ESCOLA POLITÉCNICA DA UNIVERSIDADE DE SÃO PAULO

Possibilidades dos FTs

Discretização

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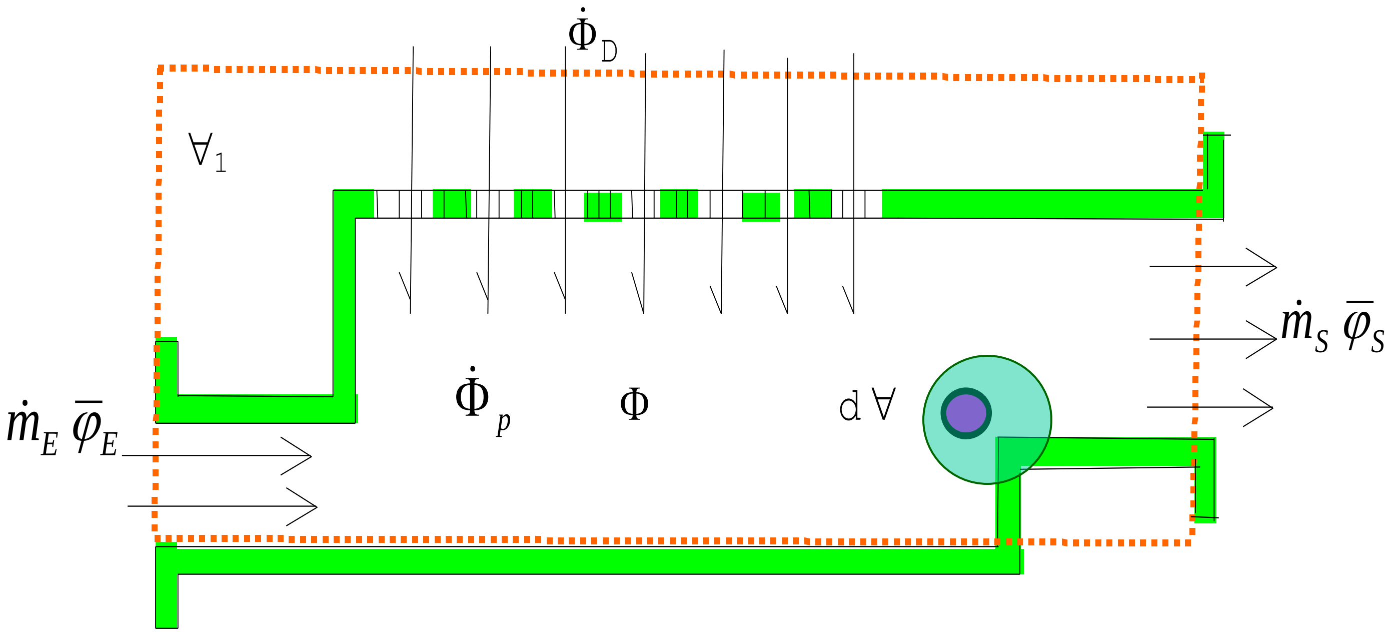
Título

$$\frac{d\Phi}{dt} = \dot{m}_E \, \overline{\varphi_E} - \dot{m}_S \, \overline{\varphi_S} + \dot{\Phi}_D + \dot{\Phi}_P$$



$$\dot{m} = \overline{\rho} \, v_b \, S = \int_S \rho \, \vec{v} \, dS \quad ; \quad \dot{m} \, \overline{\varphi} = \overline{\rho} \, \varphi_b \, v_b \, S = \int_S \rho \, \varphi \, \vec{v} \, dS$$

$$v_b = \frac{1}{\overline{\rho} \, S} \int_S \rho \, \vec{v} \, dS \quad ; \quad \varphi_b = \frac{1}{\overline{\rho} \, v_b \, S} \int_S \rho \, \varphi \, \vec{v} \, dS$$

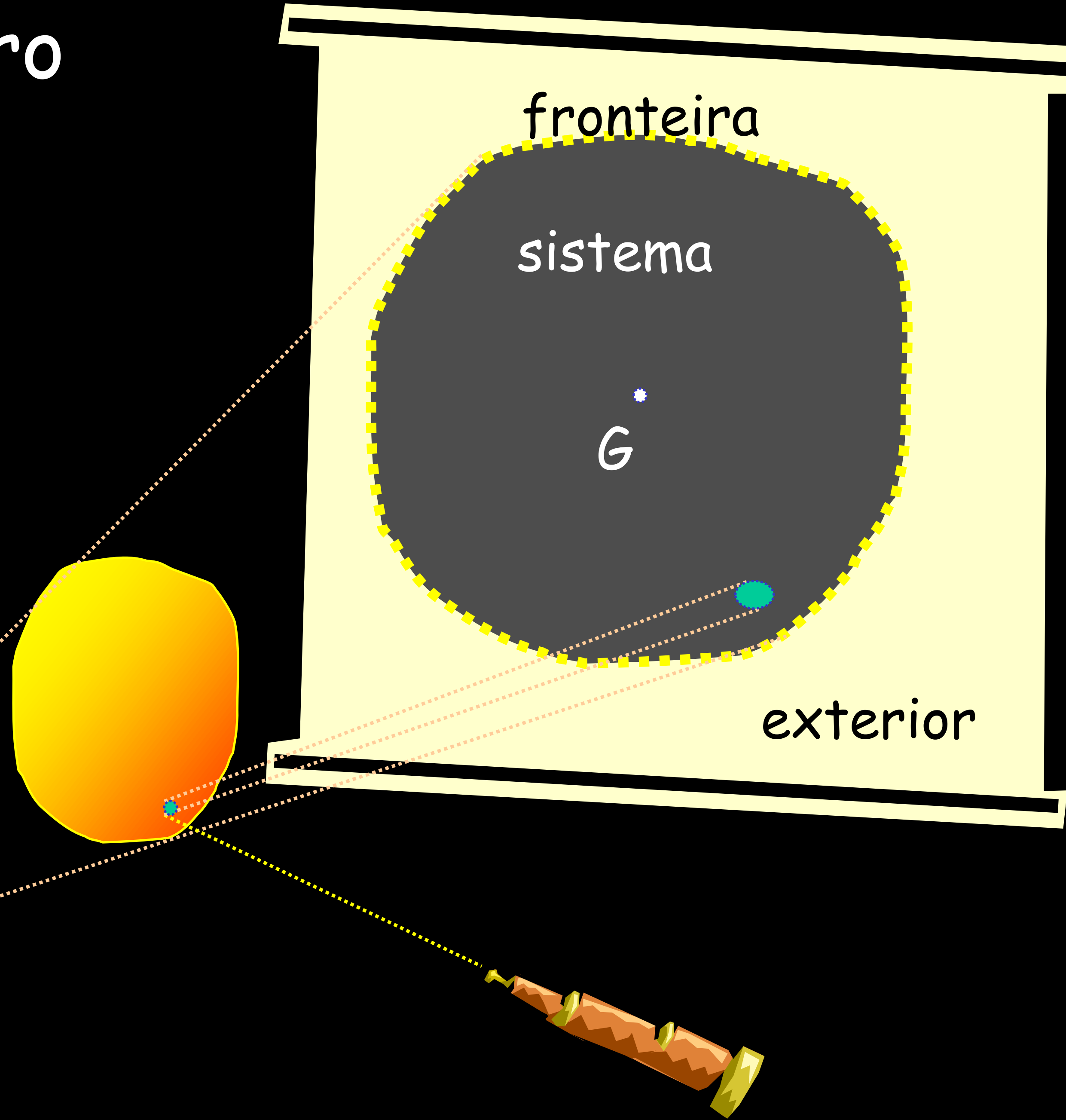
$$\text{macro} = \int \text{micro}$$

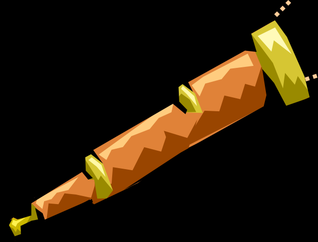
$$m = \int_{sist} dm$$

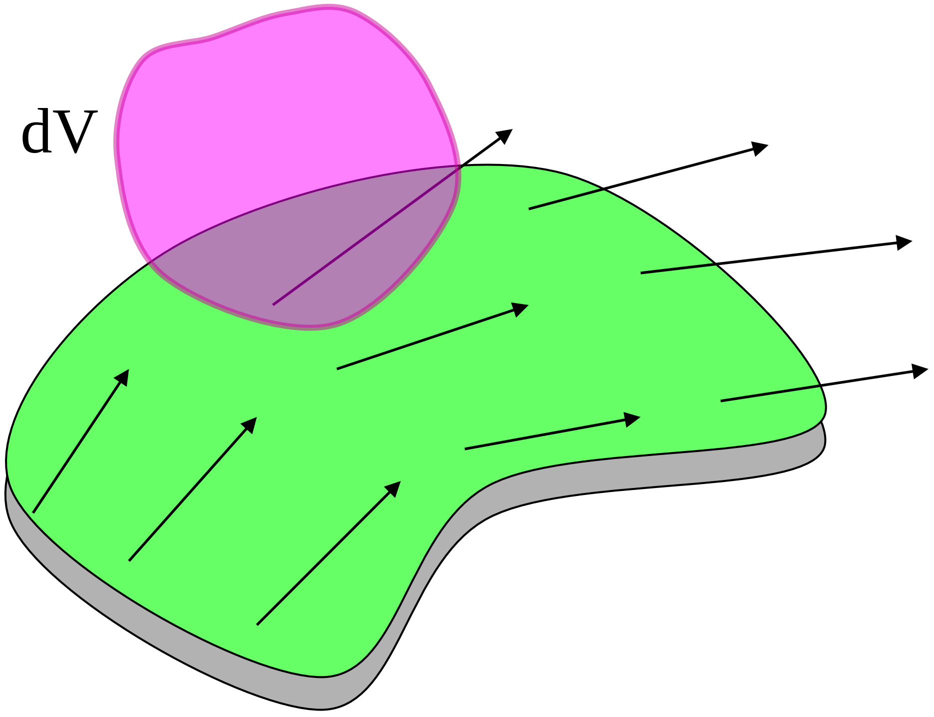
$$\forall = \int_{sist} dV$$

$$m = \int_{\forall} \rho \, dV$$

$$\Phi = \int_{\forall} \rho\varphi \, dV$$





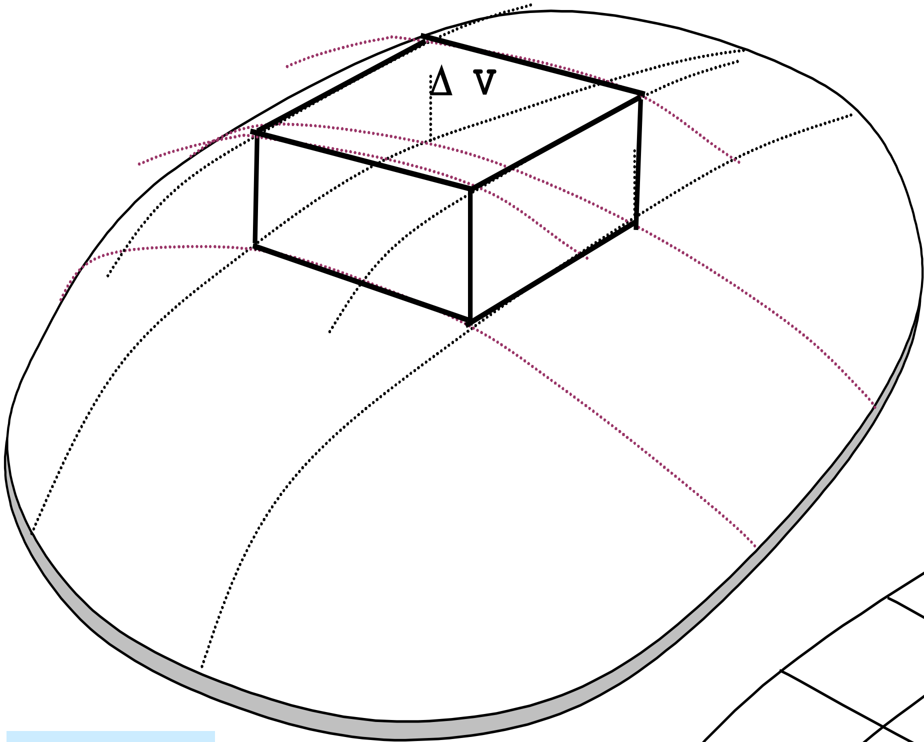


$$\rho \frac{D\,\varphi}{Dt} = \rho \left(\frac{\partial\,\varphi}{\partial t} + \vec{v}\,.\,\mathrm{gr\vec{a}d}\,\varphi\right) = \frac{\partial\,\rho\,\varphi}{\partial t} + \mathrm{div}\,\rho\,\vec{v}\,\varphi = \mathrm{div}\,\rho\,\lambda_\Phi\,\mathrm{gr\vec{a}d}\,\varphi + \dot{\sigma}_{\forall\Phi}$$

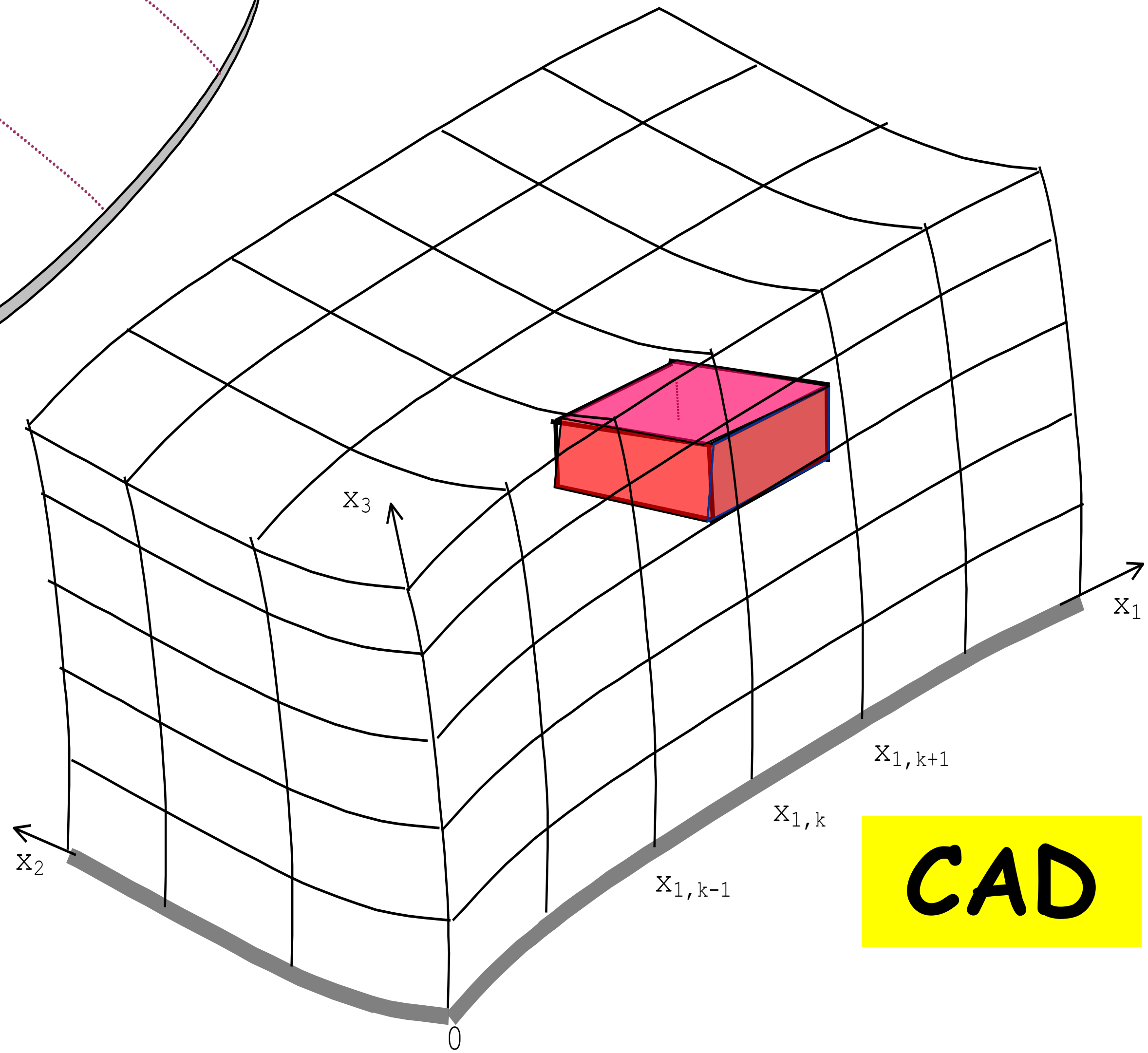
onde $\mathbf{j}_\Phi = -\,\rho\,\lambda_\Phi\,\boldsymbol{\nabla}\varphi$.

sendo $\varphi = 1$ a equação da continuidade:

$$\frac{\partial\,\rho}{\partial t} + \mathrm{div}\,\rho\,\vec{v} = \frac{D\,\rho}{Dt} + \rho\,\mathrm{div}\,\vec{v} = 0$$



construir a malha a partir da fronteira

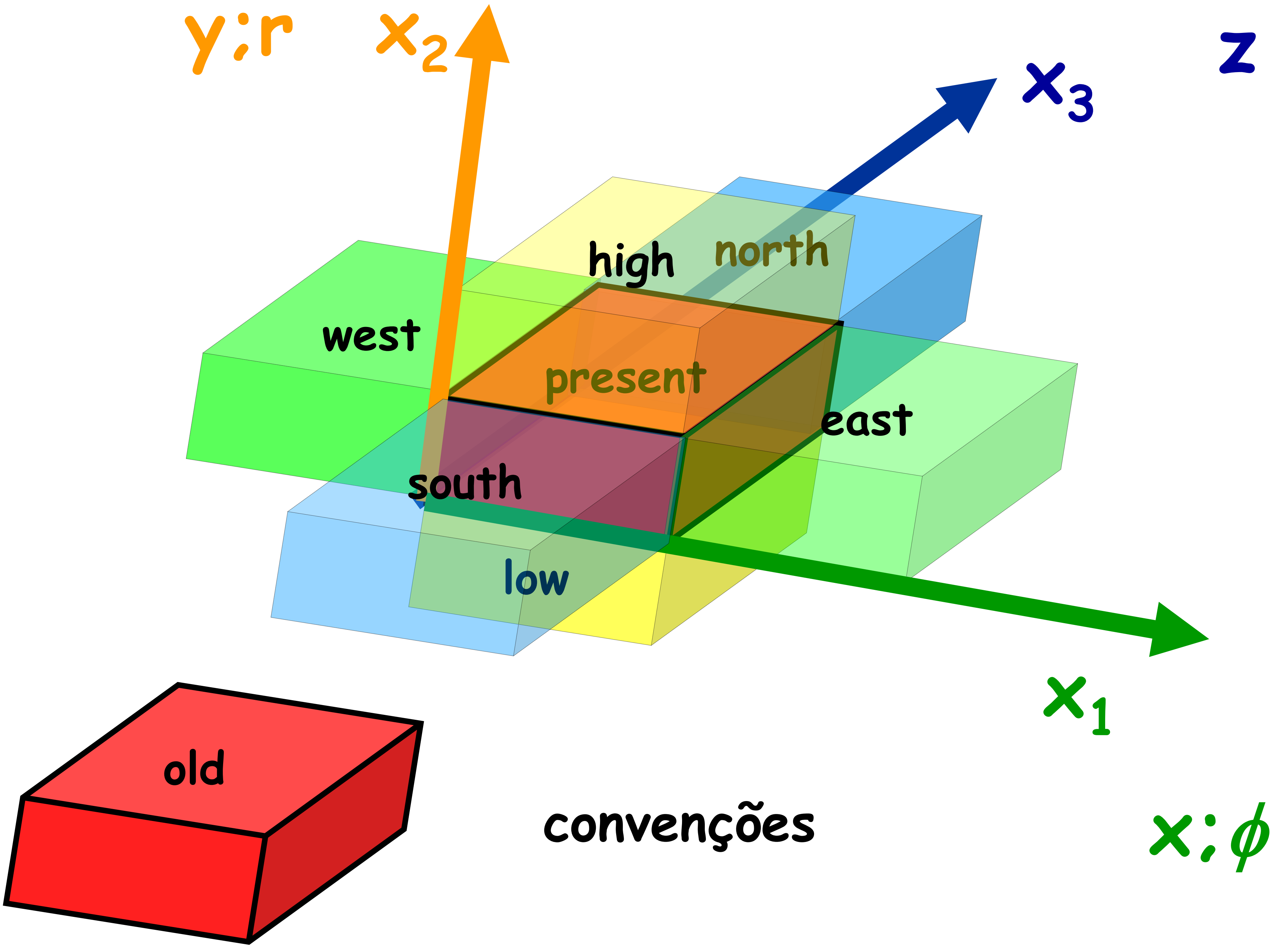


Δ∀

cada célula é um batch

$$\dot{\sigma}_{V\Phi} = c_* (\varphi_* - \varphi)$$

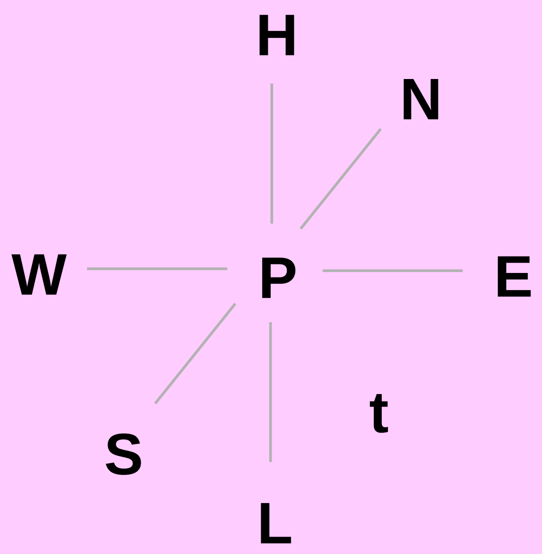
CAD



y;r
x2
x3
z
high
north
west
present
east
south
low
x1
old
convenções
x;ϕ

PNSEWHLt

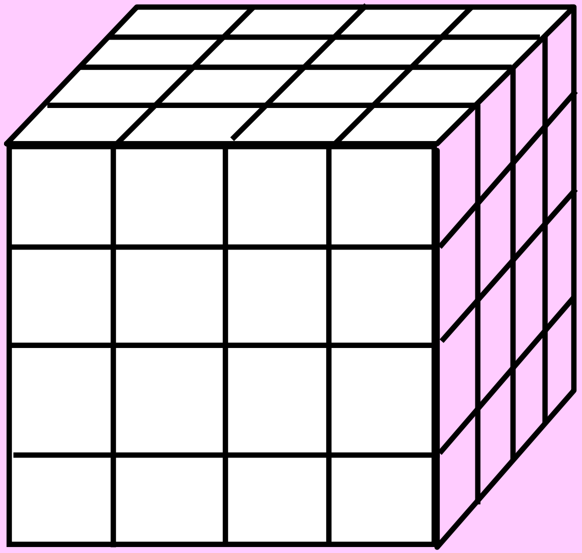
Os elementos de volume formam um conjunto ordenado de pontos no tempo e no espaço. Para o caso de elementos hexaédricos:



P - elemento central
N - elemento ao norte
S - elemento ao sul
E - elemento ao leste
W - elemento ao oeste
H - elemento acima
L - elemento abaixo
t - instante de tempo

Relação de um ponto do *grid* com suas vizinhanças:

$$A_P\phi_P = A_N\phi_N + A_S\phi_S + A_E\phi_E + A_W\phi_W + A_H\phi_H + A_L\phi_L + A_t\phi_t + \text{fontes}$$

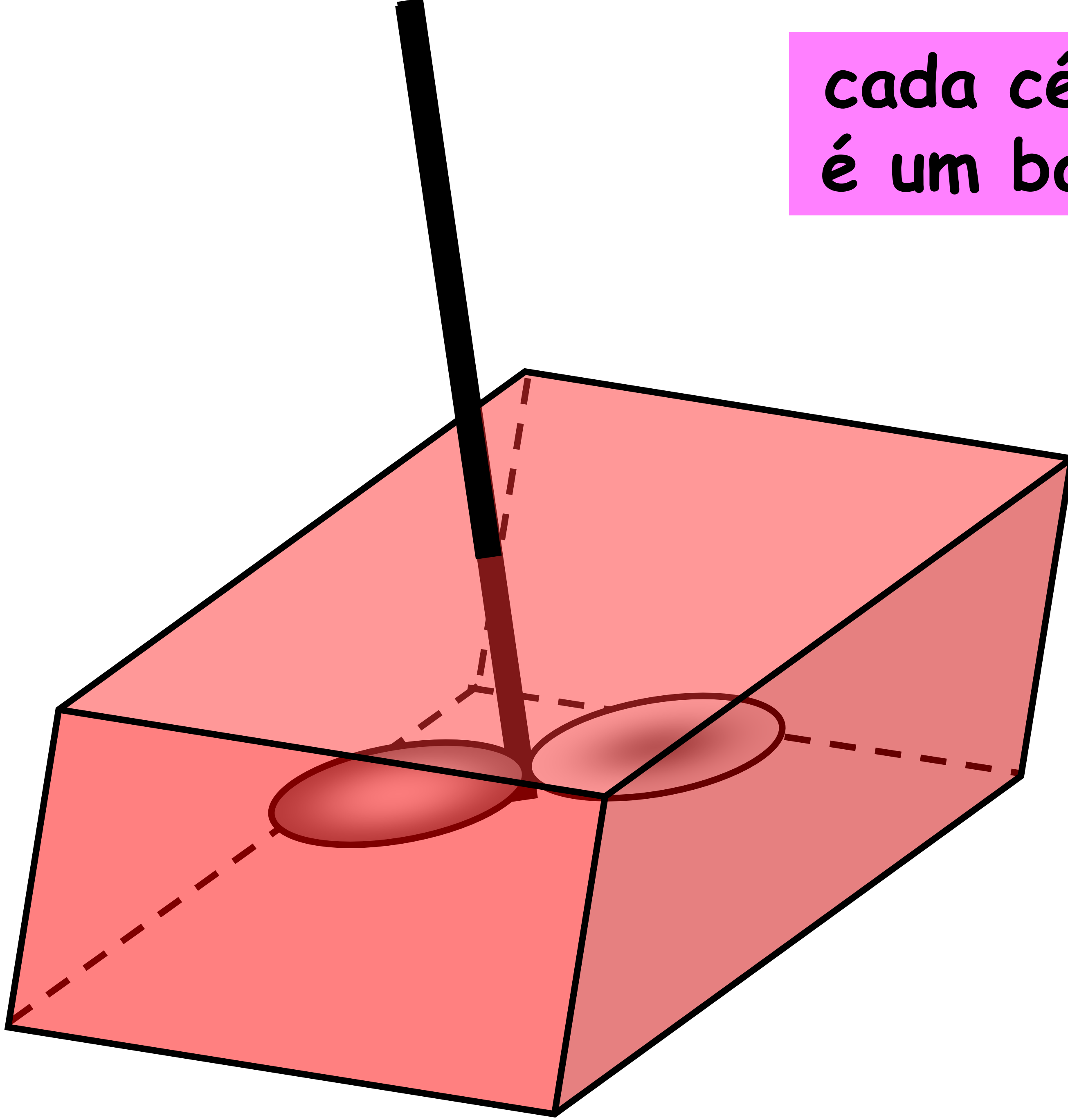


Como as equações de conservação não podem ser aplicadas na forma diferencial, elas são discretizadas em um número finito de elementos de volume, definidos de forma que preencham todo o espaço pelo qual o fluido escoa (domínio).

