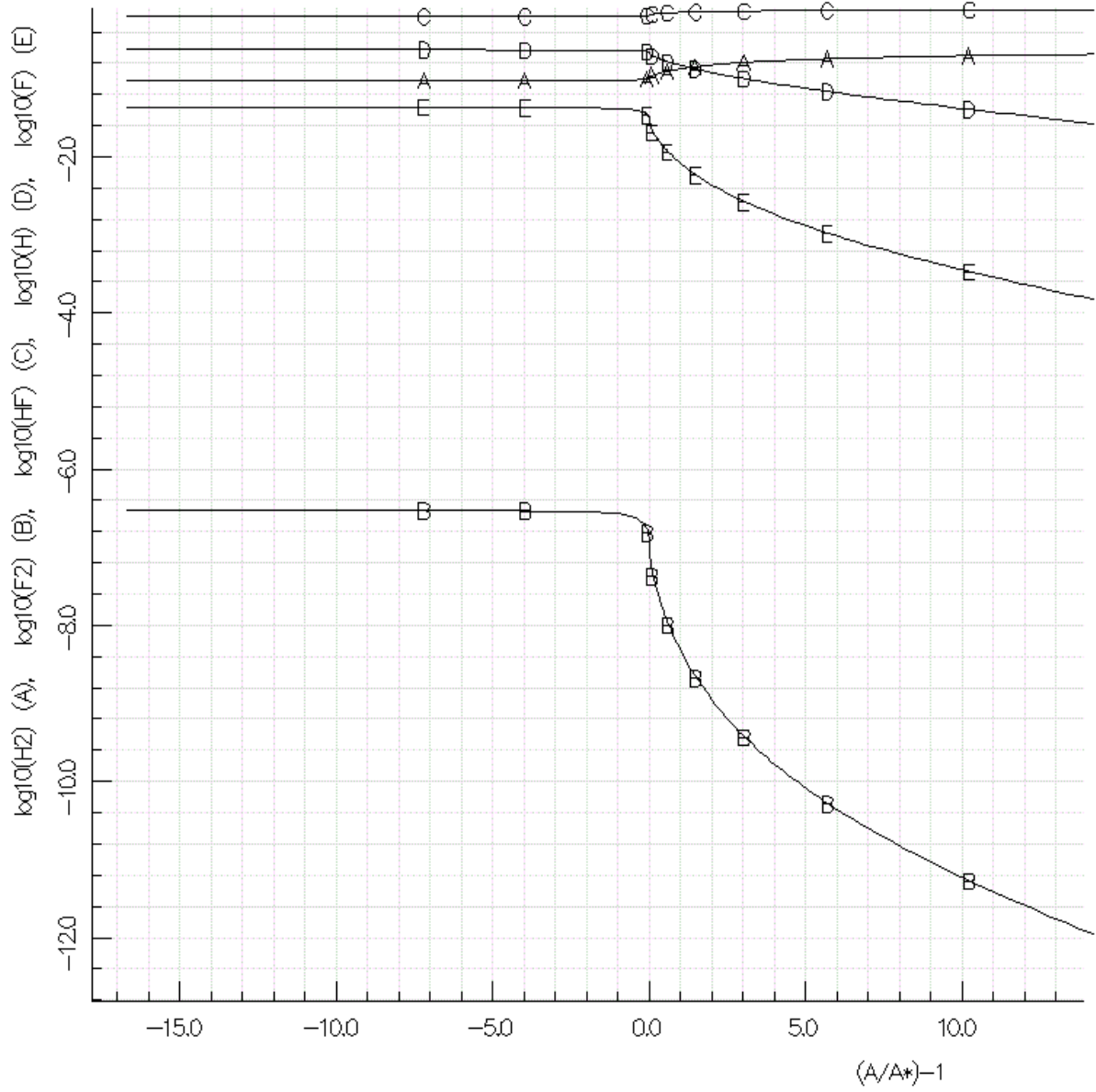


Figure 3: Equilibrium flow ala Zucrow and Hoffman, species

Nozzle flow, frozen,  $t=1.00004$ ,  $dt=0.0061$