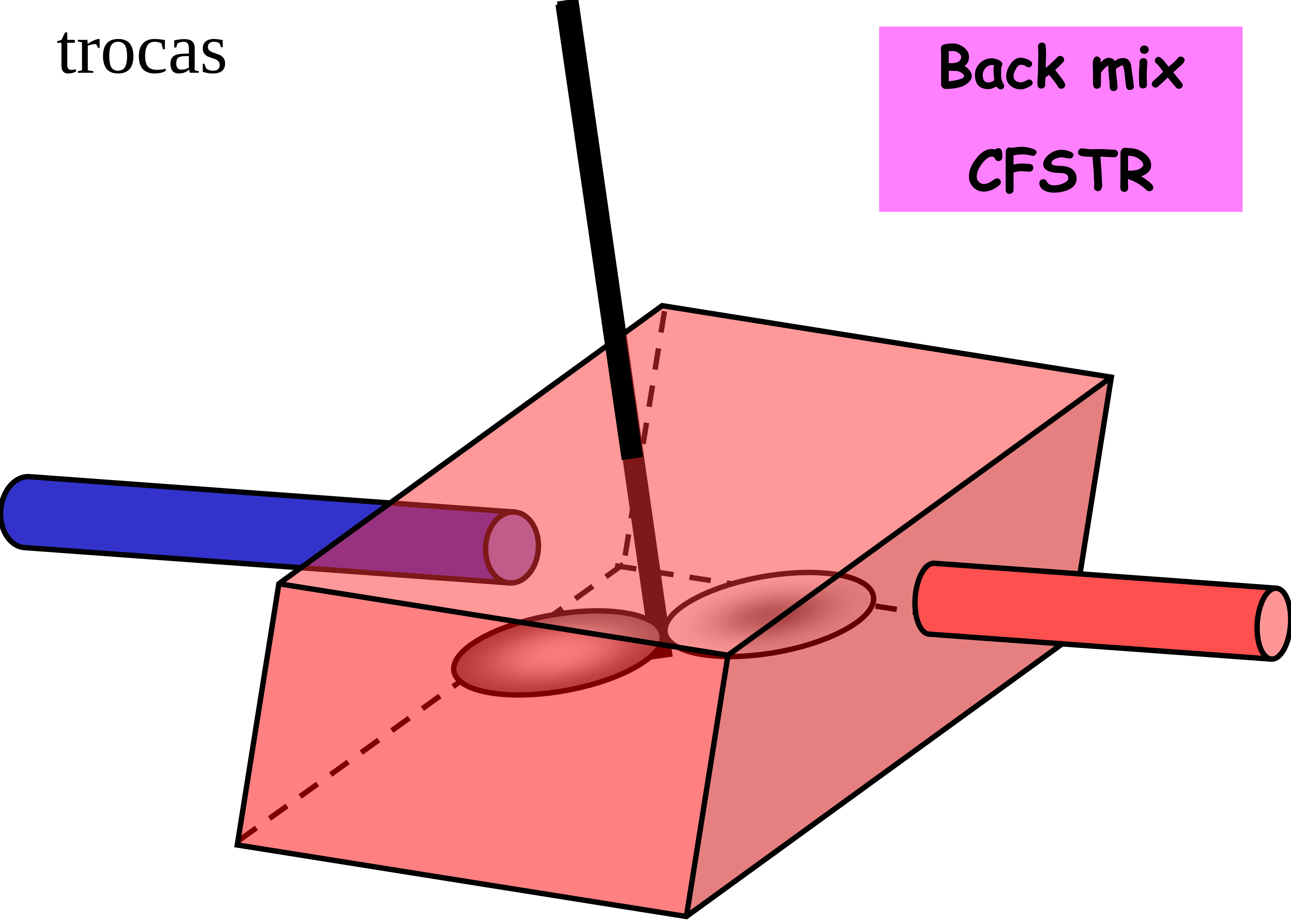
Quando o número de elementos de volume tende a infinito, a equação de conservação tende a forma diferencial. É, no entanto, atualmente inviável a resolução computacional de um domínio infinitesimalmente discretizado.

batelada

cada célula
é um batch



trocas



des-divergir

$$\frac{\partial \rho \varphi}{\partial t} + \mathrm{div}\, \rho\, \vec{v}\, \varphi = -\,\mathrm{div}\ \dot{\vec{j}}_{\Phi} + \dot{\sigma}_{\forall_{\Phi}}$$

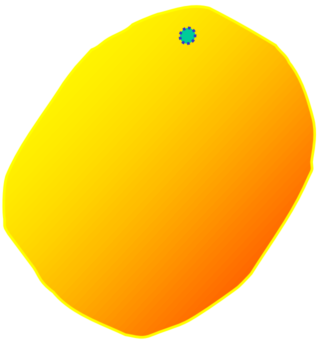
$$\dot{\vec{j}}_{\varphi} = -\rho \lambda_{\Phi}\, \mathrm{gr\vec{a}d}\, \varphi$$

$$\dot{\sigma}_{V\Phi} = c_{*} \left(\varphi_{*} - \varphi \right)$$

$$\frac{\partial \rho \varphi}{\partial t} = -\,\mathrm{div}\, \rho \left(\vec{v}\, \varphi - \lambda_{\Phi}\, \mathrm{gr\vec{a}d}\, \varphi \right) + c_{*} \left(\varphi_{*} - \varphi \right)$$

$$d\forall$$

$$\int_{\forall} \frac{\partial \rho \varphi}{\partial t}\, dV = -\int_{\forall} \mathrm{div}\ \rho \left(\vec{v}\, \varphi - \lambda_{\Phi}\, \mathrm{gr\vec{a}d}\, \varphi \right) dV + \int_{\forall} c_{*} \left(\varphi_{*} - \varphi \right) dV$$

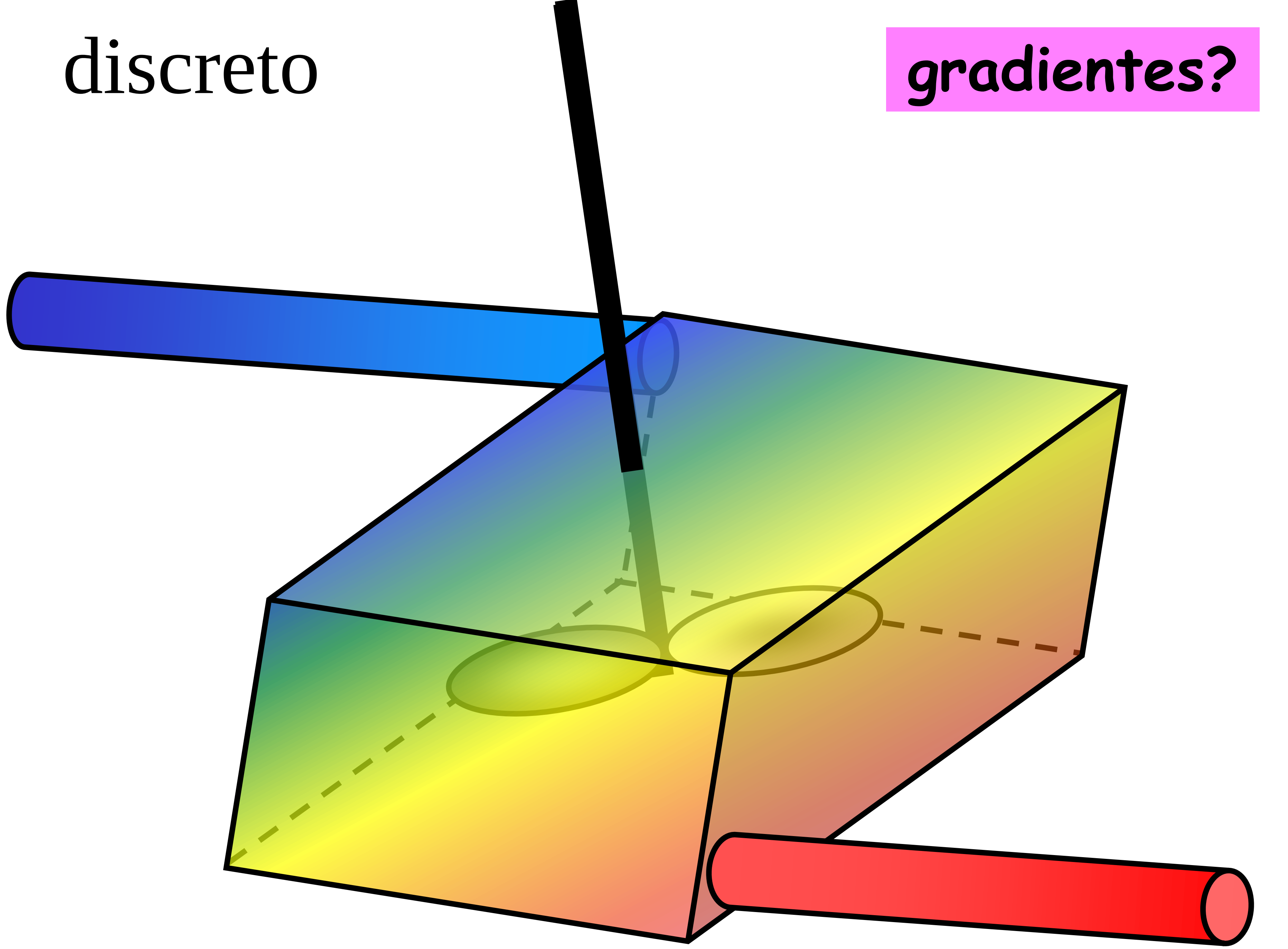


$$\int_{\forall} \frac{\partial \rho \varphi}{\partial t}\, dV = -\int_{\$} \rho \left(\vec{v}\, \varphi - \lambda_{\Phi}\, \mathrm{gr\vec{a}d}\, \varphi \right) . d\vec{S} + c_{*} \left(\varphi_{*} \int_{\forall} dV - \int_{\forall} \varphi\, dV \right)$$

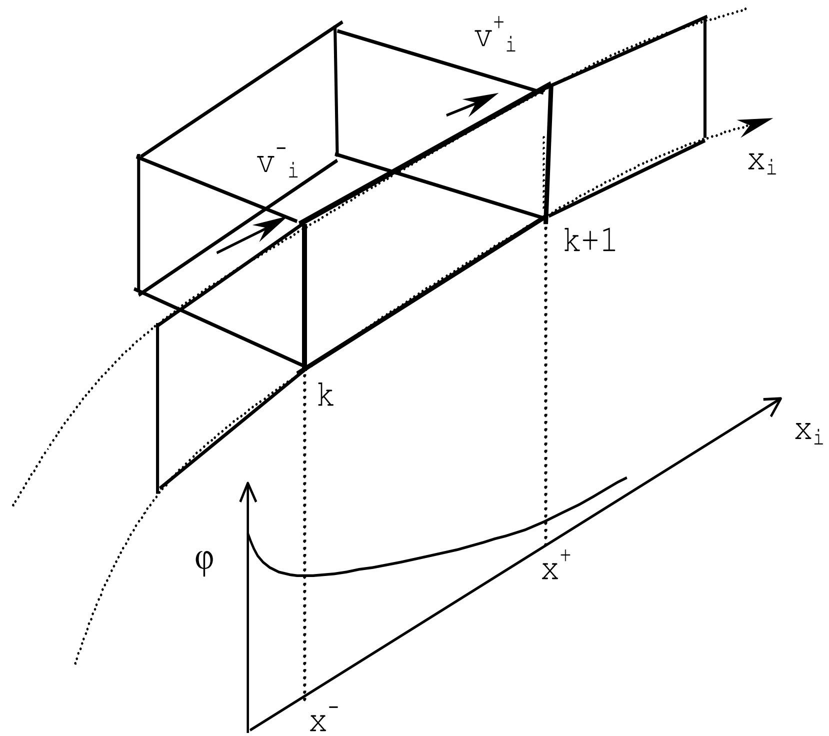
$$\vec{v}\, .\, d\vec{S} = \sum_{i=1}^{3} v_i\, dS_i \qquad \text{e} \qquad \mathrm{gr\vec{a}d}\, \varphi\, .\, d\vec{S} = \sum_{i=1}^{3} \frac{\partial \varphi}{\partial x_i}\, dS_i$$

$$\int_{\forall} \frac{\partial \rho \varphi}{\partial t}\, dV = -\int_{\$} \sum_{i=1}^{3} \rho \left(v_i\, \varphi - \lambda_{\Phi} \frac{\partial \varphi}{\partial x_i} \right) dS_i + c_{*} \left(\varphi_{*} \int_{\forall} dV - \int_{\forall} \varphi\, dV \right)$$

$$\Delta\forall$$


discreto
gradientes?

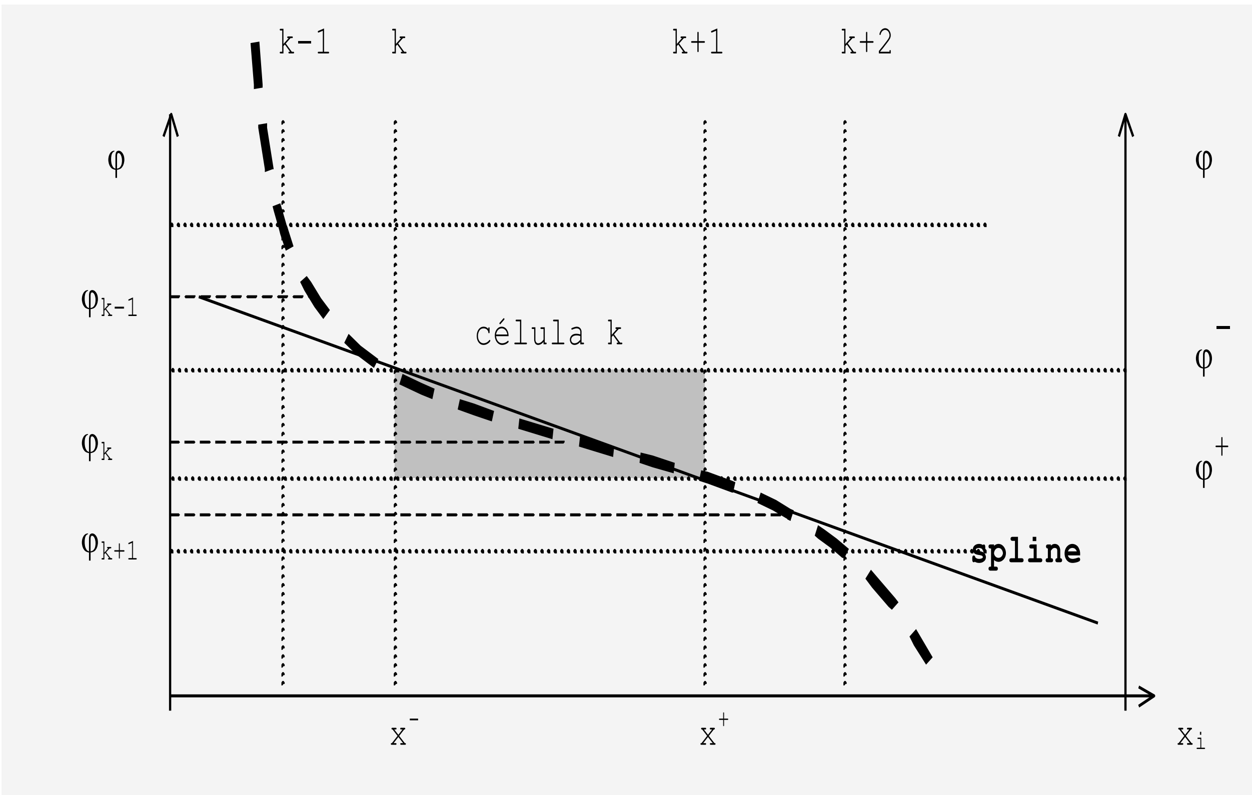
$$\int_{\forall} \frac{\partial \, \rho\varphi}{\partial t} \, dV = -\int_{\$} \sum_{i=1}^{3} \rho \left(v_i \, \varphi - \lambda_{\Phi} \frac{\partial \varphi}{\partial x_i} \right) dS_i + c_* \left(\varphi_* \int_{\forall} dV - \int_{\forall} \varphi \, dV \right)$$



$$\forall = \frac{\left(S_i^- + S_i^+ \right)}{2} \left(x_i^- - x_i^+ \right) = \prod_{i=1}^{3} \left(x_i^- - x_i^+ \right)$$

$$\frac{\partial \, \rho\varphi}{\partial t} \forall = \sum_{i=1}^{3} \left\{ \rho^- \left(v_i^- \varphi_i^- - \lambda_{\Phi}^- \left. \frac{\partial \varphi}{\partial x_i} \right|_- \right) \$_i^- + \rho^+ \left(-v_i^+ \varphi_i^+ + \lambda_{\Phi}^+ \left. \frac{\partial \varphi}{\partial x_i} \right|_+ \right) \$_i^+ \right\} + c_* \left(\varphi_* - \varphi \right) \forall$$

$$\frac{\partial \; \rho\varphi}{\partial t}\forall = \sum_{i=1}^{3}\left\{ \rho^{-}\left(v_i^{-}\varphi_i^{\;-} - \lambda_{\Phi}^{-} \left.\frac{\partial\varphi}{\partial x_i}\right|_{-} \right) \$_i^{-} + \rho^{+}\left(-v_i^{+}\varphi_i^{\;+} + \lambda_{\Phi}^{+} \left.\frac{\partial\varphi}{\partial x_i}\right|_{+} \right) \$_i^{+} \right\} + c_{*}\left(\varphi_{*} - \varphi\right)\forall$$



$$v_i^{-} = v_k$$

$$v_i^{+} = v_{k+1}$$

$$\varphi \cong \varphi_k$$

$$\lambda_i^{-} = \frac{\lambda_k + \lambda_{k-1}}{2}$$

$$\lambda_i^{+} = \frac{\lambda_{k+1} + \lambda_{k+2}}{2}$$

$$\frac{\partial \; \rho \; \varphi}{\partial t}\forall = \sum_{i=1}^{6} \pm\, \rho^{\pm}\left(v_i^{\pm}\varphi^{\pm} - \lambda_{\Phi}^{\pm} \left.\frac{\partial\varphi}{\partial x_i}\right|_{\pm} \right) \$_i^{\pm} + c_{*}\left(\varphi_{*} - \varphi\right)\forall$$

$$\frac{\partial \rho \varphi}{\partial t} \forall = \sum_{i=1}^{6} \pm \left(\rho^{\pm} v_i^{\pm} \varphi^{\pm} - \rho^{\pm} \lambda_{\Phi}^{\pm} \left. \frac{\partial \varphi}{\partial x_i} \right|_{\pm} \right) S_i^{\pm} + c_* \left(\varphi_* - \varphi \right) \forall$$

$$\Gamma_{\Phi}^{\pm} = \rho^{\pm} \lambda_{\Phi}^{\pm}$$

$$\frac{\partial \rho \varphi}{\partial t} \cong \frac{\Delta \rho \varphi}{\Delta t} = \frac{\rho \varphi - (\rho \varphi)_o}{\Delta t}$$

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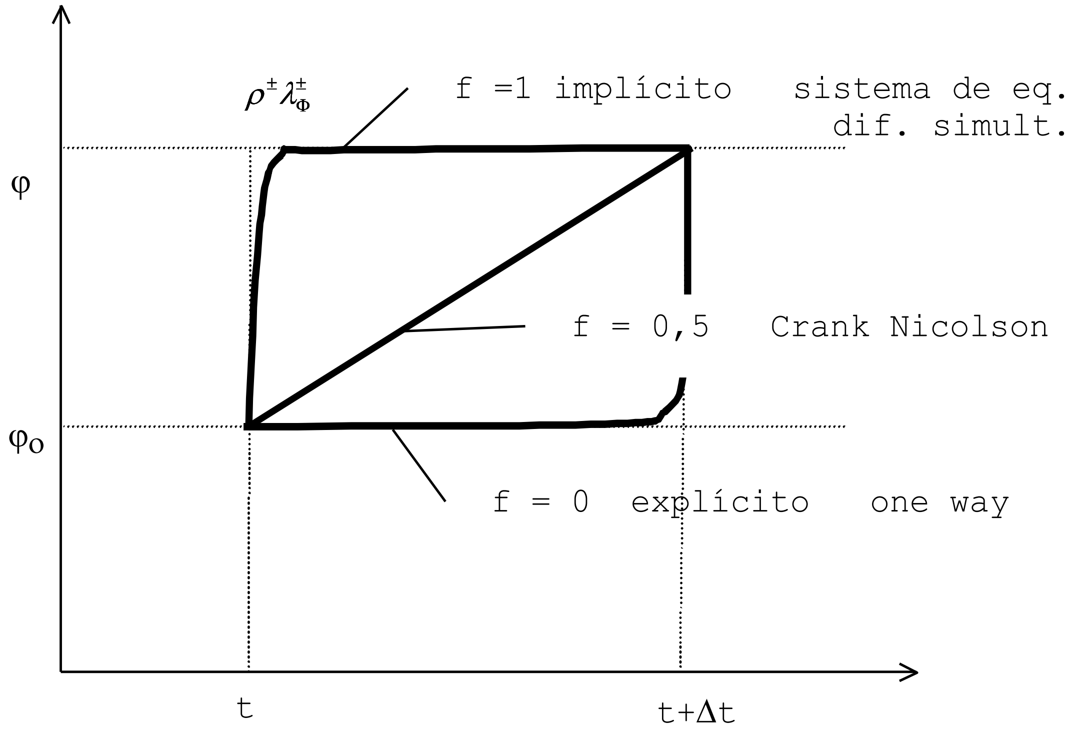
f = 0 -> método **explicito**

$$\bar{\varphi} = \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \varphi \, dt \cong$$

$$\cong f \varphi + (1 - f) \varphi_o$$

$$\Delta t < \frac{(\Delta x)^2}{2 \lambda_{\Phi}}$$



$$\frac{\partial \ \rho\varphi}{\partial t} \forall = \sum_{i=1}^{3} \left\{ \rho^{-} \left(v_i^{-} \varphi_i^{\ -} - \lambda_{\Phi}^{-} \left. \frac{\partial \varphi}{\partial x_i} \right|_{-} \right) \$_i^{-} + \rho^{+} \left(-v_i^{+} \varphi_i^{\ +} + \lambda_{\Phi}^{+} \left. \frac{\partial \varphi}{\partial x_i} \right|_{+} \right) \$_i^{+} \right\} + c_{\star} \left(\varphi_{\star} - \varphi \right) \forall$$

difusão

$$\lambda_i^{-} = \frac{\lambda_k + \lambda_{k-1}}{2}$$

$$\lambda_i^{+} = \frac{\lambda_{k+1} + \lambda_{k+2}}{2}$$

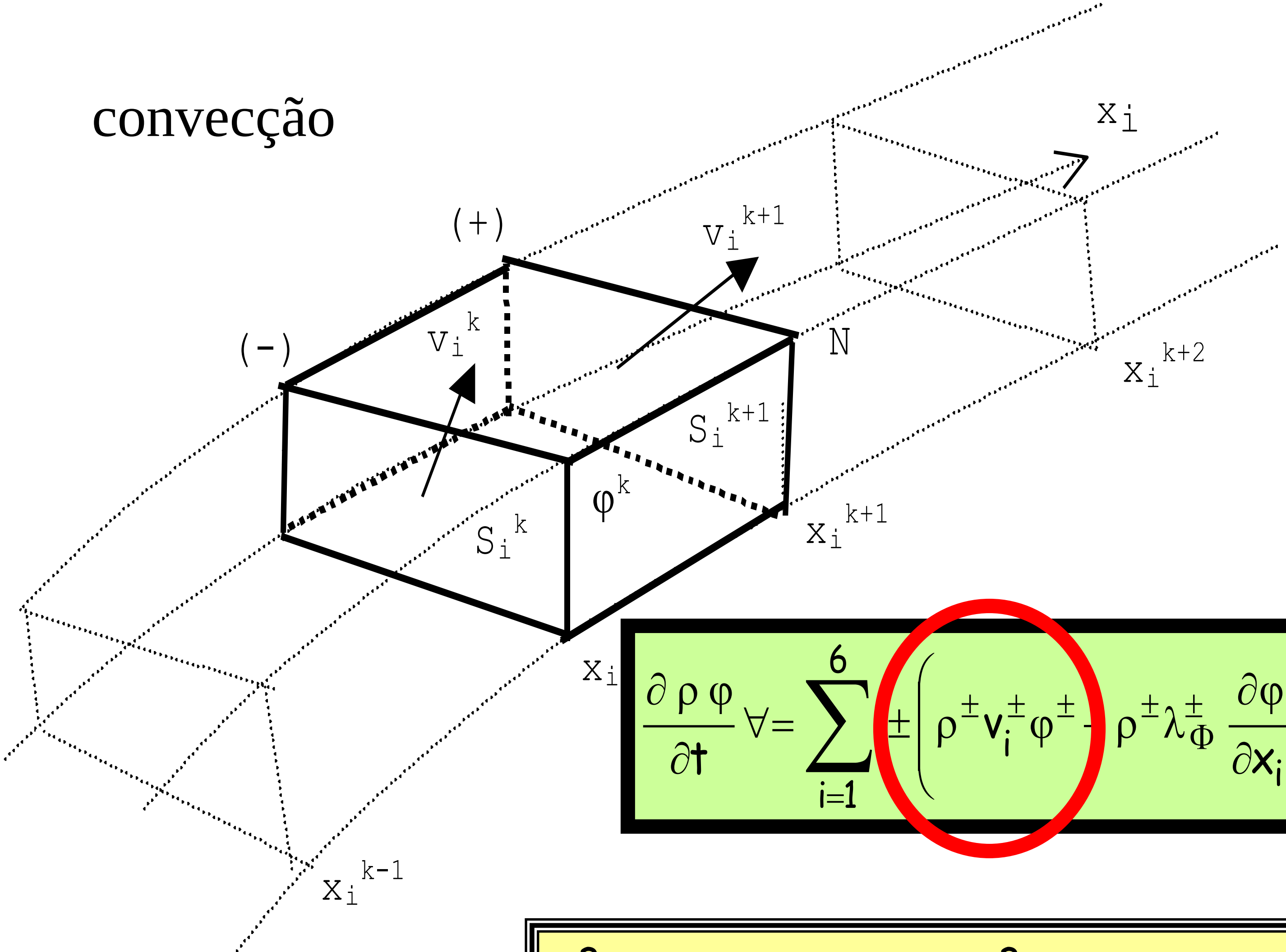
$$\frac{\partial \ \rho \ \varphi}{\partial t} \forall = \sum_{i=1}^{6} \pm \rho^{\pm} \left(v_i^{\pm} \varphi^{\pm} - \lambda_{\Phi}^{\pm} \left. \frac{\partial \varphi}{\partial x_i} \right|_{\pm} \right) \$_i^{\pm} + c_{\star} \left(\varphi_{\star} - \varphi \right) \forall$$

tempo

$$\frac{\partial \rho \varphi}{\partial t} \forall = \sum_{i=1}^{6} \pm \left(\rho^{\pm} v_i^{\pm} \varphi^{\pm} - \rho^{\pm} \lambda_{\Phi}^{\pm} \left. \frac{\partial \varphi}{\partial x_i} \right|_{\pm} \right) S_i^{\pm} + c_{*} \left(\varphi_{*} - \varphi \right) \forall$$

$$\frac{\partial \rho\varphi}{\partial t} \cong \frac{\Delta \rho \varphi}{\Delta t} = \frac{\rho\varphi - \left(\rho\varphi\right)_0}{\Delta t}$$

convecção

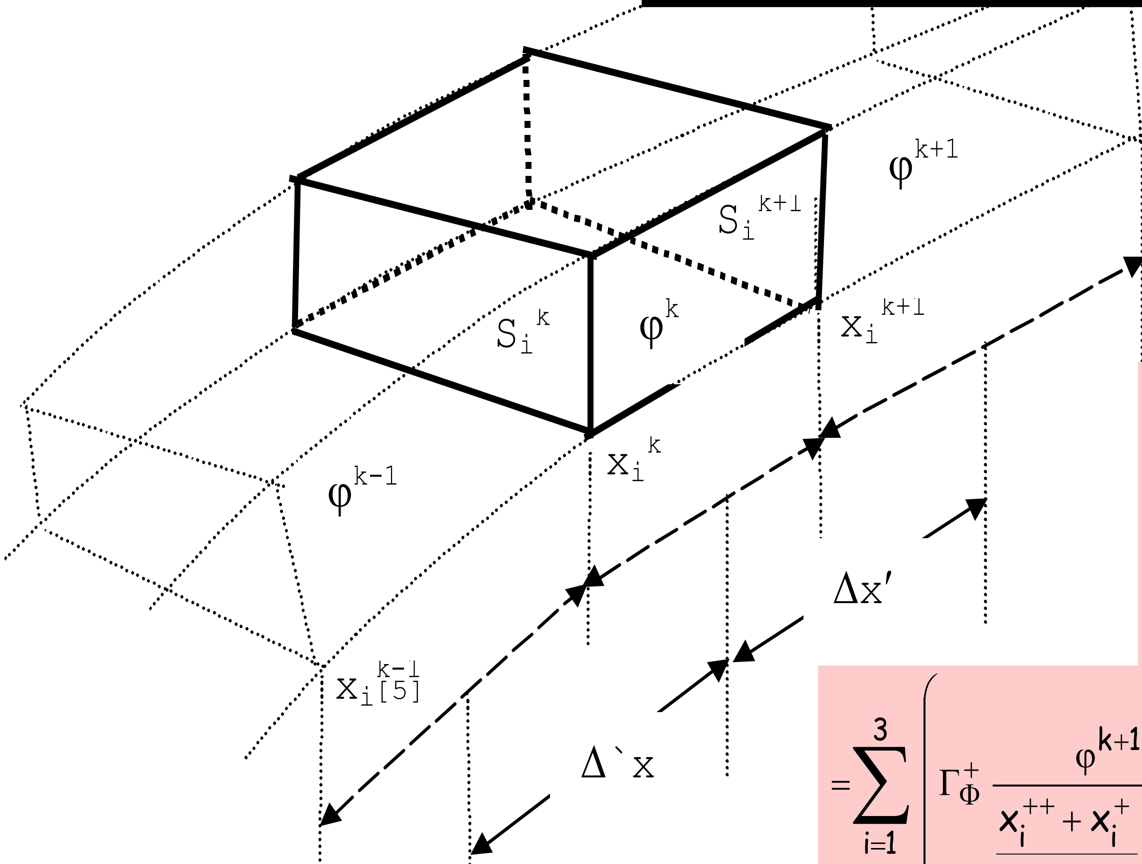


$$\frac{\partial \rho \varphi}{\partial t}\forall = \sum_{i=1}^{6} \pm\left(\rho^{\pm} v_i^{\pm} \varphi^{\pm} - \rho^{\pm} \lambda_{\Phi}^{\pm} \left.\frac{\partial\varphi}{\partial x_i}\right|_{\pm}\right) S_i^{\pm} + c_*\left(\varphi_* - \varphi\right)\forall$$

$$\sum_{i=1}^{3} \pm\rho^{\pm} v_i^{\pm} \varphi^{\pm} S_i^{\pm} \cong \sum_{i=1}^{3}\left(\rho^{-} \varphi^{-} v_i^{-} S_i^{-} - \rho^{+}\varphi^{+} v_i^{+} S_i^{+}\right)$$

difusão

$$\frac{\partial \rho\,\varphi}{\partial t}\forall = \sum_{i=1}^{6} \pm\left(\rho^{\pm} v_i^{\pm} \varphi^{\pm} - \rho^{\pm}\lambda_{\Phi}^{\pm} \left.\frac{\partial\varphi}{\partial x_i}\right|_{\pm}\right) S_i^{\pm} + c_{\star}\left(\varphi_{\star} - \varphi\right)\forall$$



$$\sum_{i=1}^{6}\pm\Gamma_{\Phi}^{\pm} \left.\frac{\partial\varphi}{\partial x_i}\right|_{\pm} S_i^{\pm} =$$

$$=\sum_{i=1}^{3}\left(\Gamma_{\Phi}^{+}\frac{\varphi^{k+1}-\varphi^{k}}{\Delta x'}S_i^{+} - \Gamma_{\Phi}^{-}\frac{\varphi^{k}-\varphi^{k-1}}{\Delta' x}S_i^{-}\right)=$$

$$=\sum_{i=1}^{3}\left(\Gamma_{\Phi}^{+}\frac{\varphi^{k+1}-\varphi^{k}}{\frac{x_i^{++}+x_i^{+}}{2}-\frac{x_i^{+}+x_i^{-}}{2}}S_i^{+} - \Gamma_{\Phi}^{-}\frac{\varphi^{k}-\varphi^{k-1}}{\frac{x_i^{+}+x_i^{-}}{2}-\frac{x_i^{-}+x_i^{--}}{2}}S_i^{-}\right)=$$

$$\sum_{i=1}^{3} 2\left(\Gamma_{\Phi}^{+}\frac{\varphi^{k+1}-\varphi^{k}}{x_i^{++}-x_i^{-}}S_i^{+} - \Gamma_{\Phi}^{-}\frac{\varphi^{k}-\varphi^{k-1}}{x_i^{+}-x_i^{--}}S_i^{-}\right)$$

juntando

$$\frac{\partial \rho \varphi}{\partial t}\forall = \sum_{i=1}^{6} \pm\rho^{\pm}\left(v_i^{\pm}\varphi^{\pm} - \lambda_{\Phi}^{\pm} \left.\frac{\partial \varphi}{\partial x_i}\right|_{\pm} \right) S_i^{\pm} + c_*\left(\varphi_* - \varphi\right)\forall$$

$$\frac{\partial \rho\varphi}{\partial t} \cong \frac{\rho^k \varphi^k - \rho_o^k \varphi_o^k}{\Delta t}$$

$$c_*\left(\varphi_*^k - \varphi^k\right)\forall$$

$$\sum_{i=1}^{3} \pm\rho^{\pm} v_i^{\pm} \varphi^{\pm} S_i^{\pm} \cong \sum_{i=1}^{3} \left(\rho^{-}\varphi^{-} v_i^{-} S_i^{-} - \rho^{+}\varphi^{+} v_i^{+} S_i^{+} \right)$$

$$\sum_{i=1}^{3} 2\left(\Gamma_{\Phi}^{+} \frac{\varphi^{k+1} - \varphi^{k}}{x_i^{++} - x_i^{-}} S_i^{+} - \Gamma_{\Phi}^{-} \frac{\varphi^{k} - \varphi^{k-1}}{x_i^{+} - x_i^{--}} S_i^{-} \right)$$

$$\frac{\rho^k \varphi^k - \rho_0^k \varphi_0^k}{\Delta t} - c_*\left(\varphi_*^k - \varphi^k\right) = \frac{1}{\forall} \sum_{i=1}^{3} \left(\rho^{-}\varphi^{-} v_i^{-} S_i^{-} - 2\Gamma_{\Phi}^{-} \frac{\varphi^{k} - \varphi^{k-1}}{x_i^{+} - x_i^{-}} S_i^{-} - \rho^{+}\varphi^{+} v_i^{+} S_i^{+} + 2\Gamma_{\Phi}^{+} \frac{\varphi^{k+1} - \varphi^{k}}{x_i^{++} - x_i^{-}} S_i^{+} \right)$$

$$\frac{\rho^k\varphi^k-\rho_0^k\varphi_0^k}{\Delta t}-c_*\left(\varphi_*^k-\varphi^k\right)=\frac{1}{\forall}\sum_{i=1}^{3}\left(\rho^-\varphi^-v_i^-S_i^- -2\Gamma_\Phi^-\frac{\varphi^k-\varphi^{k-1}}{x_i^+-x_i^{--}}S_i^- -\rho^+\varphi^+v_i^+S_i^+ +2\Gamma_\Phi^+\frac{\varphi^{k+1}-\varphi^k}{x_i^{++}-x_i^-}S_i^+\right)$$

$$\varphi^-=\frac{\varphi^k+\varphi^{k-1}}{2}\quad ; \quad \varphi^+=\frac{\varphi^{k+1}+\varphi^k}{2}$$

$$\frac{\rho^k\varphi^k-\rho_0^k\varphi_0^k}{\Delta t}-c_*\left(\varphi_*^k-\varphi^k\right)=\frac{1}{\forall}\sum_{i=1}^{3}\left(\frac{\varphi^k+\varphi^{k-1}}{2}\rho^-v_i^-S_i^- -2\Gamma_\Phi^-\frac{\varphi^k-\varphi^{k-1}}{x_i^+-x_i^{--}}S_i^- -\frac{\varphi^{k+1}+\varphi^k}{2}\rho^+v_i^+S_i^+ +2\Gamma_\Phi^+\frac{\varphi^{k+1}-\varphi^k}{x_i^{++}-x_i^-}S_i^+\right)$$

$$\varphi^k\left[\underbrace{c_*+\frac{\rho^k}{\Delta t}+\sum_{i=1}^{3}\left(\frac{2\Gamma_\Phi^+}{\forall}\frac{S_i^+}{x_i^{++}-x_i^-}+\frac{\rho^+v_i^+S_i^+}{2\forall}+\frac{2\Gamma_\Phi^-}{\forall}\frac{S_i^-}{x_i^+-x_i^{--}}-\frac{\rho^-v_i^-S_i^-}{2\forall}\right)}_{a_k}\right]=$$

$$=\underbrace{c_*}_{a_*}\varphi_*^k+\underbrace{\frac{\rho_0^k}{\Delta t}}_{a_0}\varphi_0^k+\sum_{i=1}^{3}\left[\varphi^{k+1}\underbrace{\left(\frac{2\Gamma_\Phi^+}{\forall}\frac{S_i^+}{x_i^{++}-x_i^-}-\frac{\rho^+v_i^+S_i^+}{2\forall}\right)}_{a_i^+}+\varphi^{k-1}\underbrace{\left(\frac{2\Gamma_\Phi^-}{\forall}\frac{S_i^-}{x_i^+-x_i^{--}}+\frac{\rho^-v_i^-S_i^-}{2\forall}\right)}_{a_i^-}\right]$$

$$\varphi^k = \frac{a_* \varphi_*^k + a_0 \varphi_0^k + \sum_{i=1}^{3} \left(a_i^+ \varphi^{k+1} + a_i^- \varphi^{k-1} \right)}{a_* + a_0 + \sum_{i=1}^{3} \left(a_i^+ + a_i^- \right)} = \frac{\sum_{j=1}^{8} a_j \varphi_j}{\sum_{j=1}^{8} a_j}$$

$$\varphi = \frac{a_o \varphi_o + a_N \varphi_N + a_S \varphi_S + a_E \varphi_E + a_W \varphi_W + a_H \varphi_H + a_L \varphi_L + a_* \varphi_*}{a_o + a_N + a_S + a_E + a_W + a_H + a_L + a_*}$$

para a discretização não há mais diferença entre entradas e produções

Batch

Condições de Contorno ou Fontes

$$0 = \sum_{i=1}^{9} S_\phi = \sum_{i=1}^{9} CO\left(VAL - \varphi\right)$$

fixed value

$CO_{BC} = 10^{20}$

$$0 = \sum_{i=1}^{9} 10^{20}\left(VAL_{BC} - \varphi\right)$$

$$\varphi = VAL_{BC}$$

fixed flux

$CO_{BC} = 10^{-20}$;

$VAL_{BC} = 10^{20}.flux$

$$S_{\phi*} = 10^{-20}\left(10^{20}.flux - \varphi\right)$$

$$S_{\phi*} = flux$$

φ = P1, U1, V1, W1, H1, KE, EP, A, ... (~10)

x, y, x = (100 . 100 . 100) t = (1000)

vetor PHI com ~ 10^7 elementos

$$\sum_{i=1}^{7} a_i \varphi_i = C_i$$

present west east low high south north sources

$$a_{111}\varphi_{111} + a_{011}\varphi_{011} + a_{211}\varphi_{211} + a_{101}\varphi_{101} + a_{121}\varphi_{121} + a_{110}\varphi_{110} + a_{112}\varphi_{112} = C_{\Phi 111}$$

$$a_{211}\varphi_{211} + a_{111}\varphi_{111} + a_{311}\varphi_{311} + a_{201o}\varphi_{201} + a_{221}\varphi_{221} + a_{210}\varphi_{210} + a_{212}\varphi_{212} = C_{\Phi 211}$$

...

$$a_{xyz}\varphi_{xyz} + a_{(x-1)yz}\varphi_{(x-1)yz} + a_{(x+1)yz}\varphi_{(x+1)yz} + \ldots + = C_{\Phi xyz}$$

• • •

$$z_{111}\psi_{111} + z_{011}\psi_{011} + z_{211}\psi_{211} + z_{101}\psi_{101} + z_{121}\psi_{121} + z_{110}\psi_{110} + z_{112}\psi_{112} = C_{\Psi 111}$$

$$z_{211}\psi_{211} + z_{111}\psi_{111} + z_{311}\psi_{311} + z_{201o}\psi_{201} + z_{221}\psi_{221} + z_{210}\psi_{210} + z_{212}\psi_{212} = C_{\Psi 211}$$

...

$$z_{xyz}\psi_{xyz} + z_{(x-1)yz}\psi_{(x-1)yz} + z_{(x+1)yz}\psi_{(x+1)yz} + \ldots + = C_{\Psi xyz}$$

BC

termos

matrizes

$$a_{ij}\,\varphi_i = C_j$$

Considerando os termos de entrada e saída como fontes eles vão para o vetor C. Resolvendo por slabs bi dimensionais a matriz a se torna tri-diagonal.

$$\begin{bmatrix} a_1 & a_2 & a_3 & \dots & 0 & 0 \\ 0 & a_4 & a_5 & \dots & 0 & 0 \\ 0 & 0 & a_7 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & a_{3N-3} & 0 \\ 0 & 0 & 0 & \dots & a_{3N-1} & a_{3N} \end{bmatrix} \cdot \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \dots \\ \dots \\ \dots \\ \varphi_N \end{bmatrix} = \begin{bmatrix} C_1 \\ C_2 \\ \dots \\ \dots \\ \dots \\ C_N \end{bmatrix}$$

TRIDIAGONAL **PHI** **S+BC**

em vez de uma matriz $10^4 \times 10^4 = 10^8$ **"apenas"** 3×10^4 **são necessários, assim a solução é possível em PCs.**

Convergência

$$\Delta t < \frac{(\Delta x)^2}{2\,\lambda_\Phi}$$

implícito x explícito

$$\overline{\varphi} \cong f\varphi + (1-f)\varphi_o$$

relaxação on line

linear f

$$S_{\phi relax} = f\left(\varphi_{old} - \varphi_p\right)\frac{\rho V}{\Delta t}$$

"dt falso"

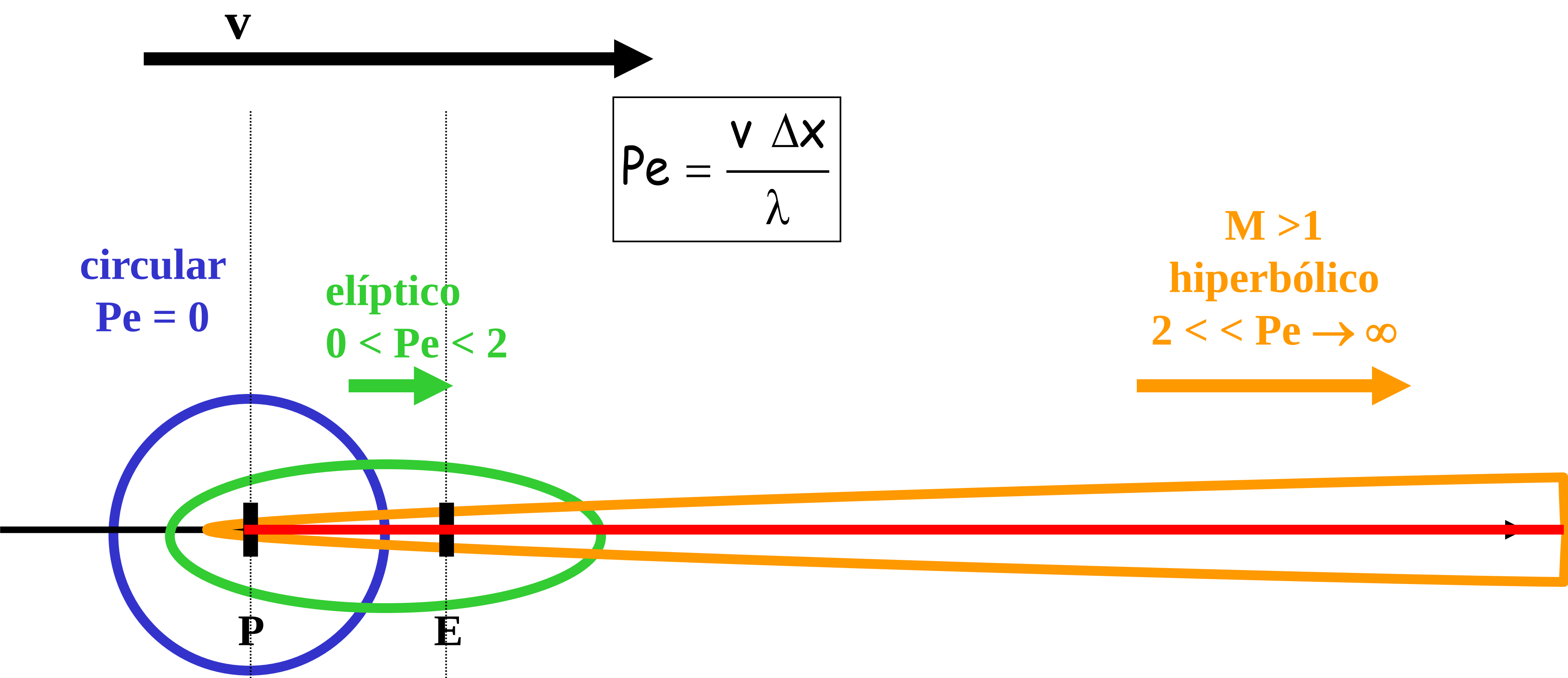
$$S_{\phi relax} = \frac{\rho V}{\left[dt_f\right]}\left(\varphi_{old} - \varphi_P\right)$$

up-wind

$$a_i^{\pm} = \frac{\overline{S_i}\;\;\overline{\lambda}}{\Delta x}\begin{cases} 1 \pm \dfrac{Pe}{2} & se\;\; Pe < 2 \\ Pe & se\;\; Pe < 2 \end{cases}$$