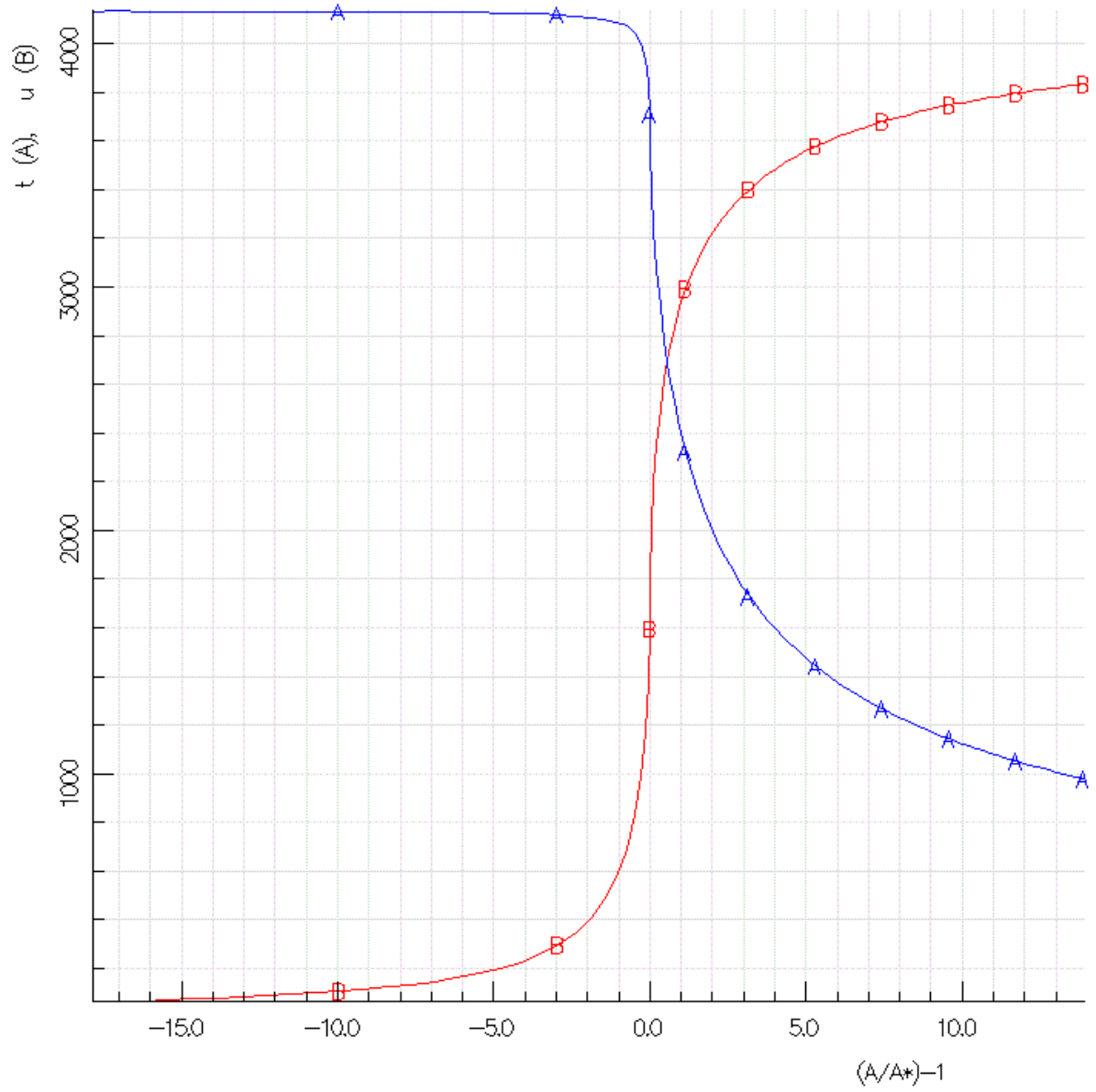


Figure 4: Frozen flow from Coso, temperature and velocity



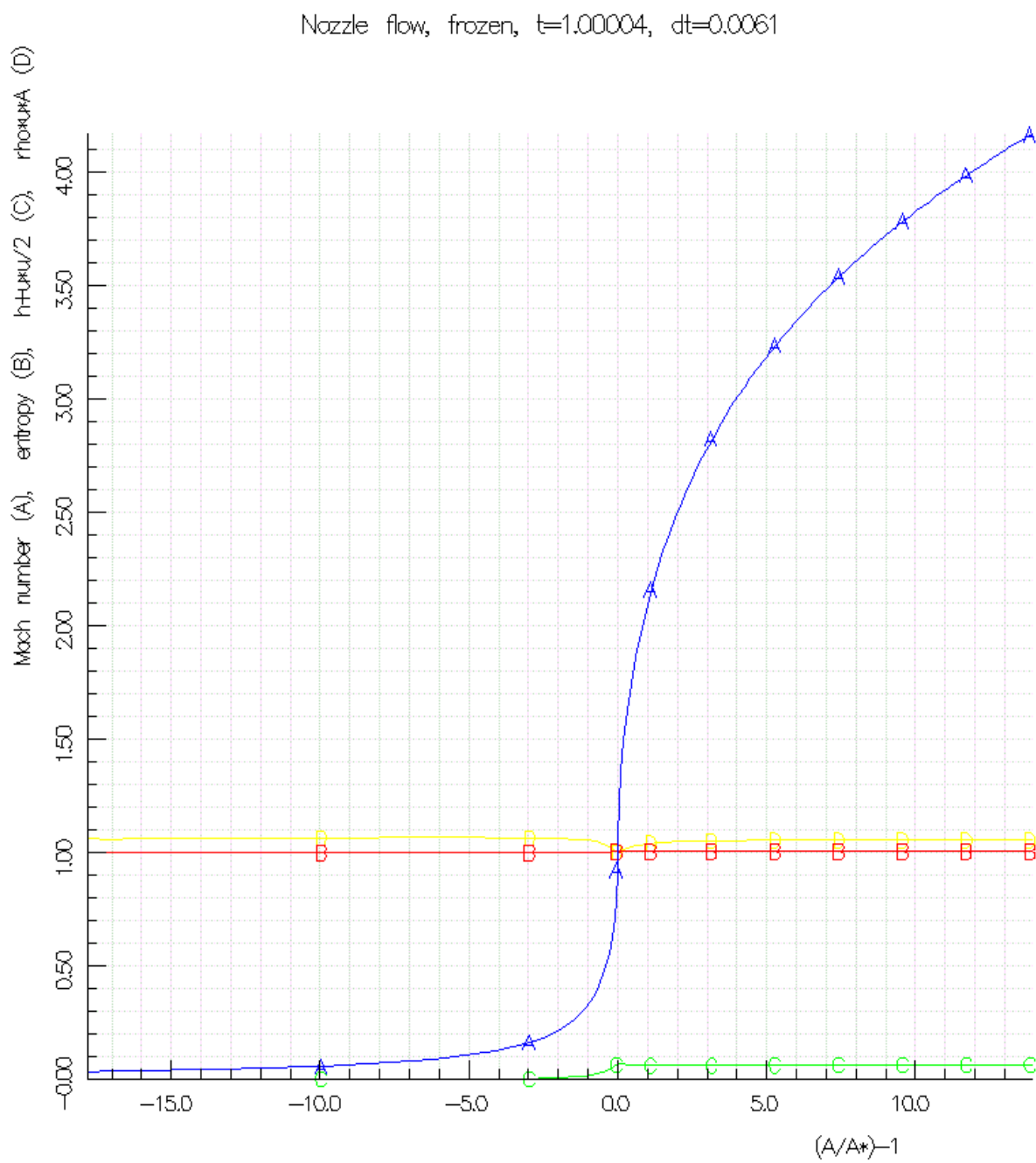


Figure 5: Frozen flow from Coso