"Pe falso"

upwind



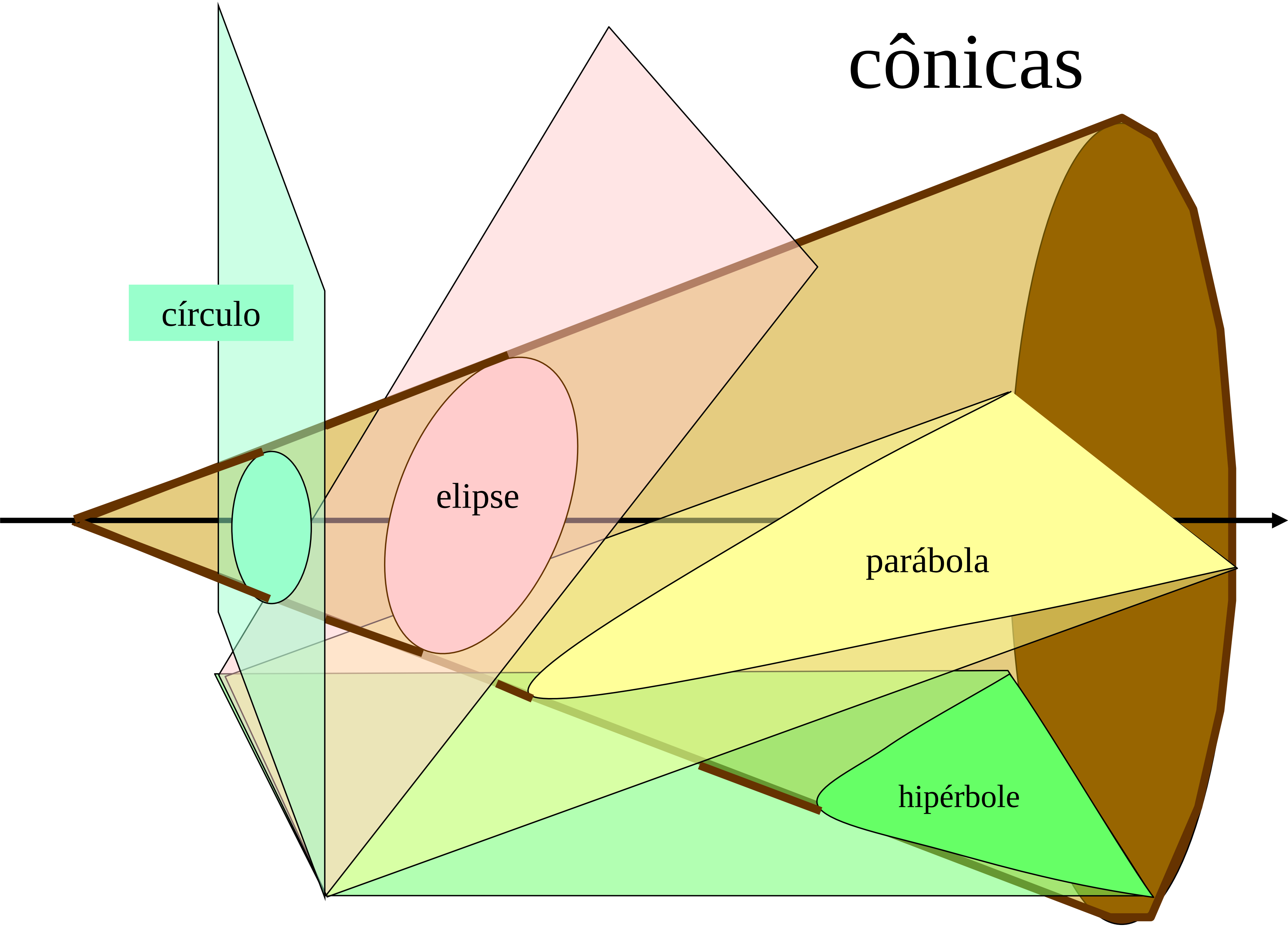
$$Pe = \frac{v\ \Delta x}{\lambda}$$

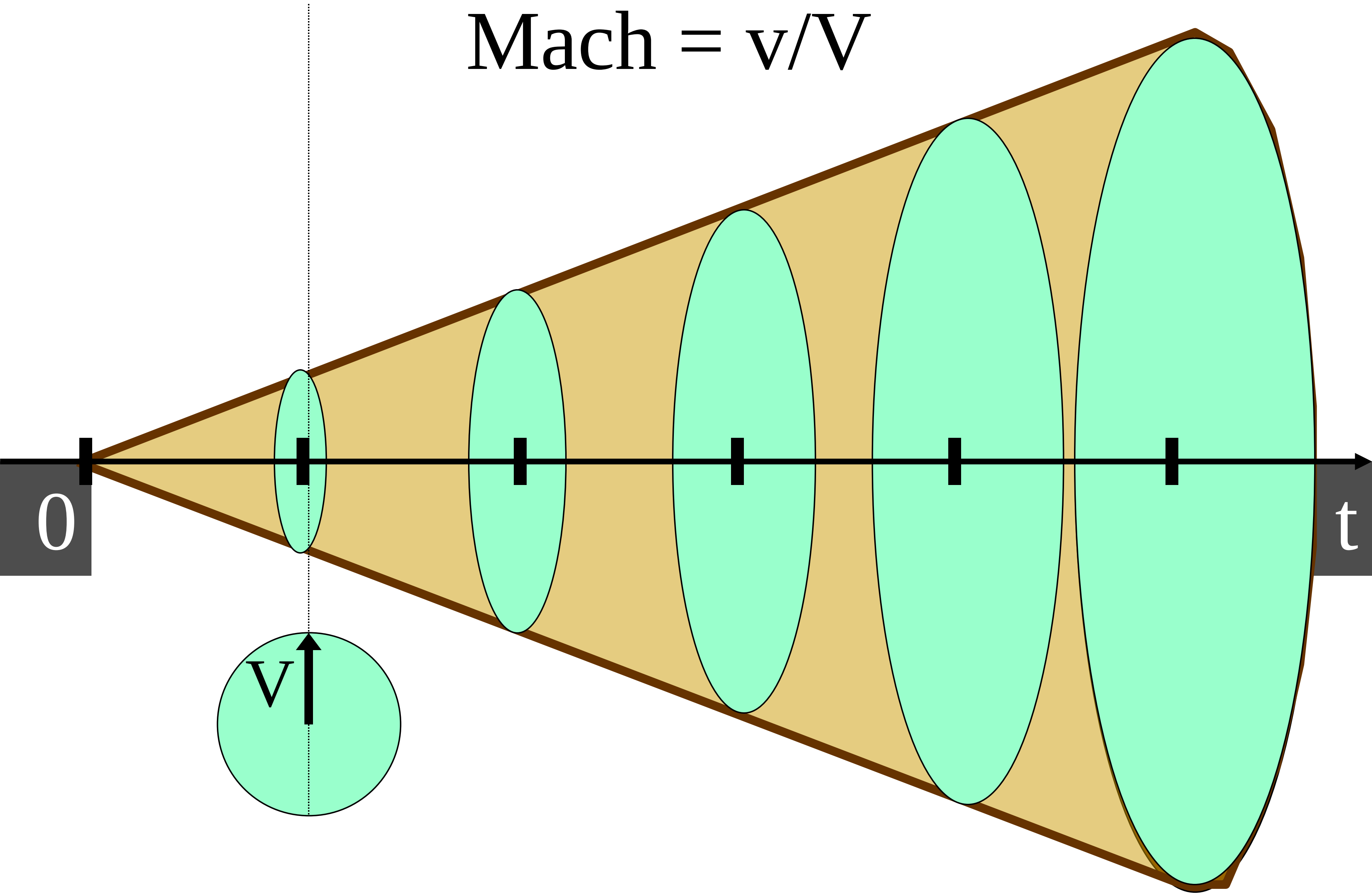
$$a_i^{\pm} = \frac{\bar{S}_i\ \bar{\lambda}}{\Delta x}\left[1 \pm \frac{Pe}{2}\right] \quad \rightarrow \quad a_i^{\pm} = \frac{\bar{S}_i\ \bar{\lambda}}{\Delta x}\ \max\left\{ \pm Pe\ ;\ 0\ ;\ \left[1 \pm \frac{Pe}{2}\right] \right\}$$

híbrido

ver pág 182 Versteeg

fig 5.9 pag 113

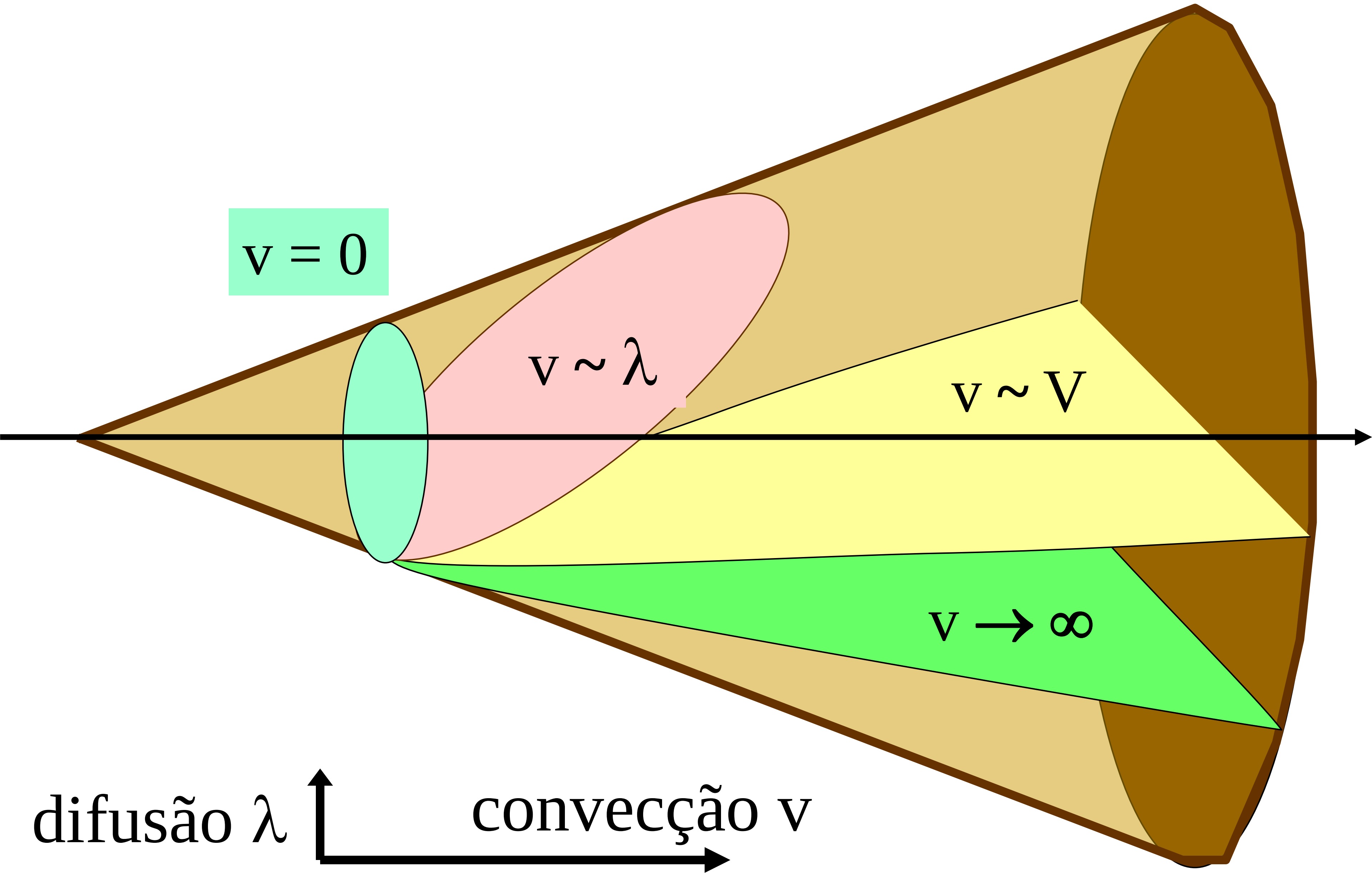

cônicas
círculo
elipse
parábola
hipérbole

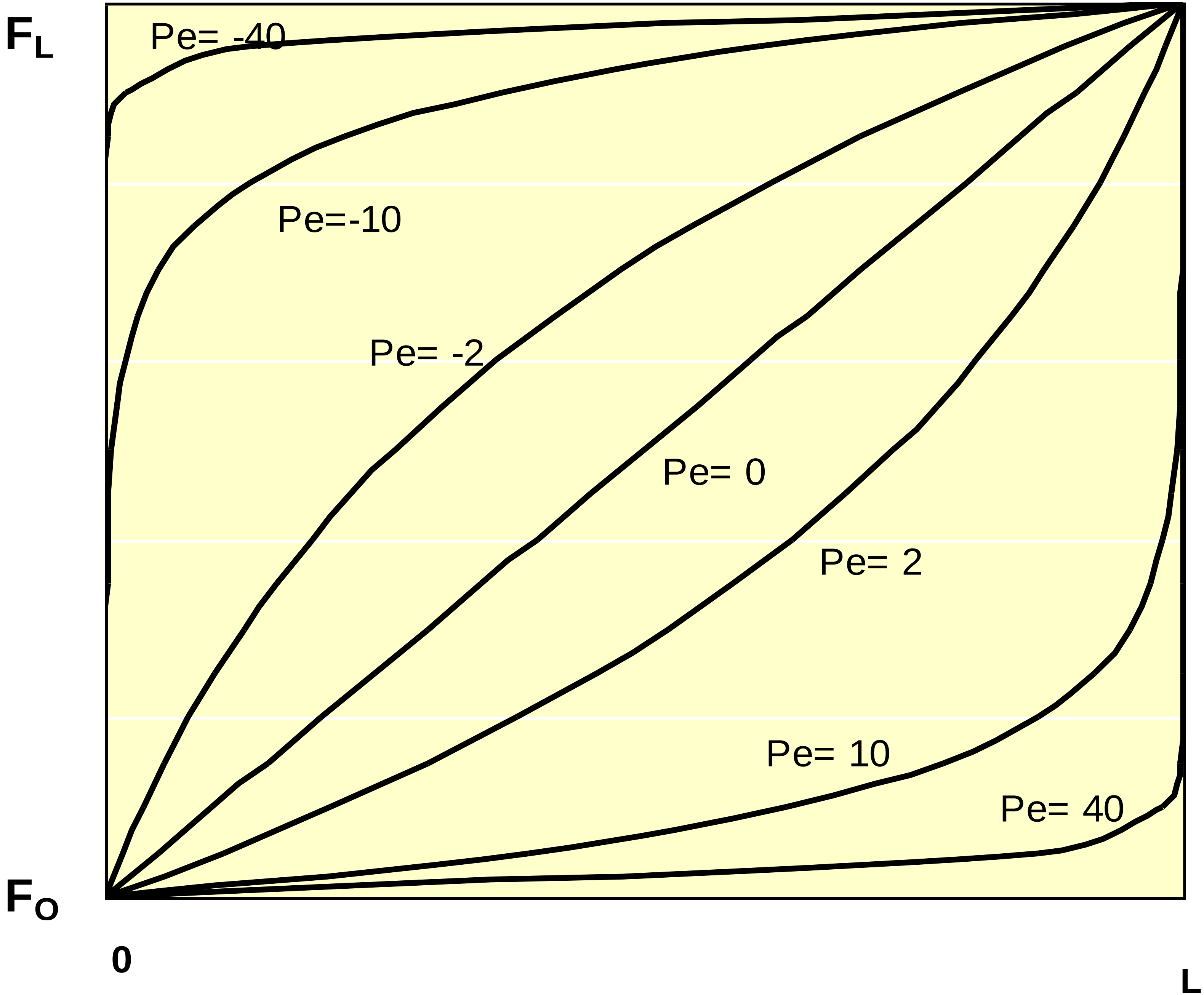


mach

caçada

upwind





F_L
Pe= -40
Pe=-10
Pe= -2
Pe= 0
Pe= 2
Pe= 10
Pe= 40
F_O
0
L

coordinate direction. The discretised equation that covers all cases is given by

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_S\phi_S + a_N\phi_N + a_B\phi_B + a_T\phi_T \tag{5.43}$$

with central coefficient

$$a_P = a_W + a_E + a_S + a_N + a_B + a_T + \Delta F$$

and the coefficients of this equation for the **hybrid differencing scheme** are as follows:

	One-dimensional flow	Two-dimensional flow	Three-dimensional flow
a_W	$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$	$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$	$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$
a_E	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$
a_S	–	$\max\left[F_s, \left(D_s + \frac{F_s}{2}\right), 0\right]$	$\max\left[F_s, \left(D_s + \frac{F_s}{2}\right), 0\right]$
a_N	–	$\max\left[-F_n, \left(D_n - \frac{F_n}{2}\right), 0\right]$	$\max\left[-F_n, \left(D_n - \frac{F_n}{2}\right), 0\right]$
a_B	–	–	$\max\left[F_b, \left(D_b + \frac{F_b}{2}\right), 0\right]$
a_T	–	–	$\max\left[-F_t, \left(D_t - \frac{F_t}{2}\right), 0\right]$
ΔF	$F_e - F_w$	$F_e - F_w + F_n - F_s$	$F_e - F_w + F_n - F_s + F_t - F_b$

In the above expressions the values of F and D are calculated with the following formulae:

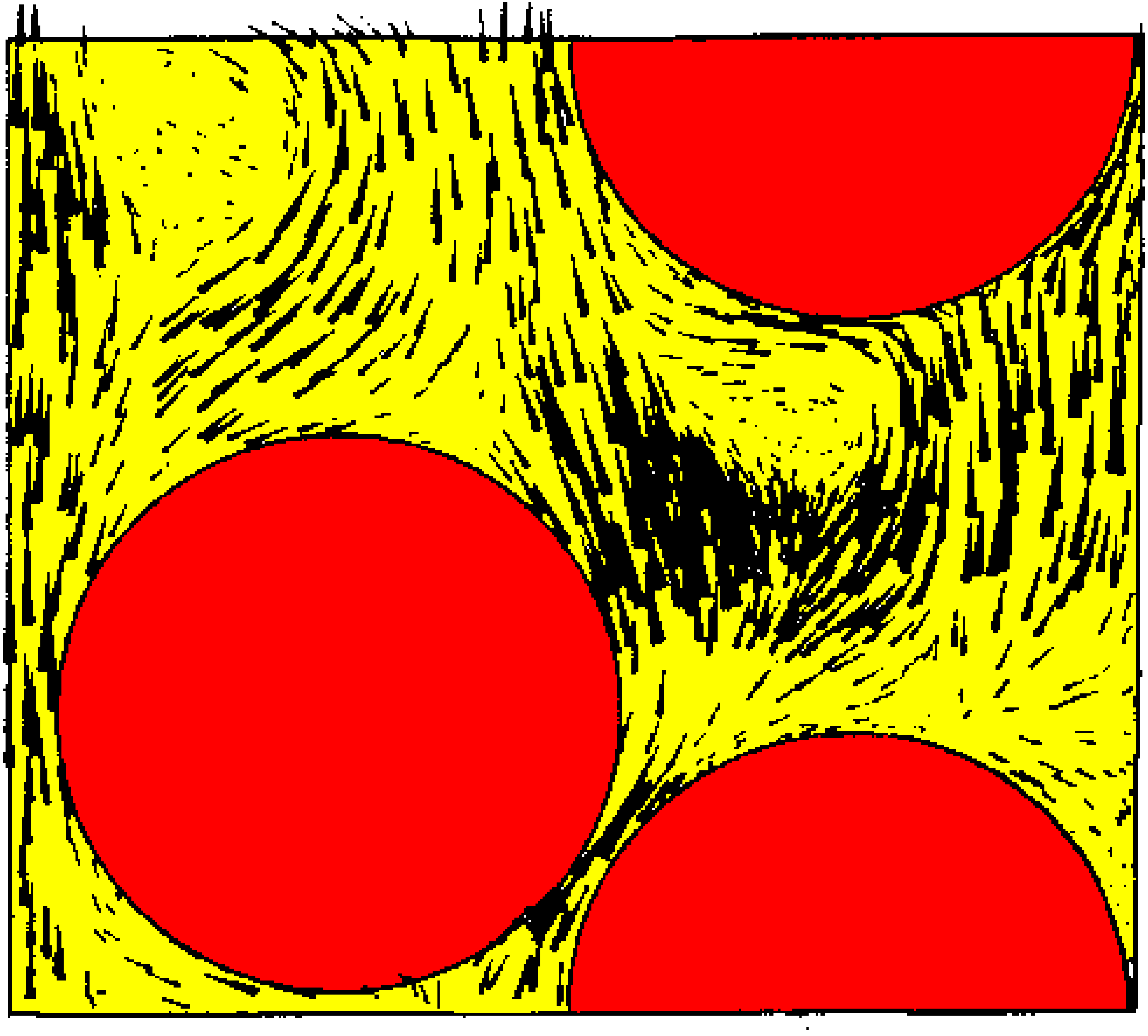
Face	w	e	s	n	b	t
F	$(\rho u)_w A_w$	$(\rho u)_e A_e$	$(\rho v)_s A_s$	$(\rho v)_n A_n$	$(\rho w)_b A_b$	$(\rho w)_t A_t$
D	$\frac{\Gamma_w}{\delta x_{WP}} A_w$	$\frac{\Gamma_e}{\delta x_{PE}} A_e$	$\frac{\Gamma_s}{\delta y_{SP}} A_s$	$\frac{\Gamma_n}{\delta y_{PN}} A_n$	$\frac{\Gamma_b}{\delta z_{PN}} A_b$	$\frac{\Gamma_t}{\delta z_{PT}} A_t$

Modifications to these coefficients to cater for boundary conditions in two and three dimensions are available in the form of expressions such as (5.40).

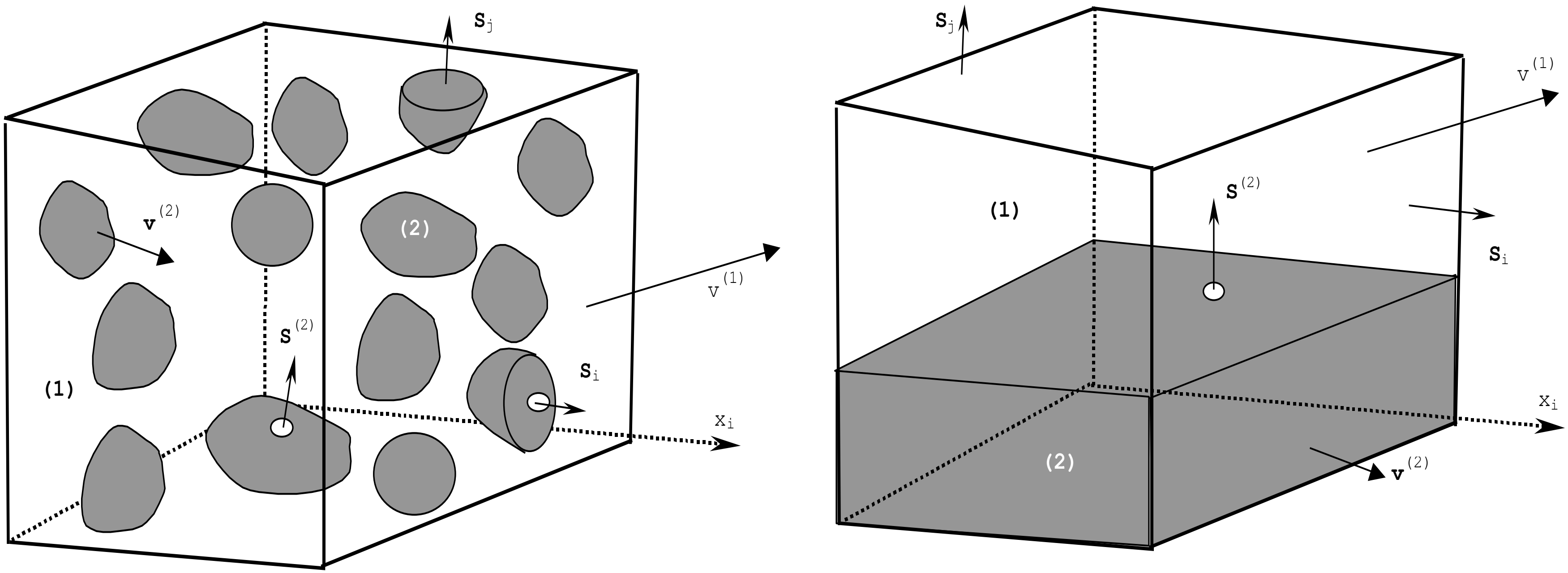
Bifásico

Bifásico

célula
mínima



bifásicos

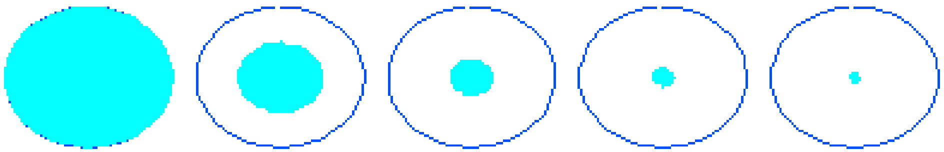


$$\frac{A^{(12)}_{efetiva}}{\forall} \cong N_p \quad \phi_p \quad \pi \quad \left\langle D_p \right\rangle^2$$

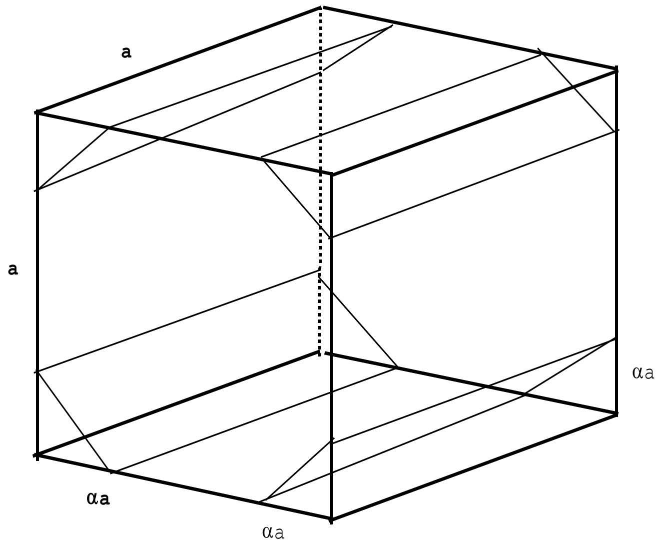
$$r = N_p \frac{4\pi}{3} \left\langle \frac{D_p}{2} \right\rangle^3 = N_p \frac{\pi}{6} \left\langle D_p \right\rangle^3$$

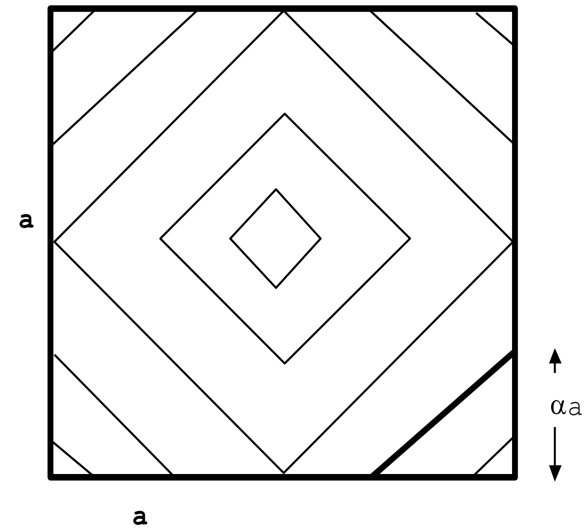
Particle Size Calculation

In many practical cases, the particle size will vary throughout the domain, as the result of combustion or evaporation/condensation.



- This can be dealt with by use of the SHADOW technique. This uses a third phase (the SHADOW phase), which behaves like the disperse phase (usually phase 2), but without interphase mass transfer.
- On the picture, the solid particles are phase 2, and the open ones the shadow phase.
- Then changes in particle size can be calculated from local volume fraction ratios:
- $D_p \ / \ D_{p,in} = (\ R2 \ / \ RS \ )^{1/3}$





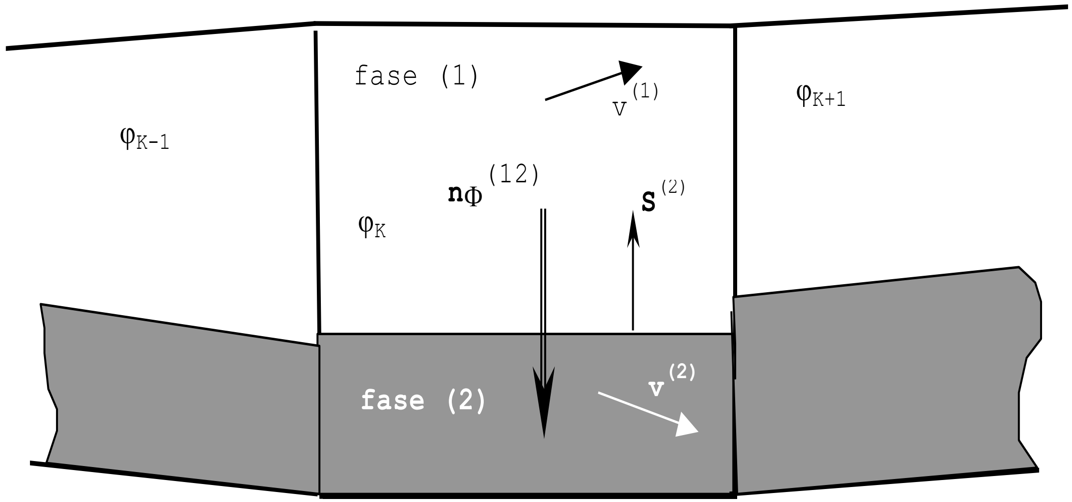
$$r = \frac{\forall^{(\alpha)}}{\forall} = \frac{4\,\frac{\alpha\, a\, \alpha\, a}{2}\, a}{a^3} \quad \rightarrow \quad \alpha = \sqrt{\frac{r}{2}}$$

$$A^{(12)} = 4\; a\; \left(2\,\alpha\, a\; \cos\, 45^o\right) = \quad 4\, a^2\, \sqrt{r} \quad \rightarrow \quad \frac{A^{(12)}}{\$} = \frac{4\, a^2\, \sqrt{r}}{6\, a^2} = \frac{2\sqrt{r}}{3}$$

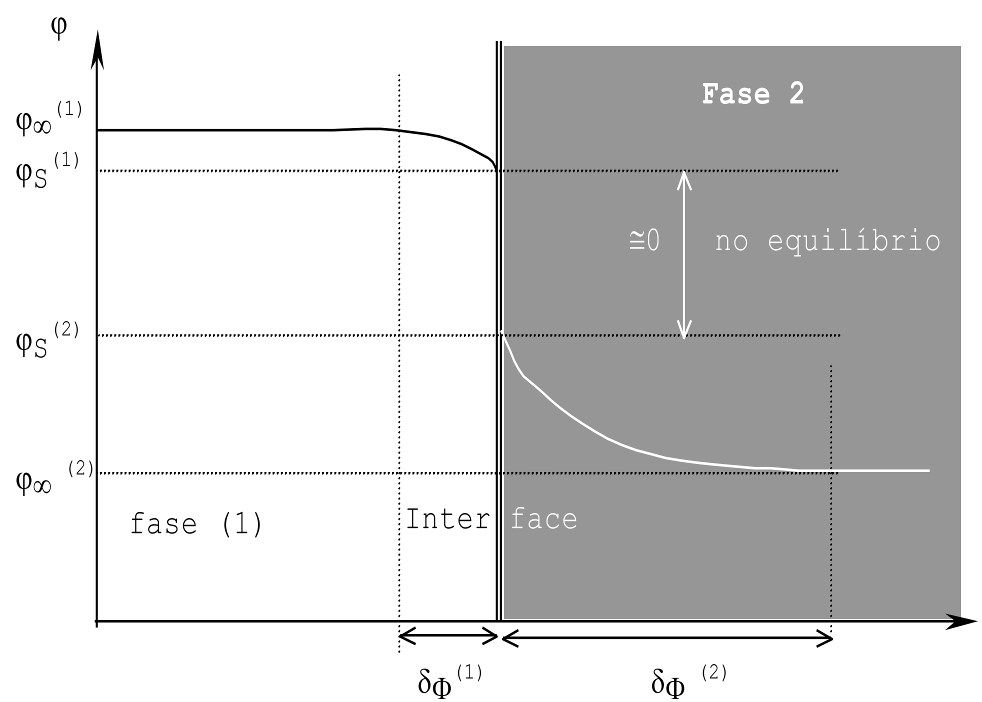
$$\frac{A^{(12)}}{\$} \cong \begin{cases} 2/3\,\sqrt{r} & p/ \quad 0 \leq r \leq 0{,}5 \\ 2/3\,\sqrt{(1-r)} & p/ \quad 0{,}5 \leq r \leq 1 \end{cases}$$

$$\frac{A^{(12)}}{\$} \cong 4\,(r - r^2)$$

$$a_p = \frac{A^{(12)}_{efetiva}}{A^{(12)}} \cong \frac{N_p\;\phi_p\;\pi\left\langle D_p\right\rangle^2}{\$\quad 4\left(r - r^2\right)} = \frac{N_p\;\phi_p\;\pi\left\langle D_p\right\rangle^2}{r\,\$\quad 4\left(1 - r\right)}$$



$$\left|\vec{n}_\Phi^{(12)}\right| \approx \lambda_\Phi^{(1)} \frac{\varphi^{(1)} - \varphi_S^{(1)}}{\delta_\Phi^{(1)}} \approx \lambda_\Phi^{(2)} \frac{\varphi^{(2)} - \varphi_S^{(2)}}{\delta_\Phi^{(2)}}$$



$$\left|\vec{n}_{\Phi}^{(12)}\right| = c_{\Phi}^{(12)}\left(\varphi_{\infty}^{(1)} - \varphi_{\infty}^{(2)}\right) \approx \lambda_{\Phi}^{(1)} \frac{\varphi_{\infty}^{(1)} - \varphi_{S}^{(1)}}{\delta_{\Phi}^{(1)}} \approx \lambda_{\Phi}^{(2)} \frac{\varphi_{S}^{(2)} - \varphi_{\infty}^{(2)}}{\delta_{\Phi}^{(2)}}$$

$$c_{\Phi}^{(12)} = \left[\frac{\delta_{\Phi}^{(1)}}{\lambda_{\Phi}^{(1)}} + \frac{\delta_{\Phi}^{(2)}}{\lambda_{\Phi}^{(2)}}\right]^{-1}$$

$$\left|\vec{n}_{\Phi}^{(12)}\right| A_{efetiva}^{(12)} = c_{\Phi}^{(12)}\left(\varphi^{(1)} - \varphi^{(2)}\right) a_{p} A^{(12)}$$

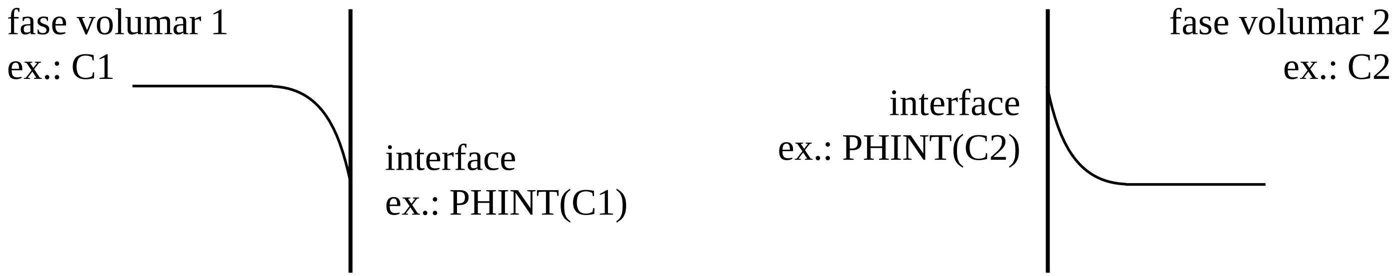
$$S_{\Phi}^{(\alpha)} = c_{\Phi}^{(12)}\left(\varphi^{(1)} - \varphi^{(2)}\right) a_{p} A^{(12)} = c_{\Phi}^{(\alpha)}\left(\varphi^{(1)} - \varphi^{(2)}\right) r\forall$$

$$c_{\Phi}^{(\alpha)} = \pm \frac{c_{\Phi}^{(12)} a_{p}}{r\forall} A^{(12)}$$

coeficiente

INTER-PHASE-SLIP ALGORITHM (IPSA) – III

A interface:



Os coeficientes de transferência da fase volumar para a interface são definidos por CINT(PHI) (ex.: CINT(C1)) - diferentes possibilidades de configuração.

Outros termos relevantes:

CMDOT, CFIPS

poderosa bifásica

termo transitório — **termo de convecção** — **termo de difusão** — **termo de fonte**

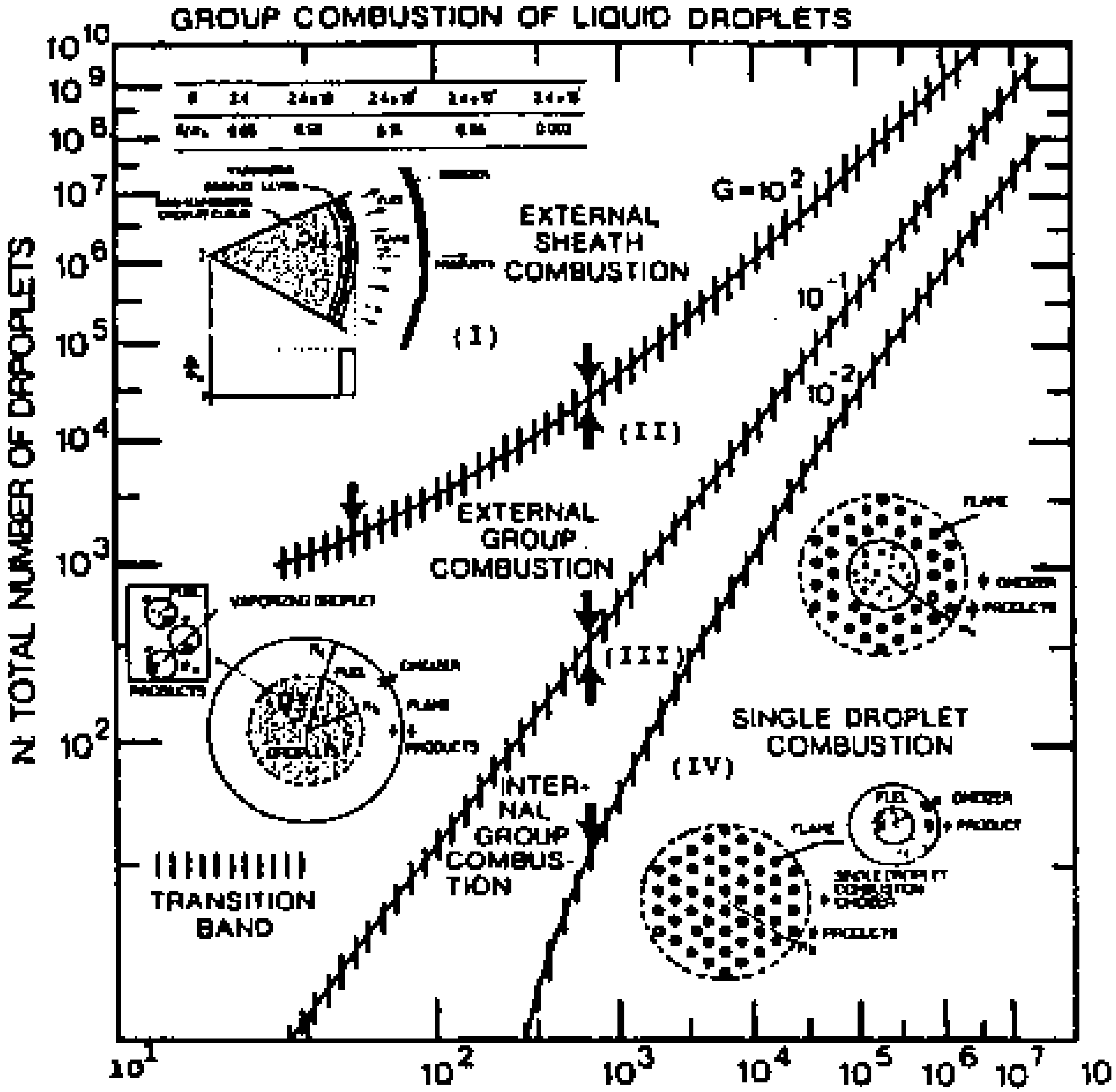
$$\frac{\partial (r_i \rho_i .\Phi)}{\partial t} + div(r_i .\rho_i .\vec{v}_i .\Phi - r_i .\Gamma .grad\,\Phi) = r_i .S_\Phi$$

$$\frac{\partial\ r\ \rho\varphi}{\partial t} = \sum_{i=1}^{6} \pm \frac{r^{\pm}\ \rho^{\pm}}{\forall} \left(v_i^{\pm} \varphi^{\pm} - \lambda_\Phi^{\pm} \left. \frac{\partial \varphi}{\partial x_i} \right|_{\pm} \right) \$_i^{\pm} + rc_{*} \left(\varphi_{*} - \varphi\right) + rc_\Phi^{(\alpha)} \left(\varphi^{(\alpha)} - \varphi\right)$$

$$\overline{\varphi} = \frac{a_O \overline{\varphi}_O + a_N \overline{\varphi}_N + a_S \overline{\varphi}_S + a_E \overline{\varphi}_E + a_W \overline{\varphi}_W + a_H \overline{\varphi}_H + a_L \overline{\varphi}_L + a_{*} \overline{\varphi}_{*} + a^{(\alpha)} \overline{\varphi}^{(\alpha)}}{a_O + a_N + a_S + a_E + a_W + a_H + a_L + a_{*} + a^{(\alpha)}}$$

spray combustion

four groups combustion modes of a droplet cloud



$$S = \frac{0{,}05}{\left(1 + 0{,}276\, Re^{0{,}5}\, Pr^{0{,}33}\right)} \left(\frac{d}{r_e}\right)$$

ábaco

CFD COMERCIAIS
chemtech

PHOENICS
Prof. Brian Spalding

FLUENT, ...

Introdução ao PHOENICS

slides da CHEMTECH

As equações diferenciais resolvidas em CFD, na sua forma mais geral, podem ser escritas do seguinte modo:

$$\frac{\partial}{\partial t}(\rho\phi)+\frac{\partial}{\partial x}(\rho u\phi)+\frac{\partial}{\partial y}(\rho v\phi)+\frac{\partial}{\partial z}(\rho w\phi)=\frac{\partial}{\partial x}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial z}\right)+S^{\phi}$$

Onde: **u**, **v** e **w** são as componentes da velocidade nas direções **x**, **y** e **z**. $\boldsymbol{\rho}$ é a densidade do fluido, $\boldsymbol{\Gamma^{\phi}}$ é o coeficiente de transferência, $\boldsymbol{\phi}$ é a variável do escoamento e $\mathbf{S^{\phi}}$ é o termo fonte.

Na realidade, os códigos de CFD nunca resolvem equações diferenciais. Só resolvem as algébricas que, quando o número de volumes é grande o suficiente, possuem as mesmas implicações que as diferenciais.

Equação de conservação	ϕ	Γ^{ϕ}	S^{ϕ}
Continuidade	1	0	0
Momento em x	u	μ	$B_x + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x} - \frac{2}{3}\mu \nabla \cdot \vec{V}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial z}\left(\mu \frac{\partial w}{\partial x}\right) - \frac{\partial P}{\partial x}$
Momento em y	v	μ	$B_y + \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial y} - \frac{2}{3}\mu \nabla \cdot \vec{V}\right) + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu \frac{\partial w}{\partial y}\right) - \frac{\partial P}{\partial y}$
Momento em z	w	μ	$B_z + \frac{\partial}{\partial z}\left(\mu \frac{\partial w}{\partial z} - \frac{2}{3}\mu \nabla \cdot \vec{V}\right) + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial z}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial z}\right) - \frac{\partial P}{\partial z}$
Energia	T	$\frac{k}{C_p}$	$\frac{1}{C_p}\frac{DP}{Dt} + \frac{\mu}{C_p}\Phi$
Massa de um componente i	C	ρD	0

$\frac{\partial}{\partial t}(\rho\phi)$	**TERMO TEMPORAL**
$\frac{\partial}{\partial x}(\rho u\phi)+\frac{\partial}{\partial y}(\rho v\phi)+\frac{\partial}{\partial z}(\rho w\phi)$	**TERMO CONVECTIVO**
$\frac{\partial}{\partial x}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial z}\right)$	**TERMO DIFUSIVO**
S^{ϕ}	**TERMO FONTE**