Nozzle flow, equilibrium,  $t=1.09943$ ,  $dt=0.0039$

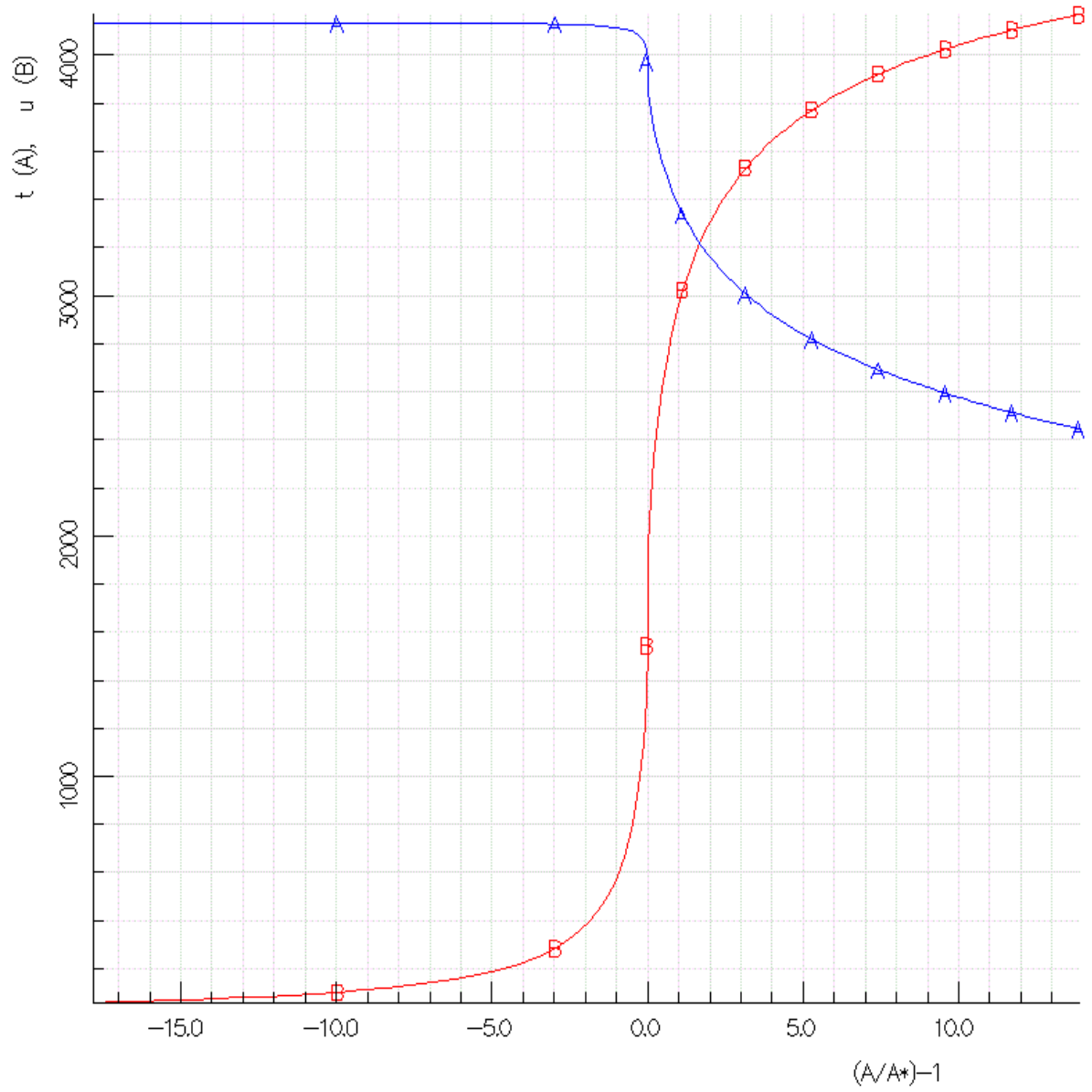


Figure 6: Equilibrium flow from Coso, temperature and velocity