Laval

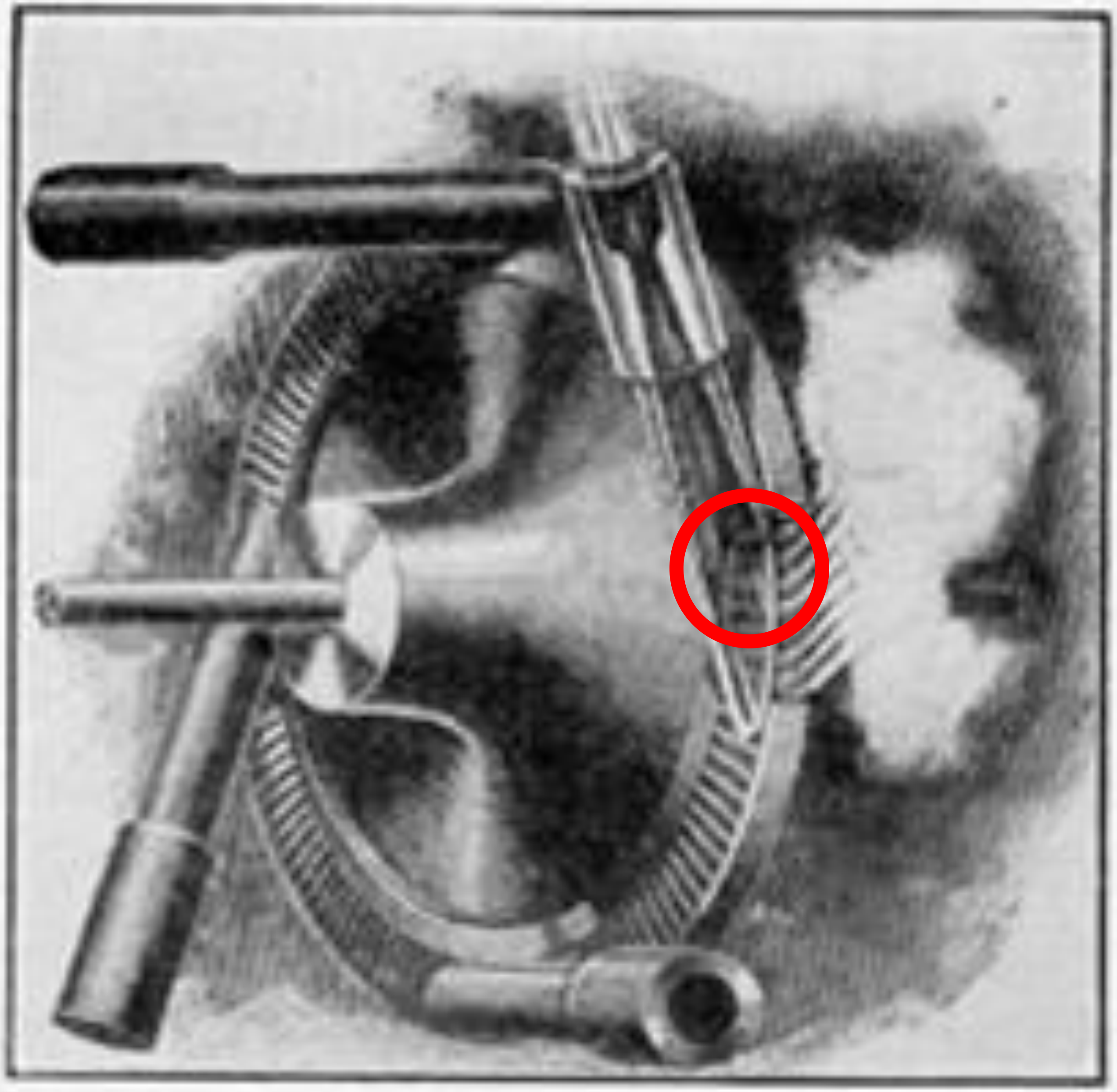
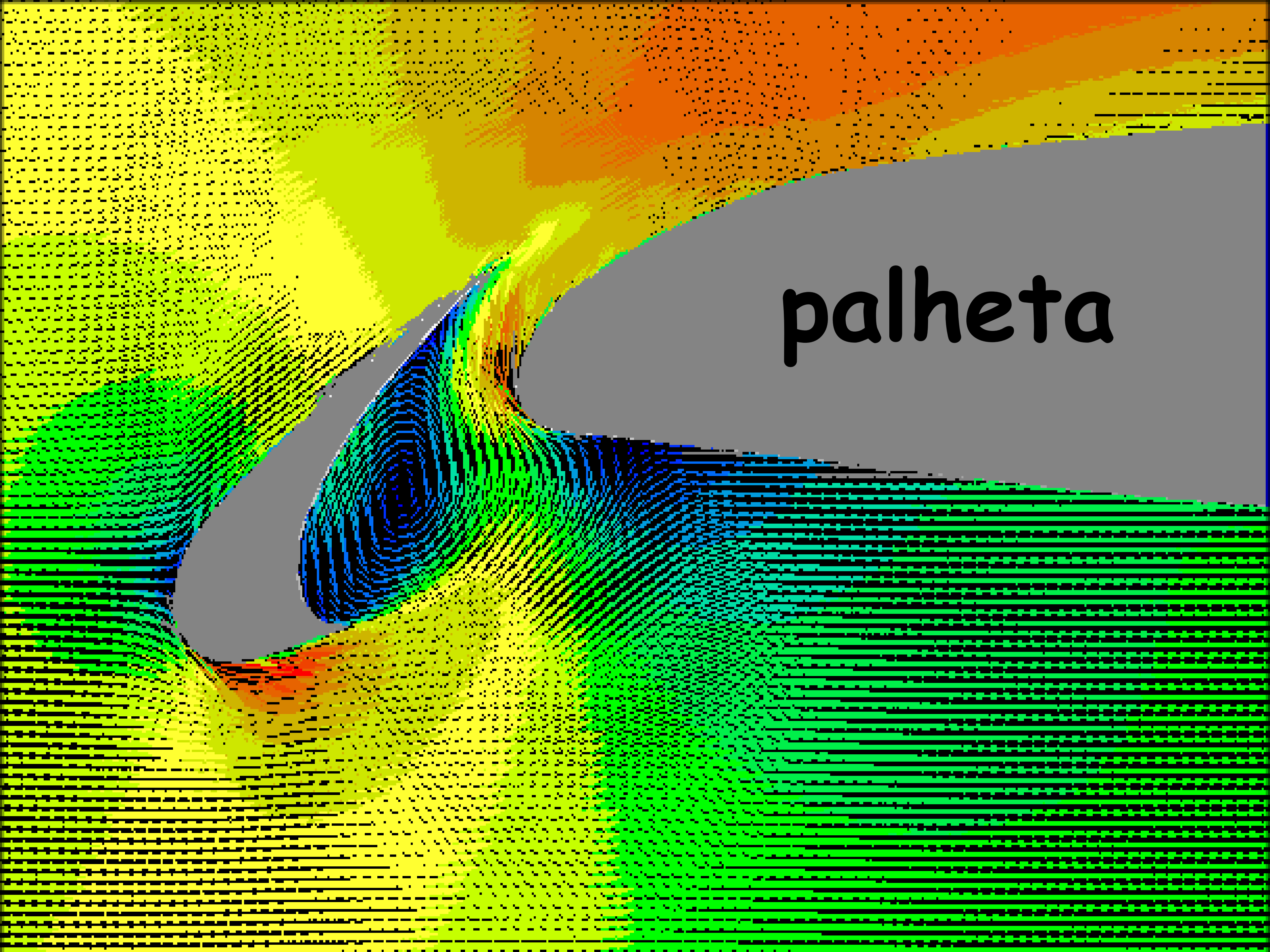
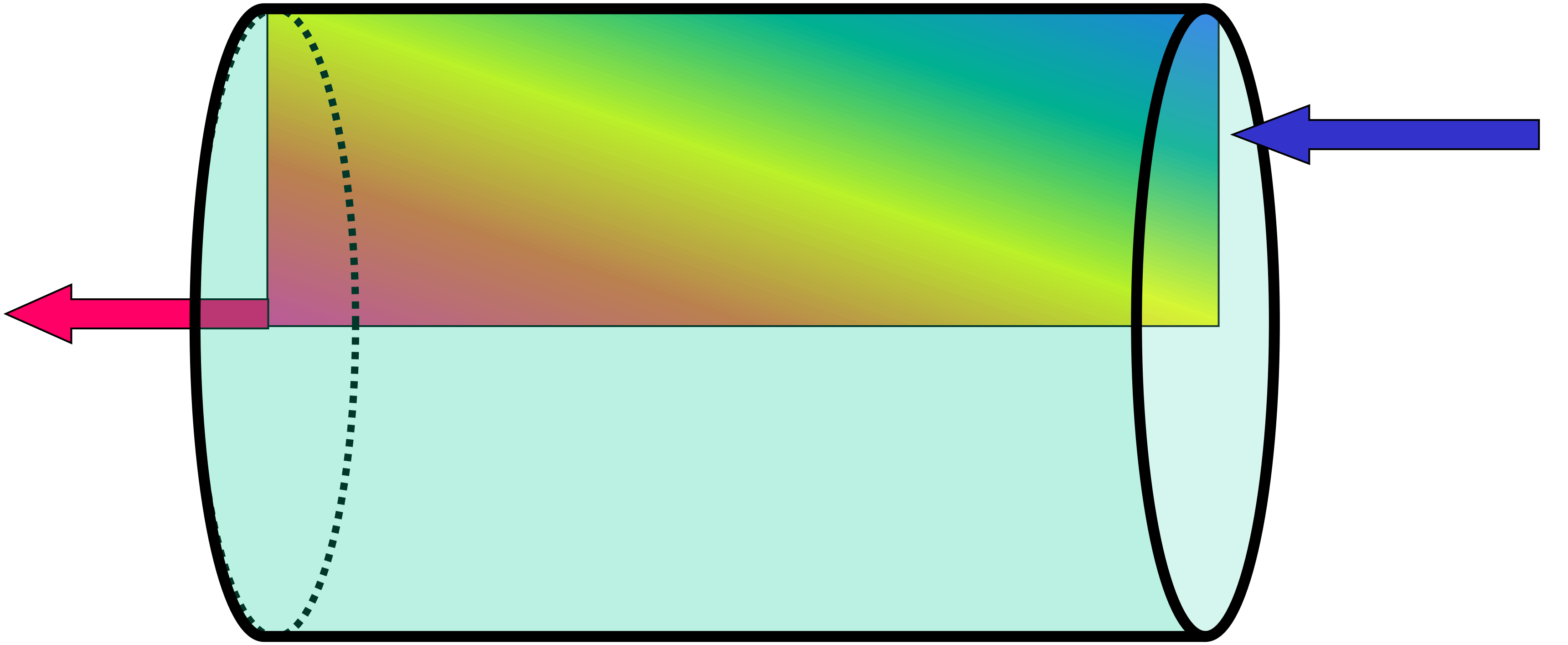
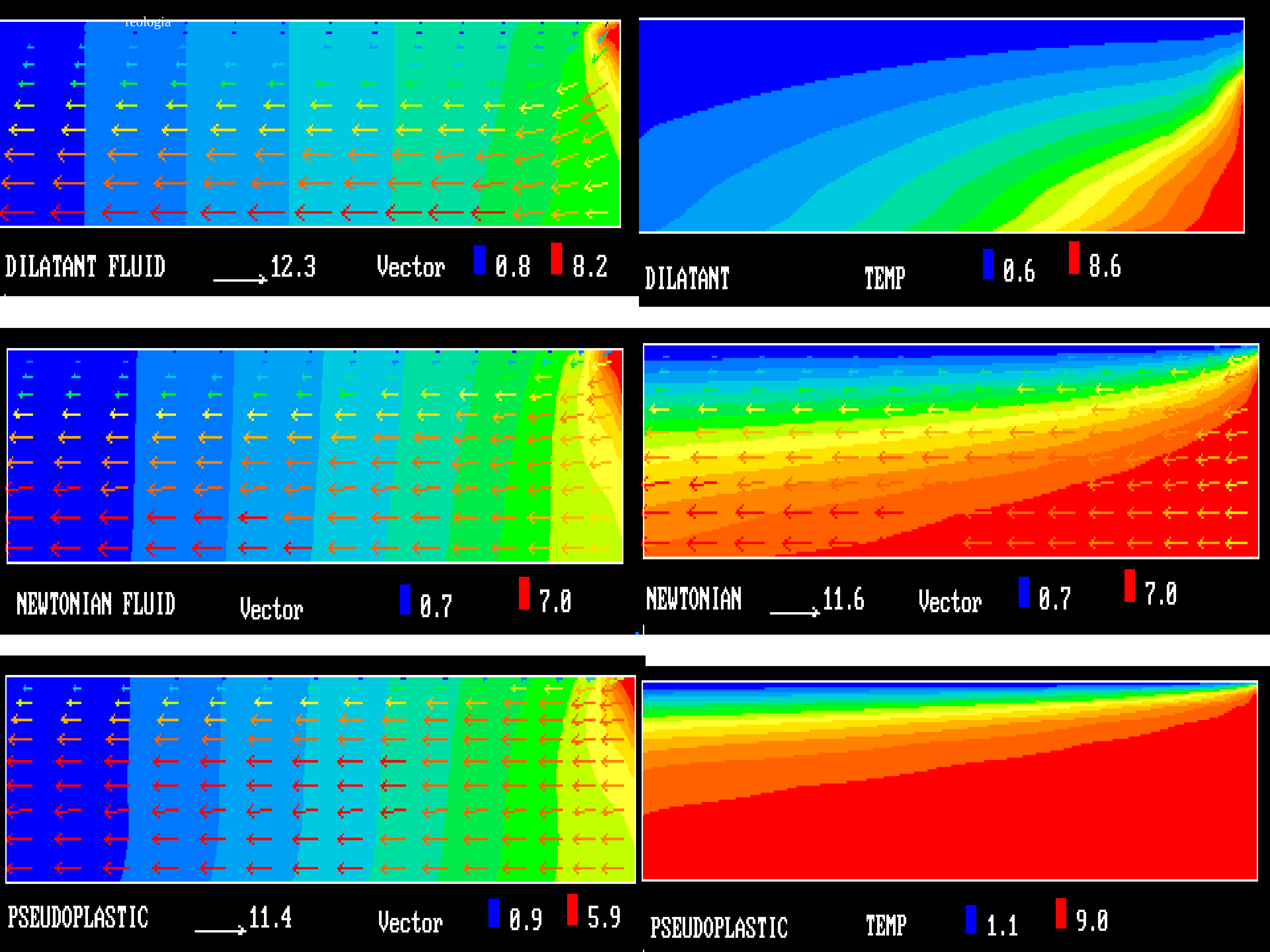


Fig. 4. Dr de Laval's Turbine.

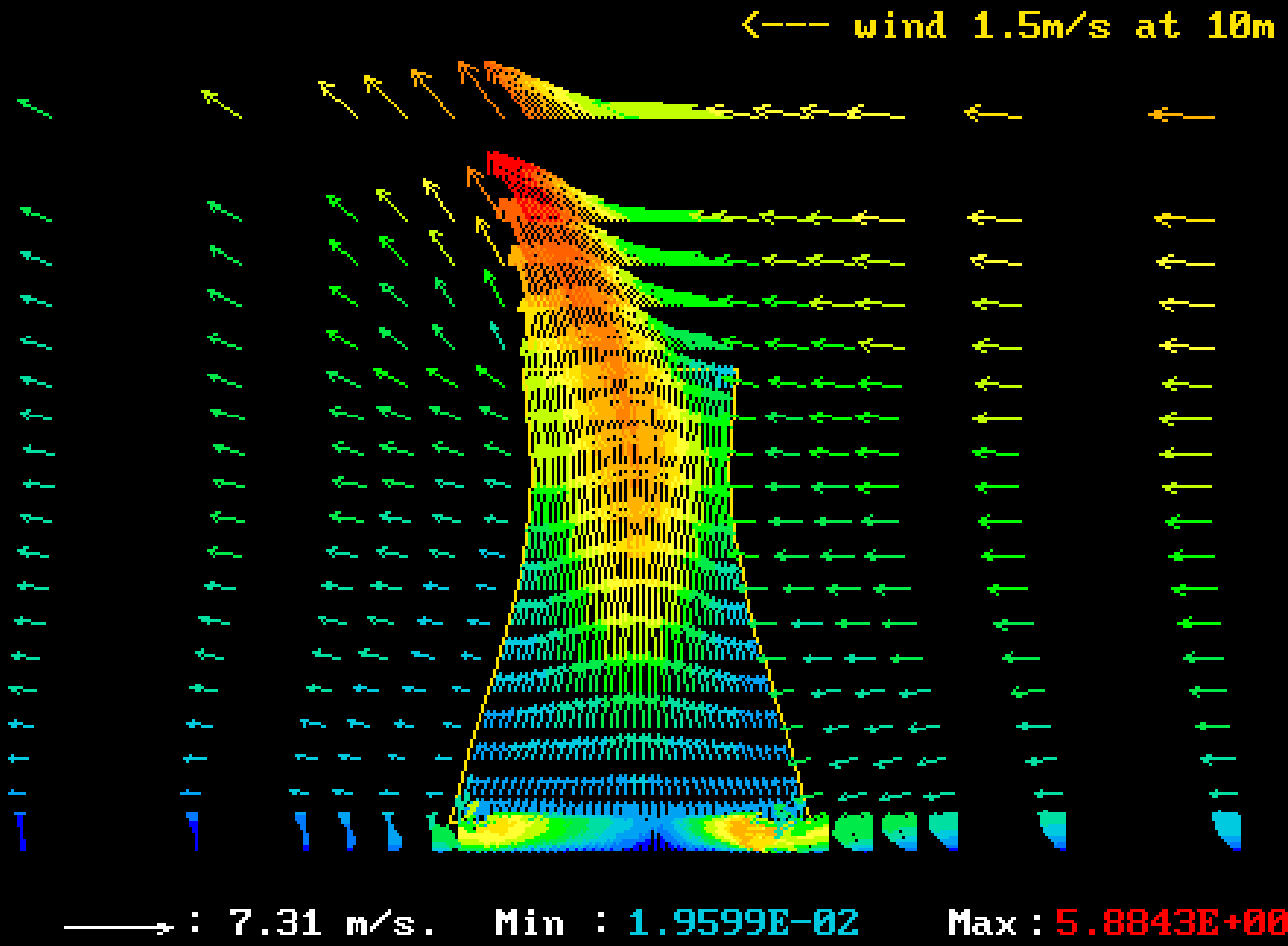

palheta

Caso 0

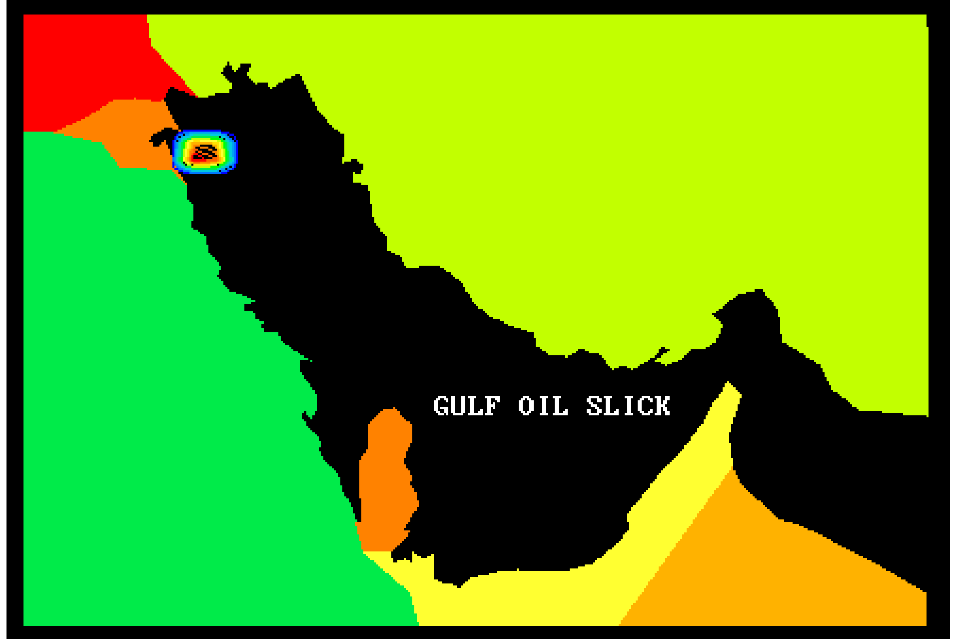


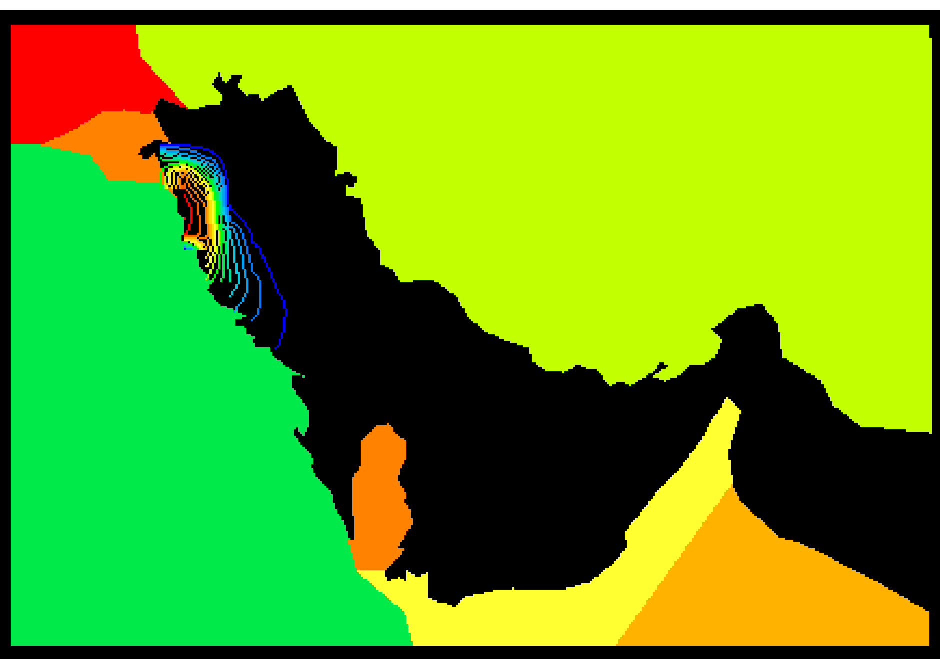

reologia
DILATANT FLUID
12.3
Vector
0.8
8.2
DILATANT
TEMP
0.6
8.6
NEWTONIAN FLUID
Vector
0.7
7.0
NEWTONIAN
11.6
Vector
0.7
7.0
PSEUDOPLASTIC
11.4
Vector
0.9
5.9
PSEUDOPLASTIC
TEMP
1.1
9.0

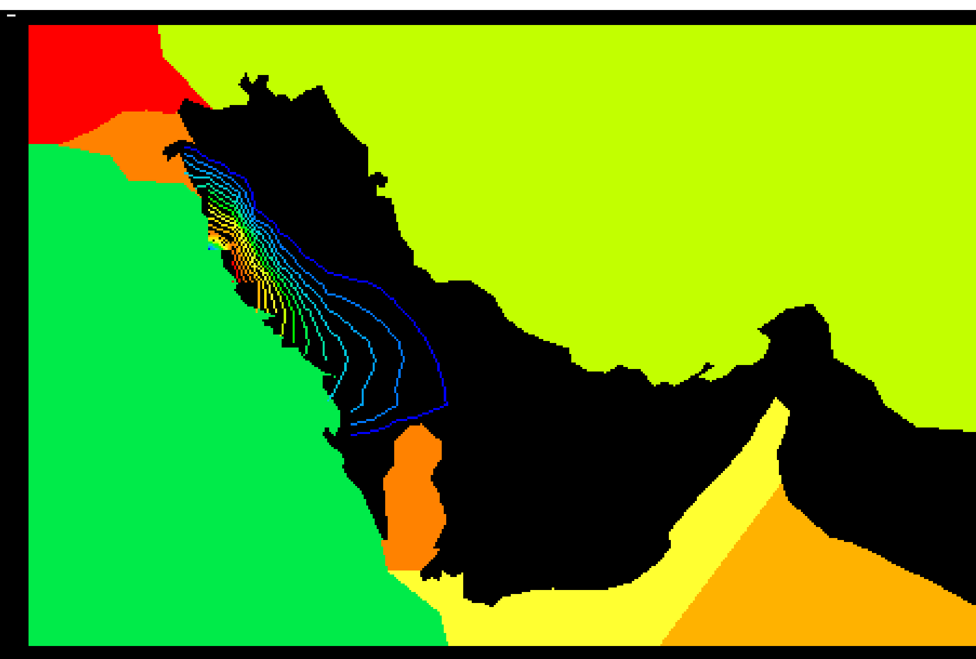
COOLING TOWER SIMULATION

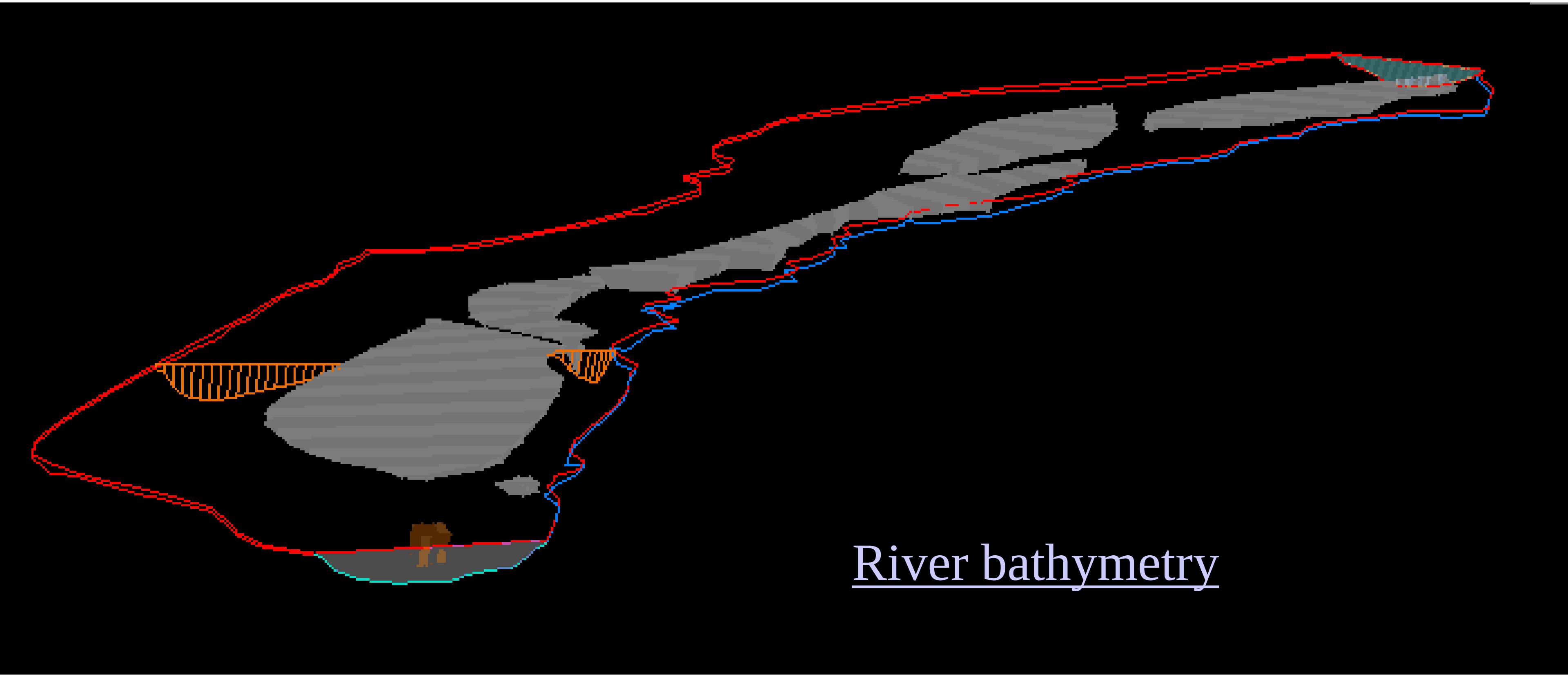


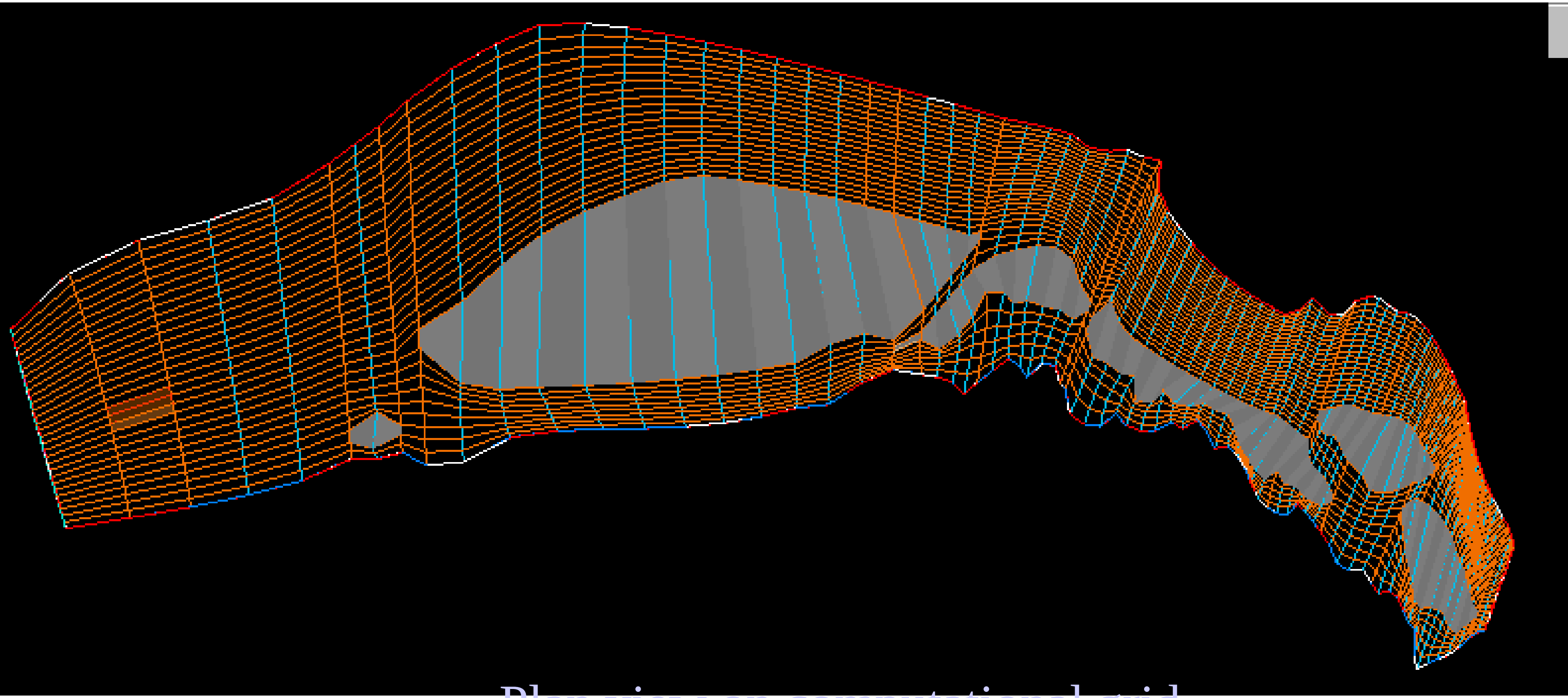
cooling tower


GULF OIL SLICK

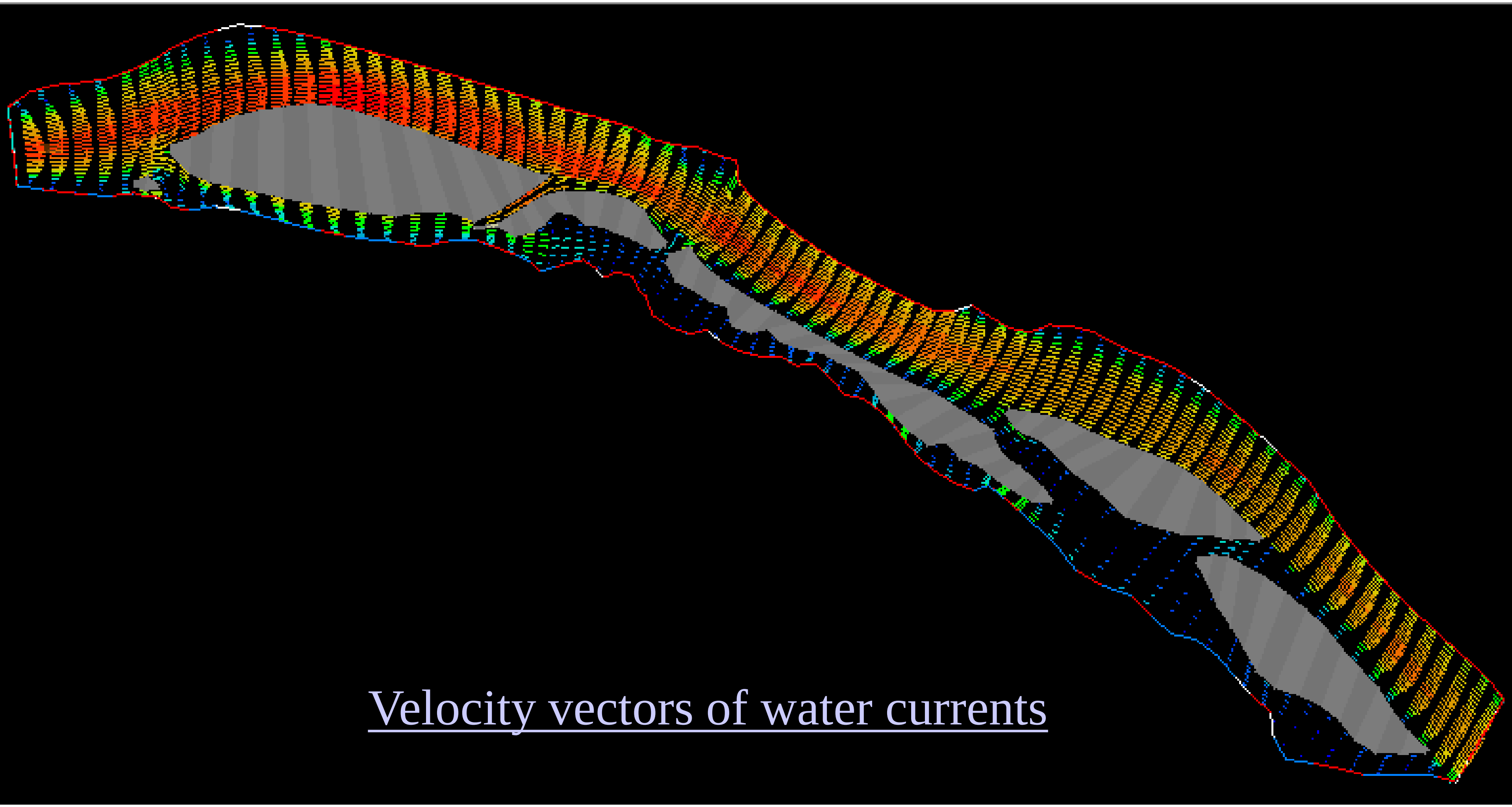




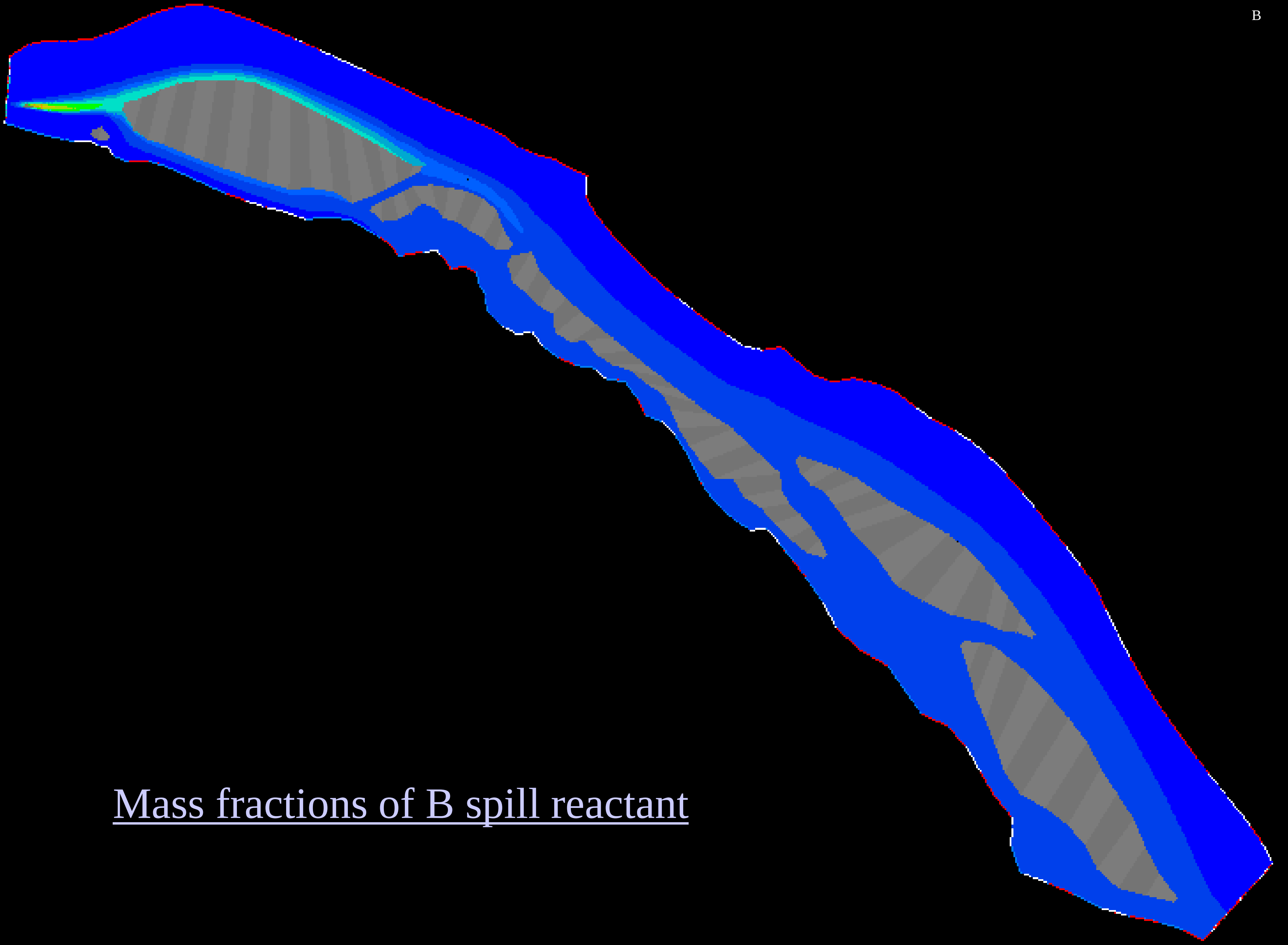

River bathymetry



Plan view on computational grid

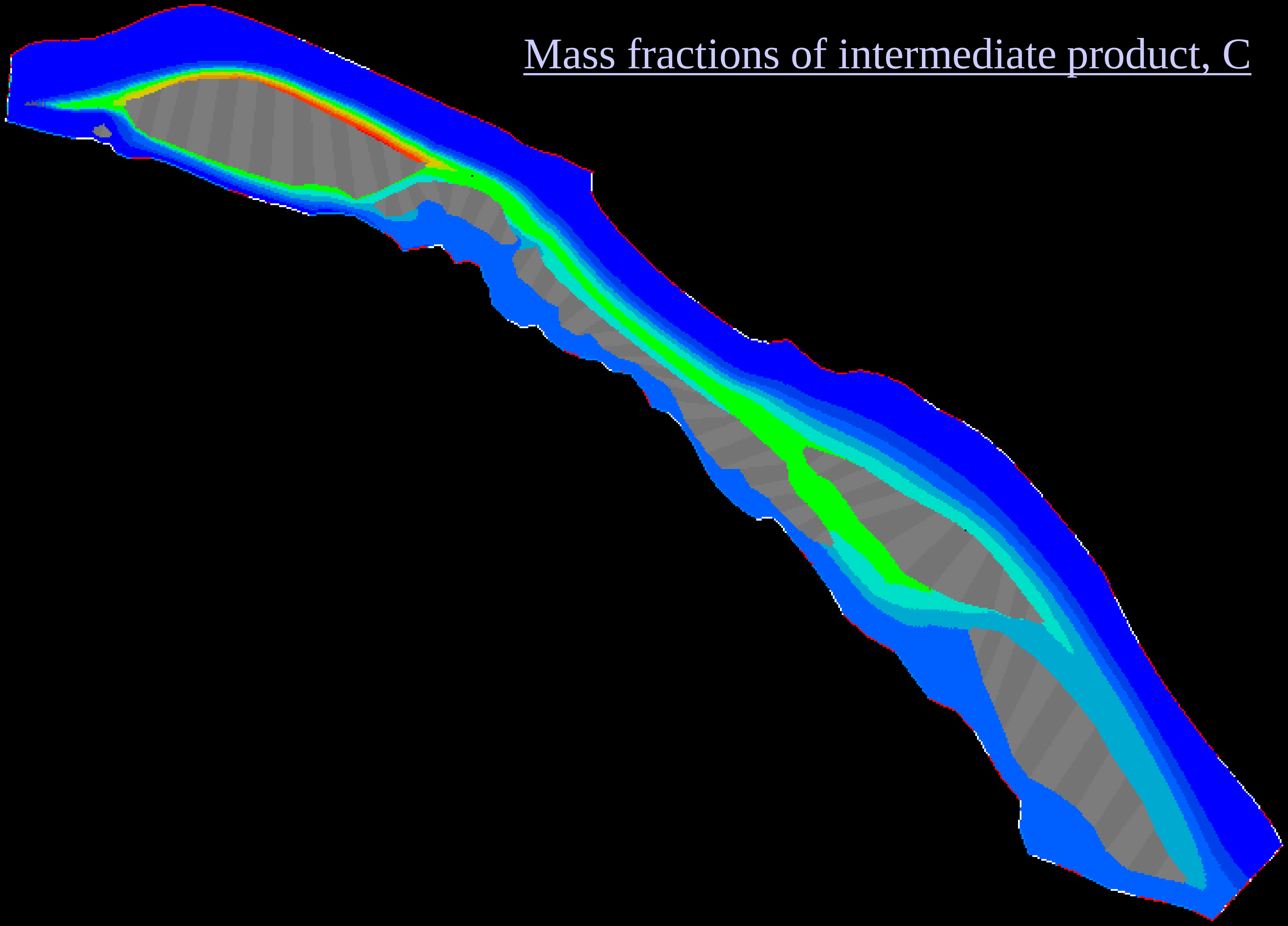


Velocity vectors of water currents

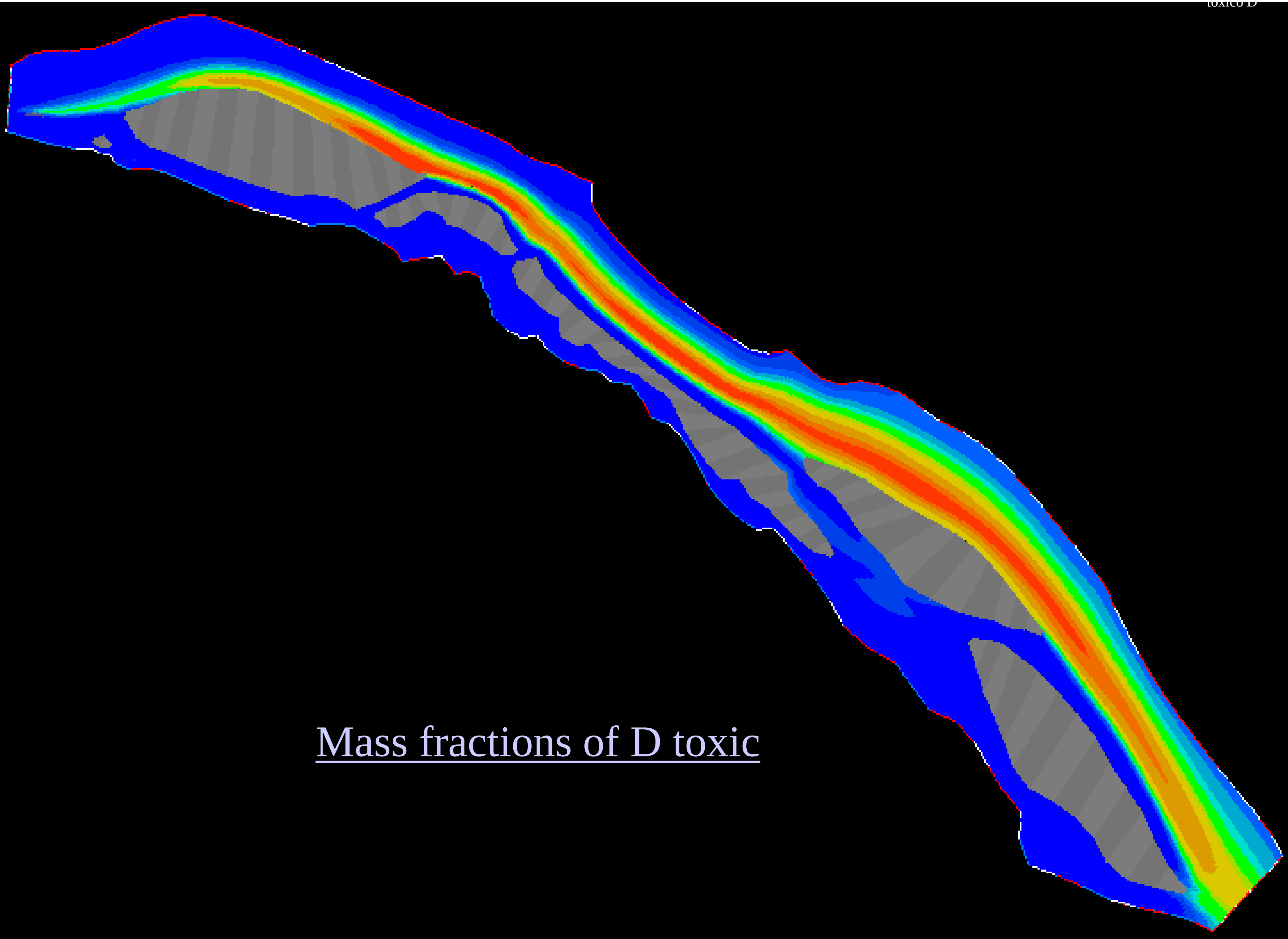


Mass fractions of B spill reactant

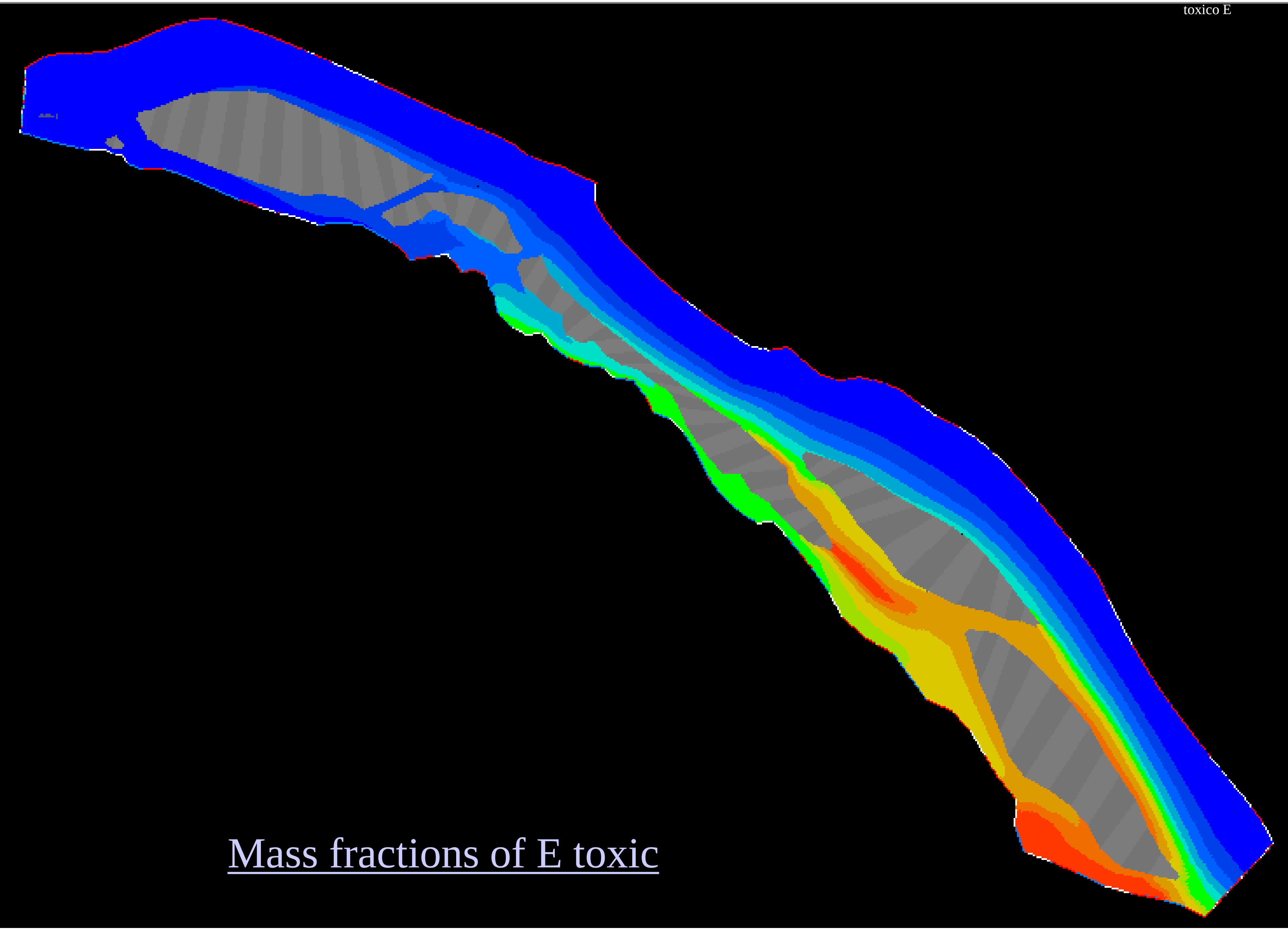
Mass fractions of intermediate product, C