Nozzle flow, equilibrium,  $t=1.09943$ ,  $dt=0.0039$

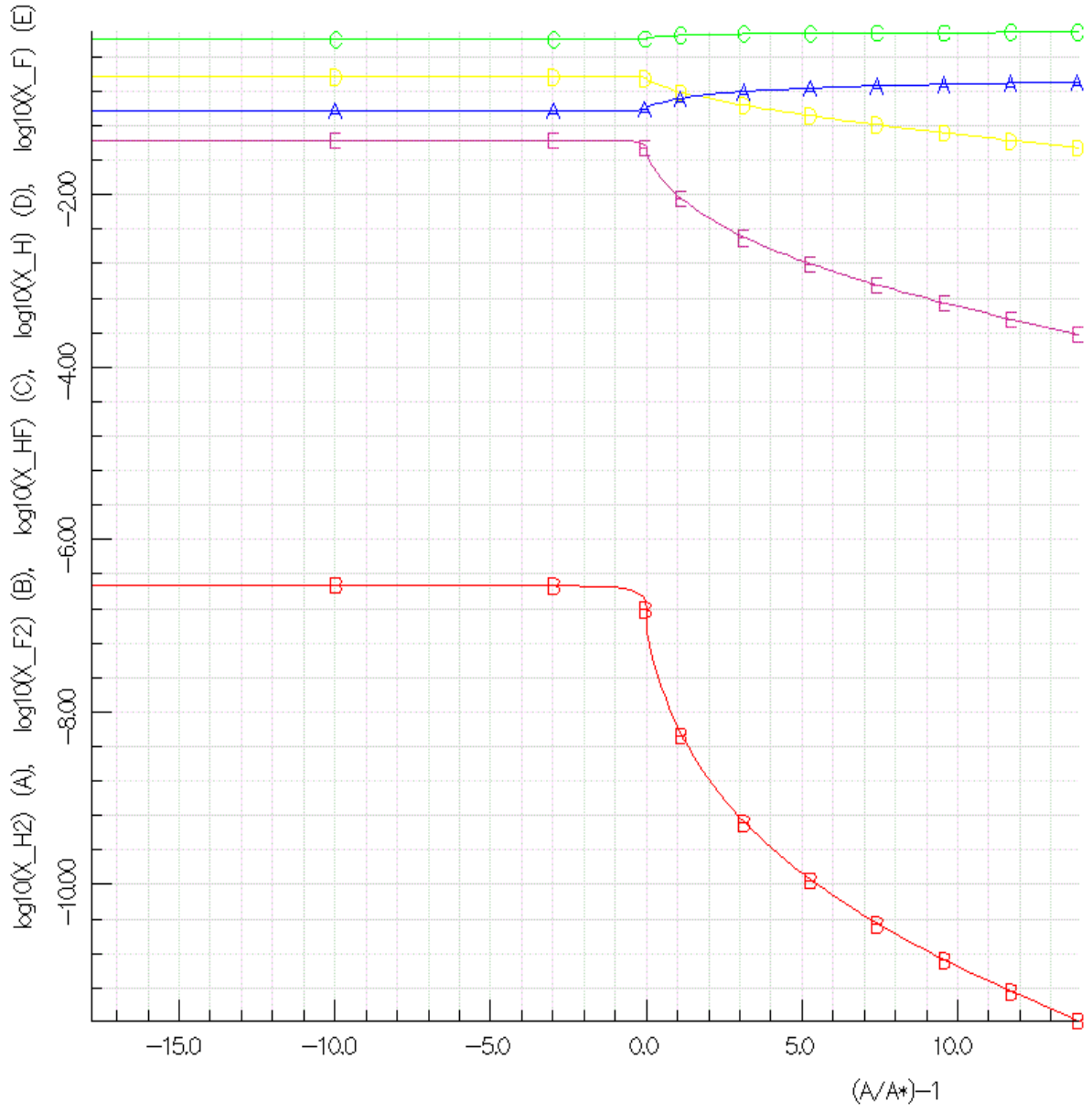


Figure 7: Equilibrium flow from Coso, species

Nozzle flow, equilibrium,  $t=1.09943$ ,  $dt=0.0039$

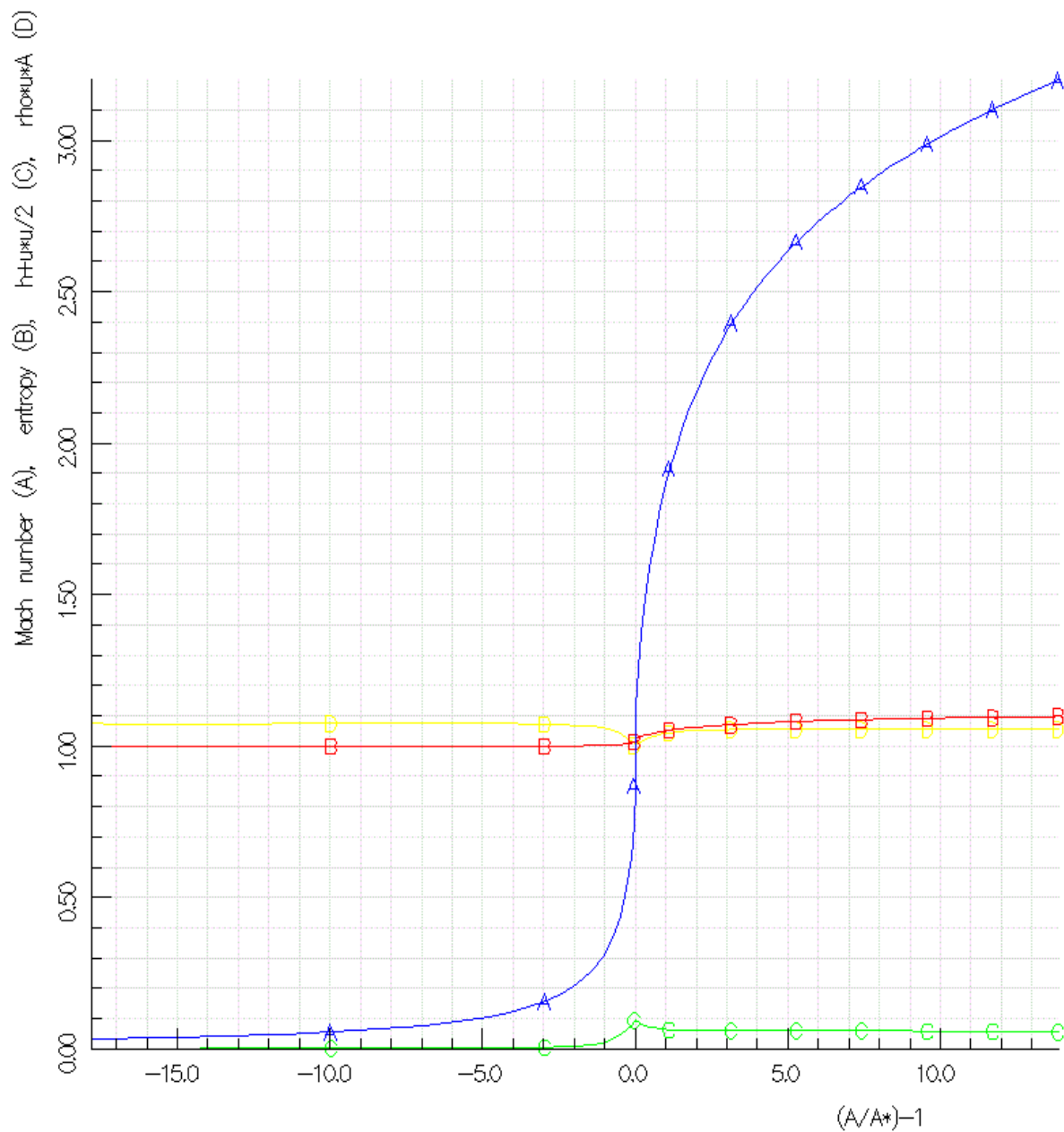


Figure 8: Equilibrium flow from Coso

Nozzle flow, nonequilibrium,  $t=1.09848$ ,  $dt=0.0059$

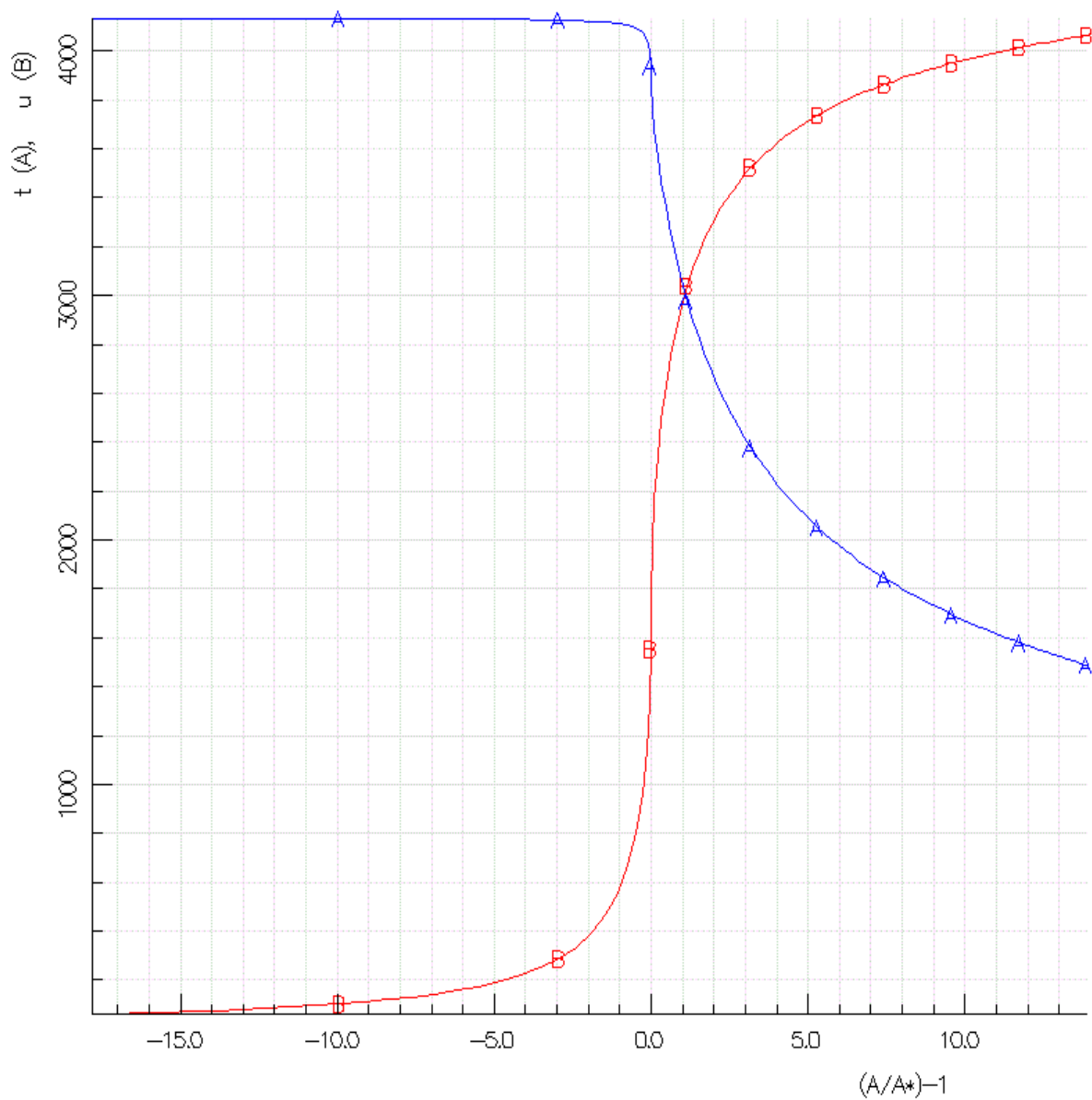


Figure 9: Non-equilibrium flow from Coso, temperature and velocity

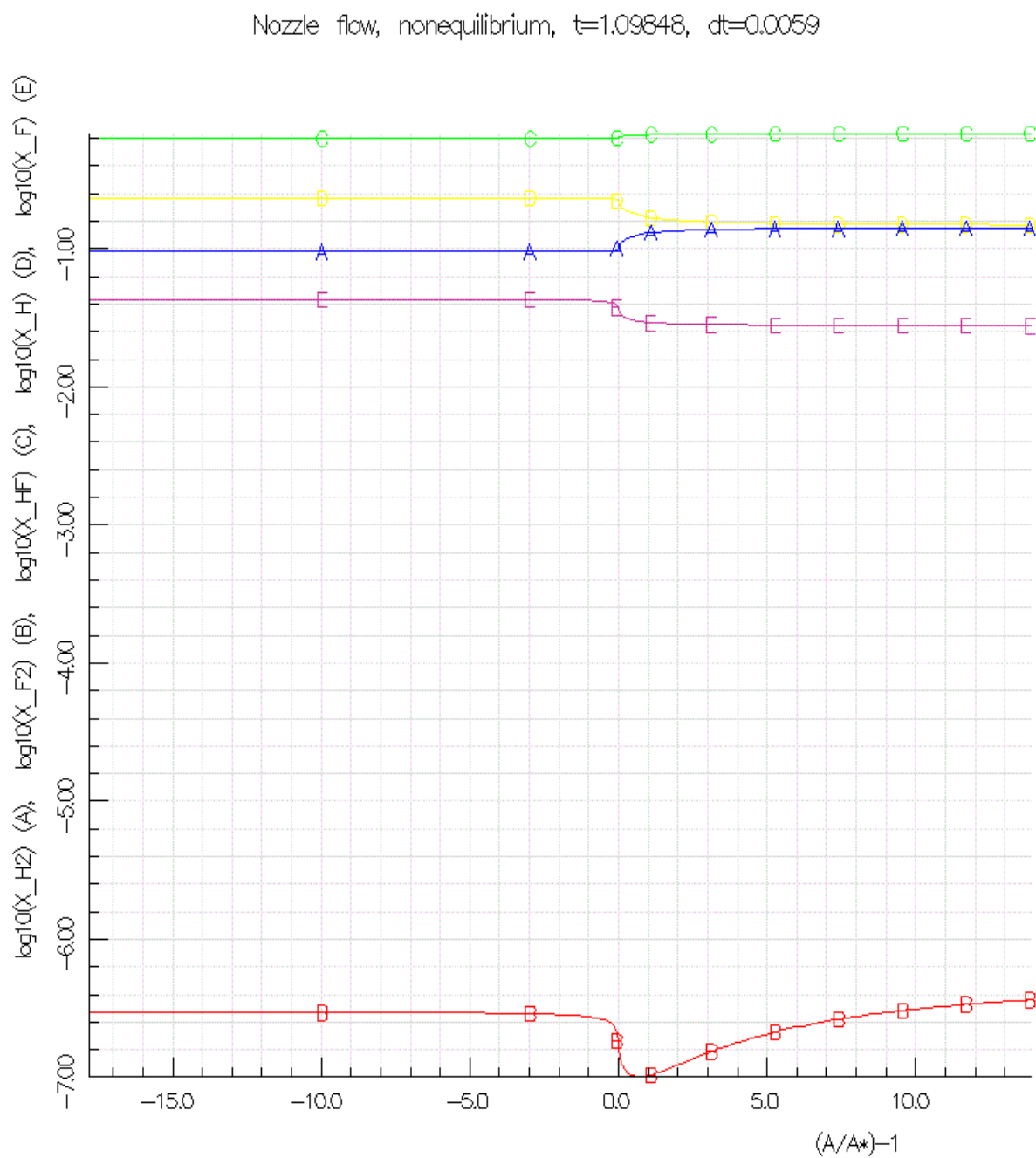


Figure 10: Non-equilibrium flow from Coso, species

Nozzle flow, nonequilibrium,  $t=1.09848$ ,  $dt=0.0059$

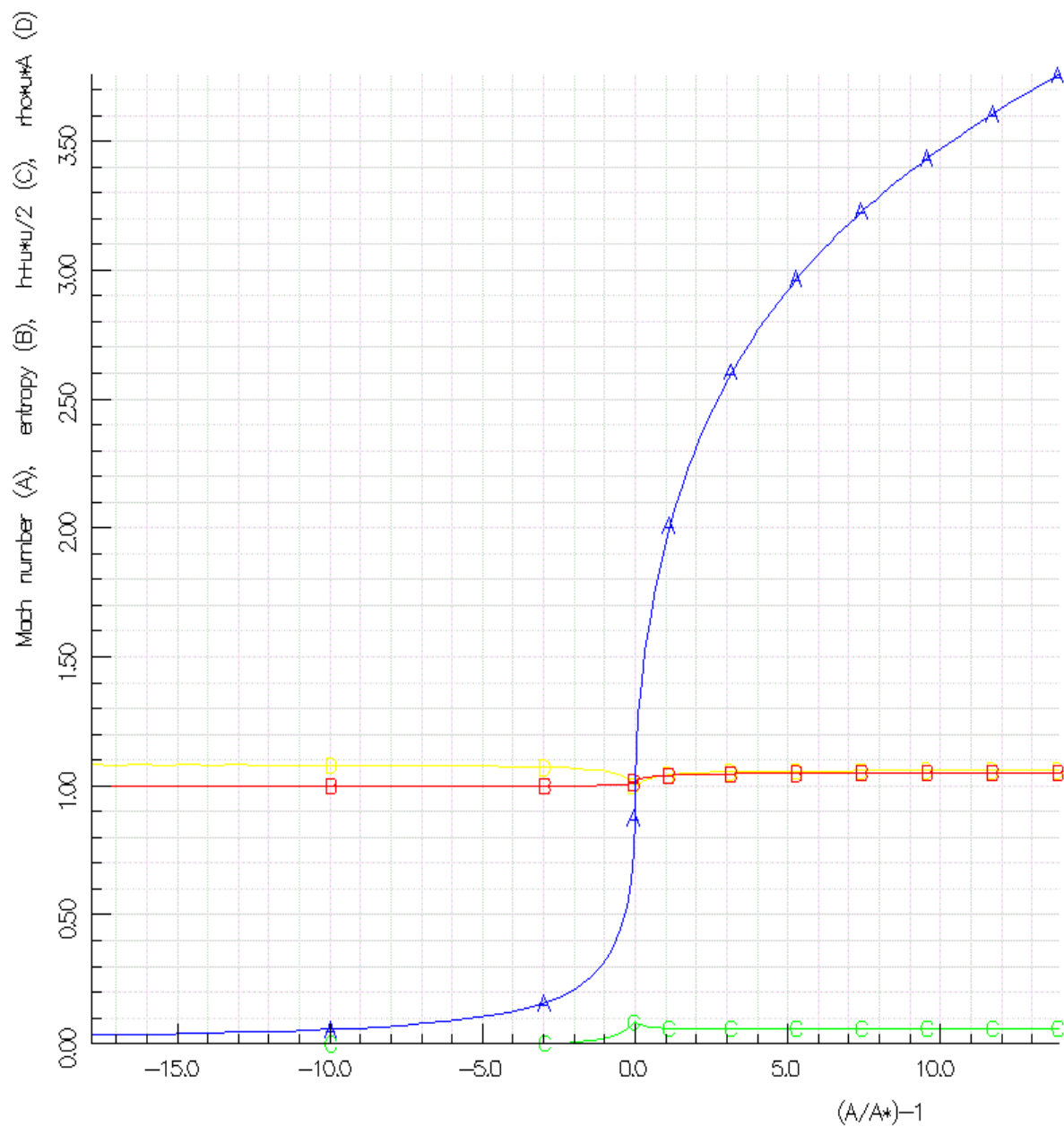


Figure 11: Non-equilibrium flow from Coso

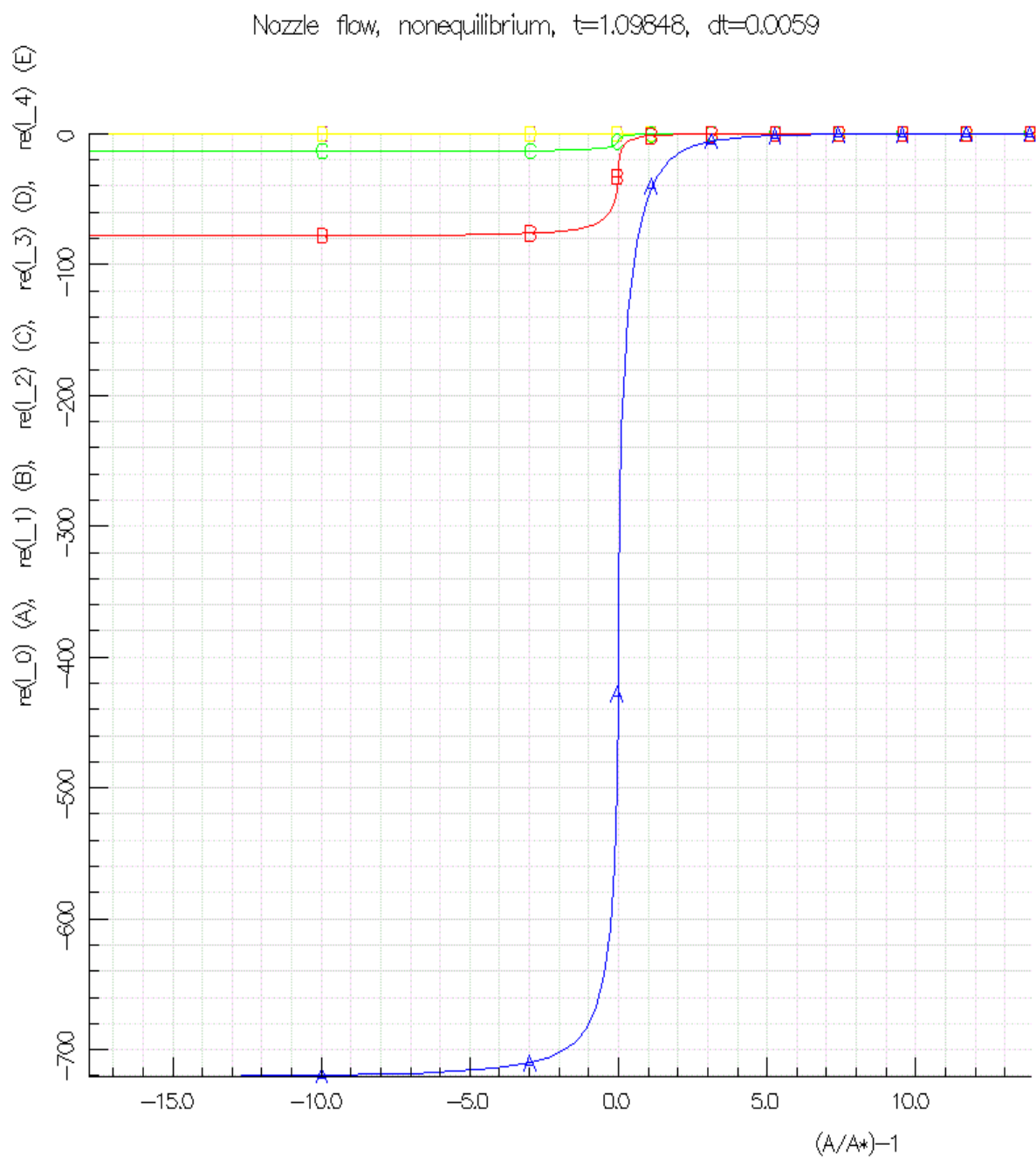


Figure 12: Non-equilibrium flow from Coso, scaled eigenvalues of the Species Jacobian