intermediário C

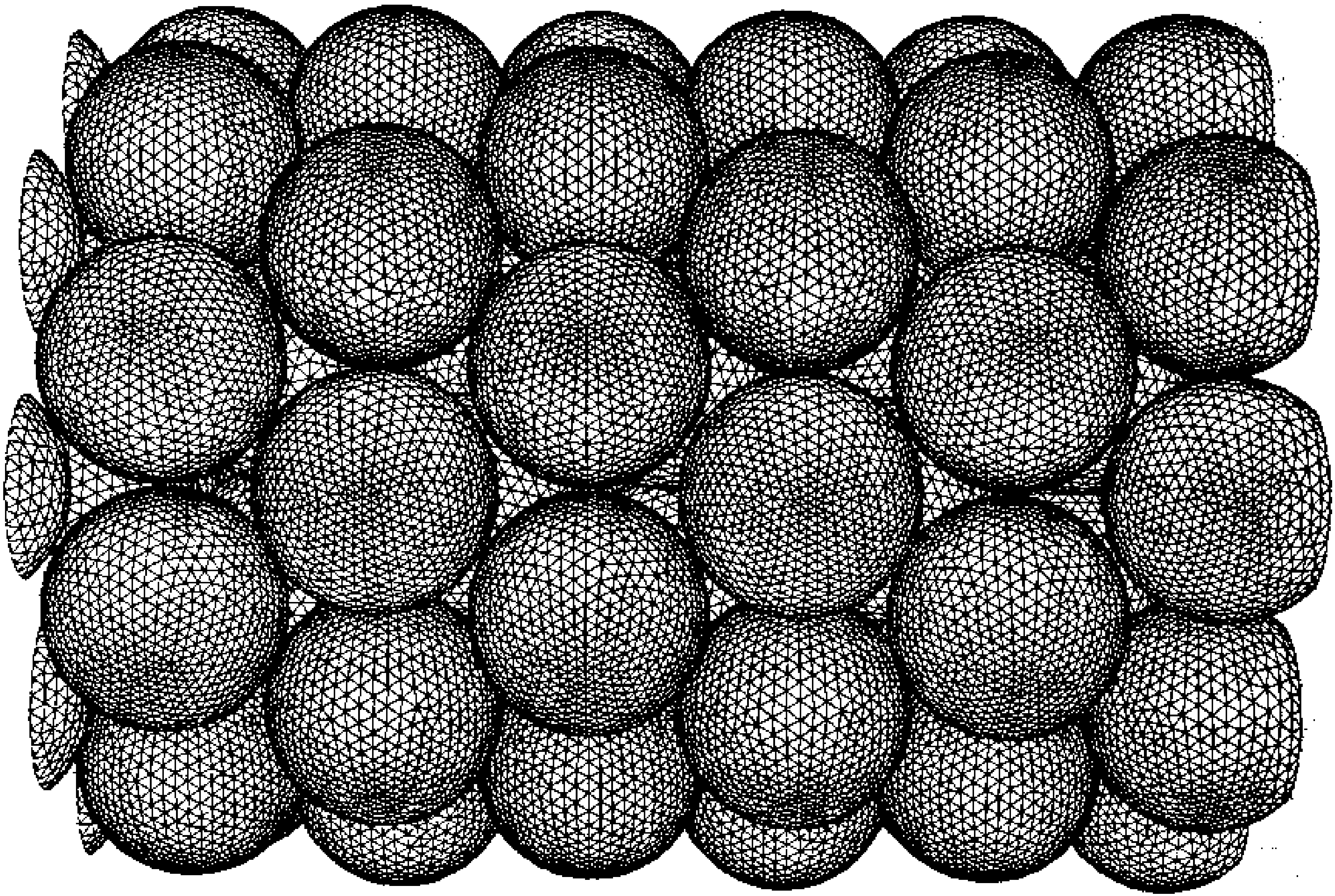


Mass fractions of D toxic



Mass fractions of E toxic


queimador

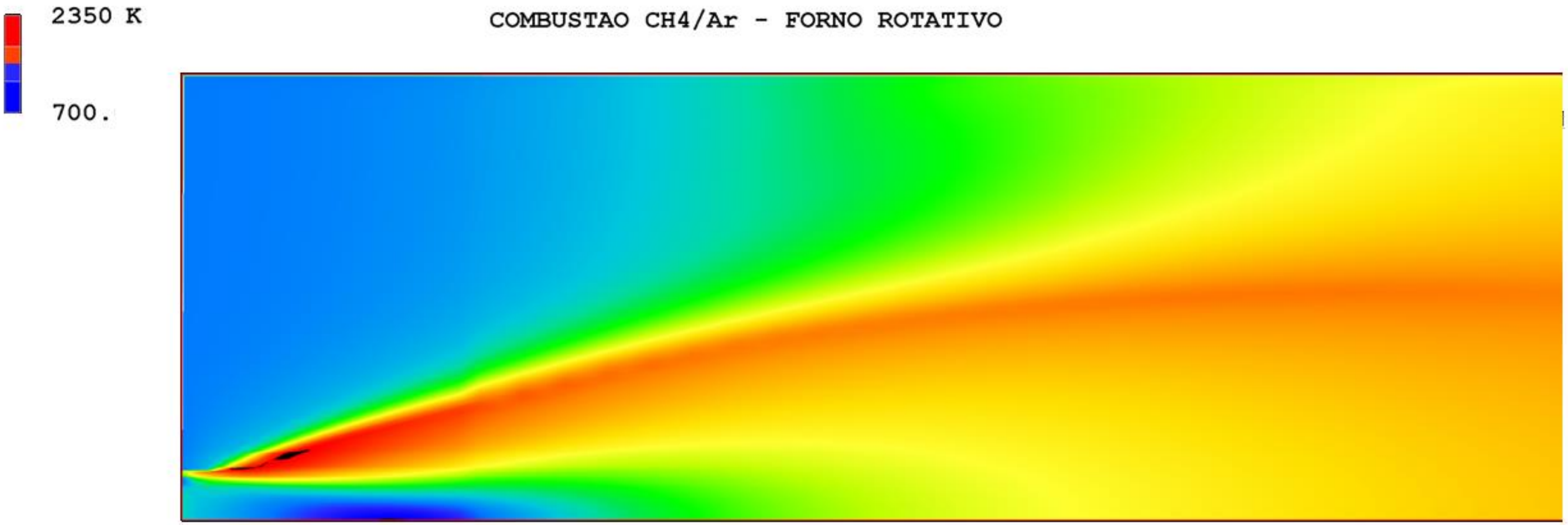


Exemplo: combustão de óleo

teste

chama

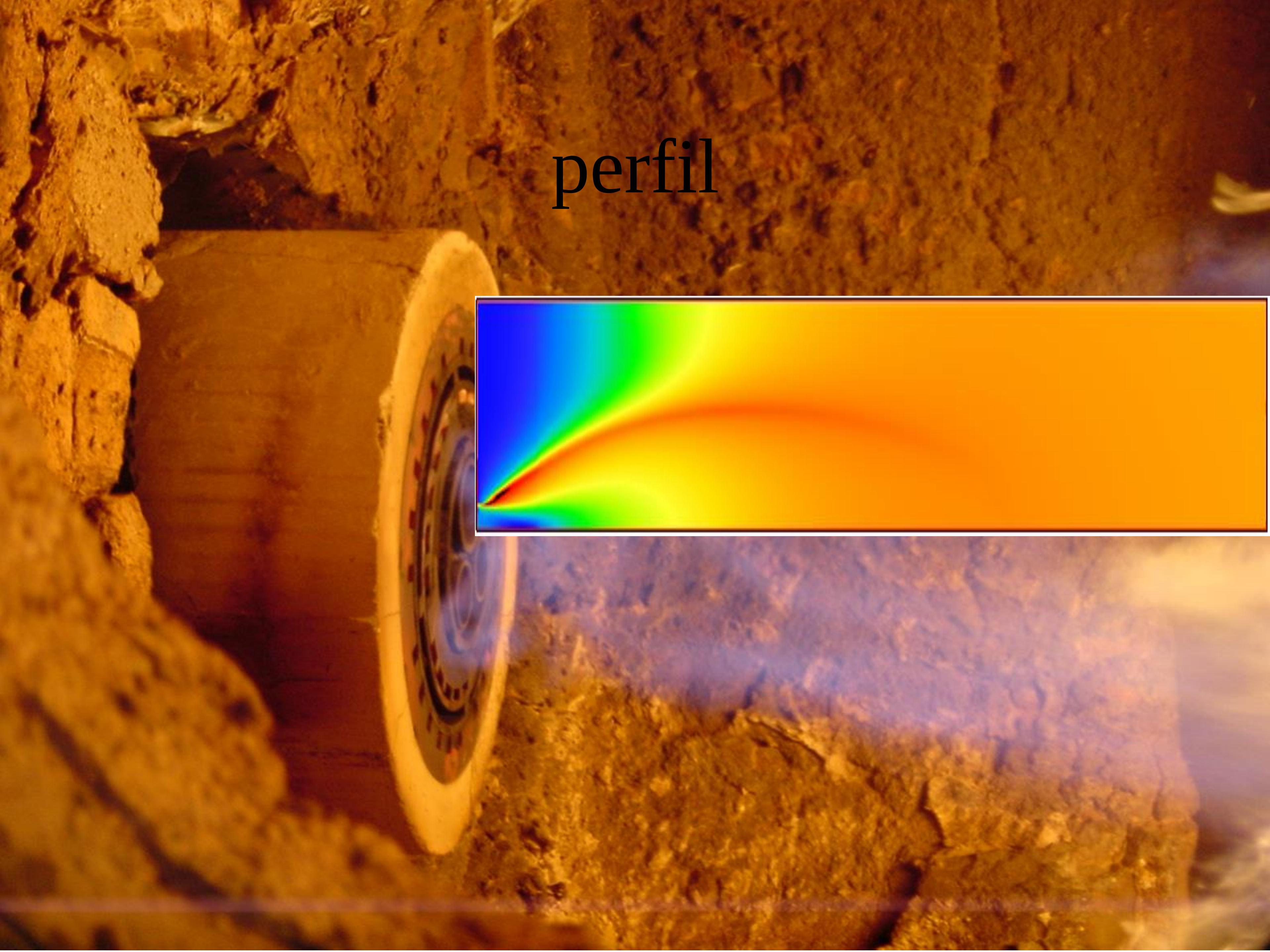
simulação



MODELOS DE RADIAÇÃO NO PHOENICS

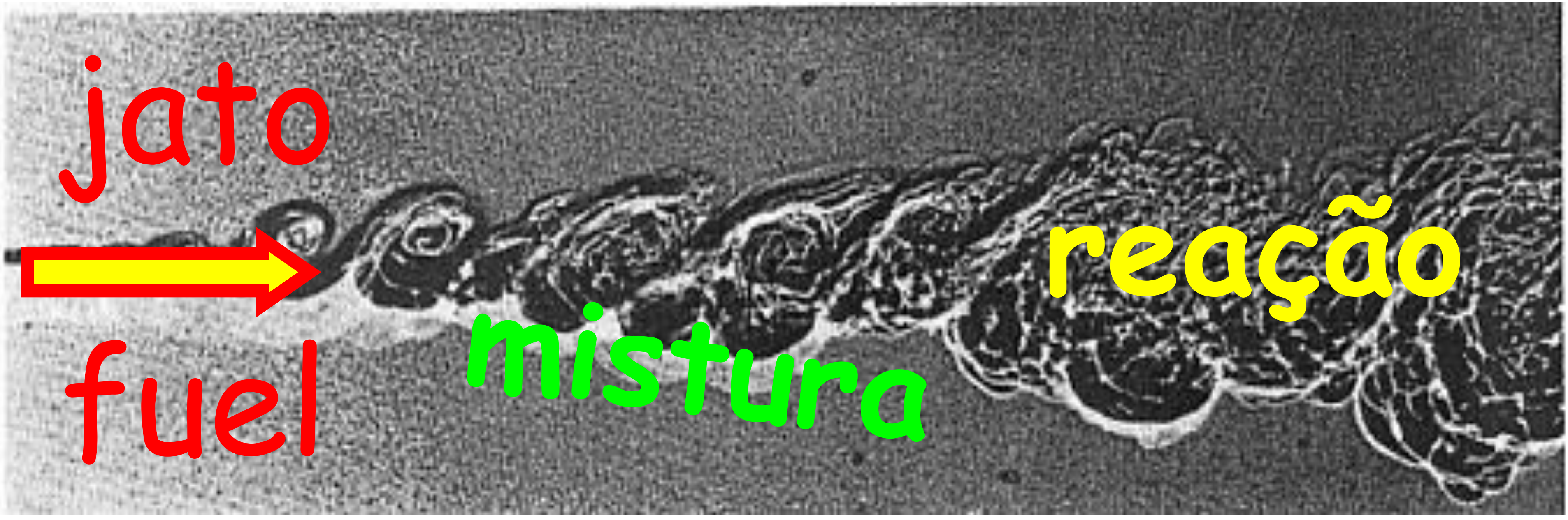
- Modelo *composite-flux* (*6-flux*) de Schuster & Hamaker, conforme formulado por Spalding (1980).
- Modelo *composite-radiosity* de Spalding (1994); este modelo é similar ao modelo P-1 harmônico-esférico de Ozisik (1973).
- Modelo de difusão de *Rosseland* (1936).
- Modelo IMMERSOL.
- Modelo de radiação superfície-para-superfície.

perfil



eddy break up

comburente



comburente

TURBULÊNCIA de **mistura**

6. Turbulent Reaction-Rate Sources

6.1 Eddy-breakup

For turbulent flows, the second form (see section 2.6 above) of the eddy-breakup reaction-rate is provided. The resulting source per unit phase mass is:

$$S_{mfu} = -a \times \min\{ mfu \, , mox / s \} \times \frac{EP}{KE}$$

This is activated by:

PATCH (CHSO, PHASEM, IF,IL, JF,JL, KF,KL, TF,TL)
COVAL (CHSO, FUEL, GRND9, GRND9)

The reaction rate constant, a and the stoichiometric ratio,s, are passed via

CHSOB = a CHSOA = 1 / (1 +s) [= fstoic]

The rate controlling parameter CHSOB is commonly set to unity.

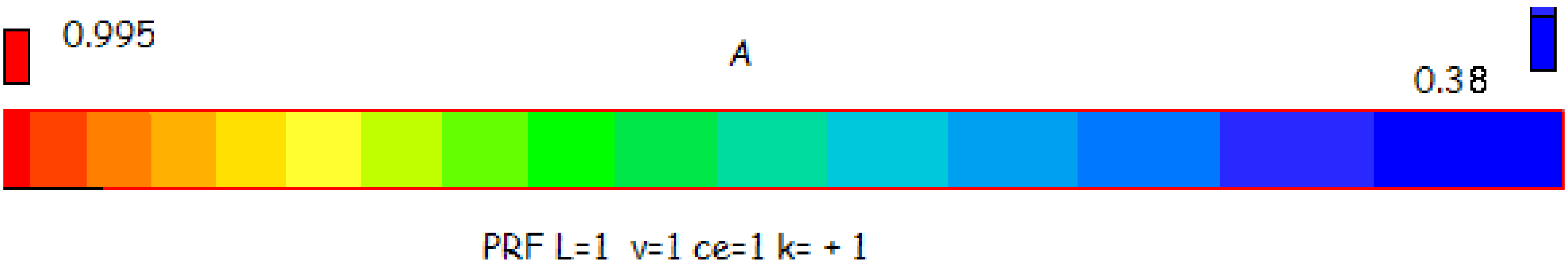
Rodando o CFD

PFR
n = 1

$$r = k\, c_A$$

$$\frac{\tilde{c}_s}{\tilde{c}_e} = e^{-\frac{Lk}{v}}$$

L=1m; v=1m/s; ce=1gmole/m3; k = 1m3/gmole/s -> cs/ce=0,37



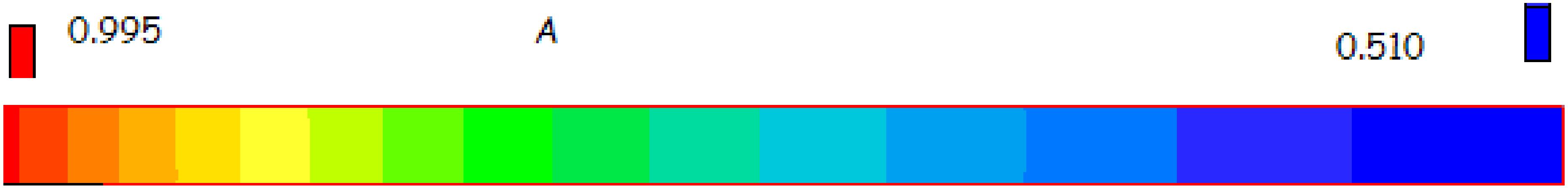
PFR 1a o

PFR n = 2

$$r = k\, c_A^{\,2}$$

$$\frac{\tilde{c}_s}{\tilde{c}_e} = \frac{1}{\dfrac{Lk\tilde{c}_e}{v} + 1}$$

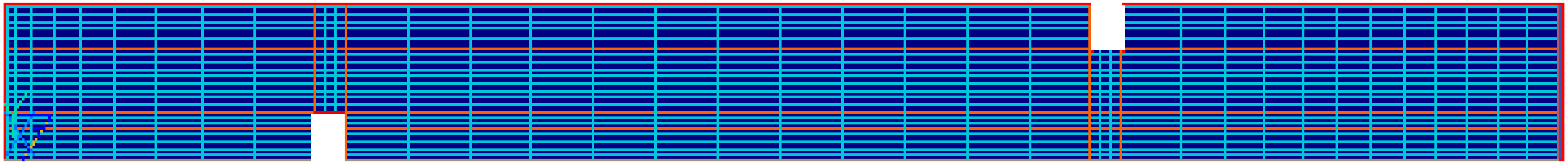
L=1m; v=1m/s; ce=1gmole/m3; k = 1m3/gmole/s -> cs/ce=0,50



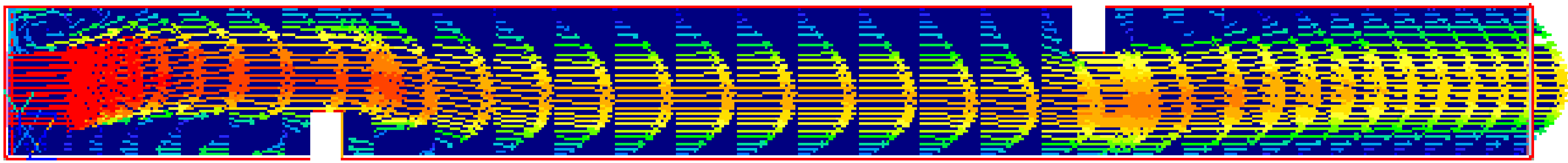
PRF L=1 v=1 ce=1 k=-1

CFD

malha



velocidades

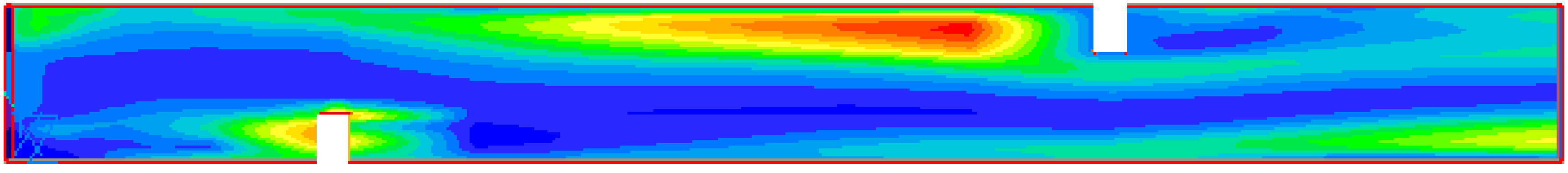


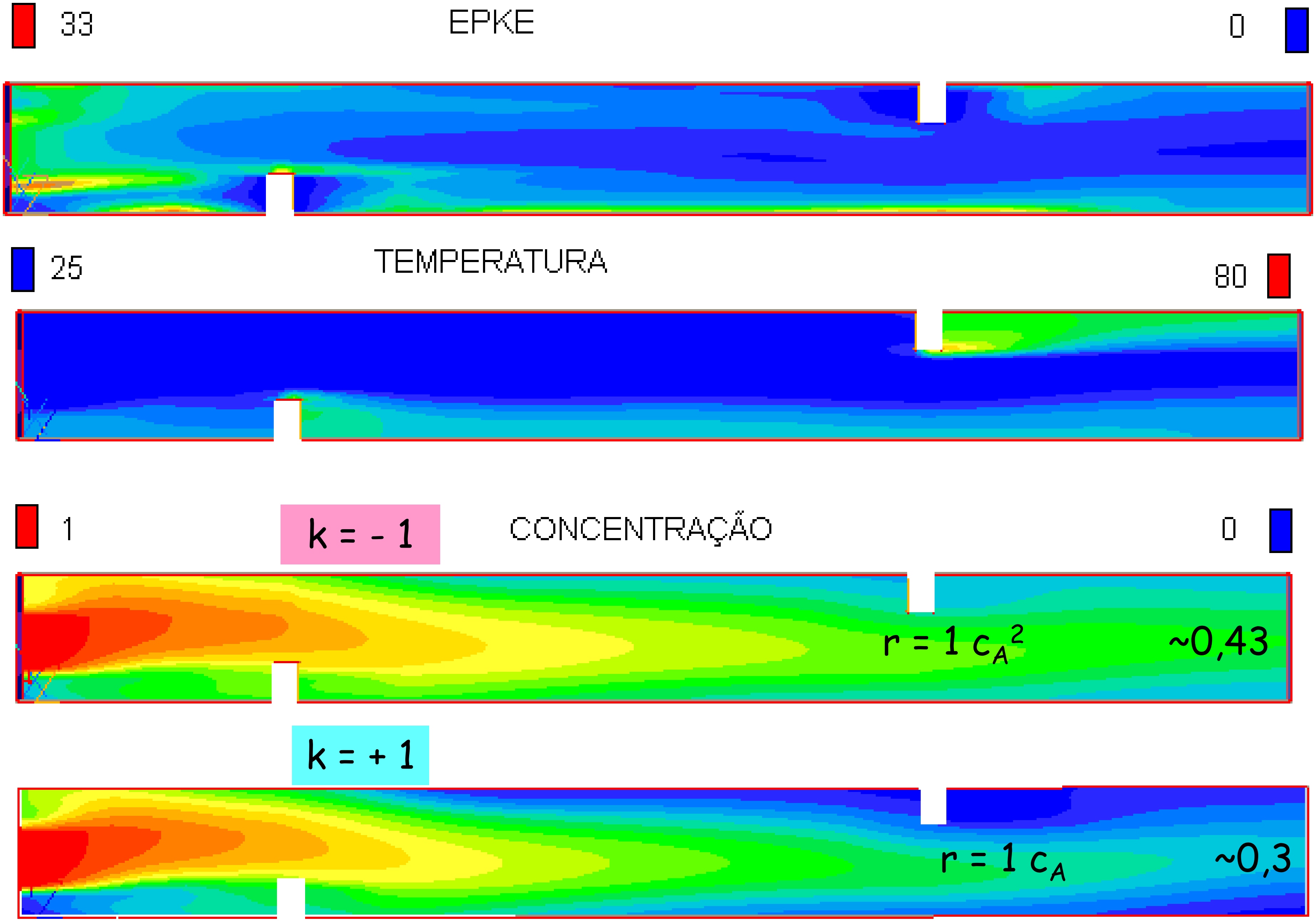
-0.37 Pa 0.027

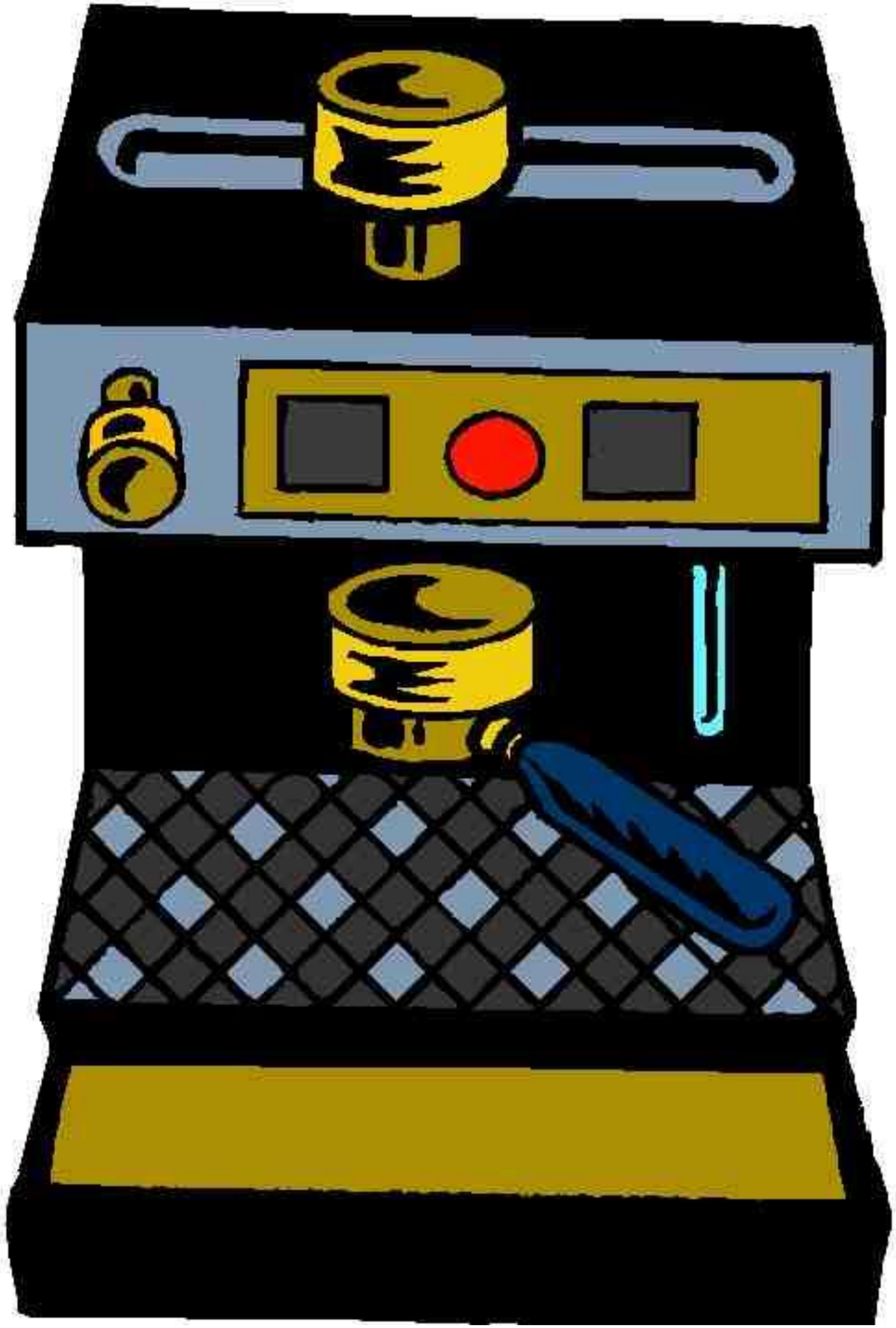
pressão

2.2E-6 8.8E-5

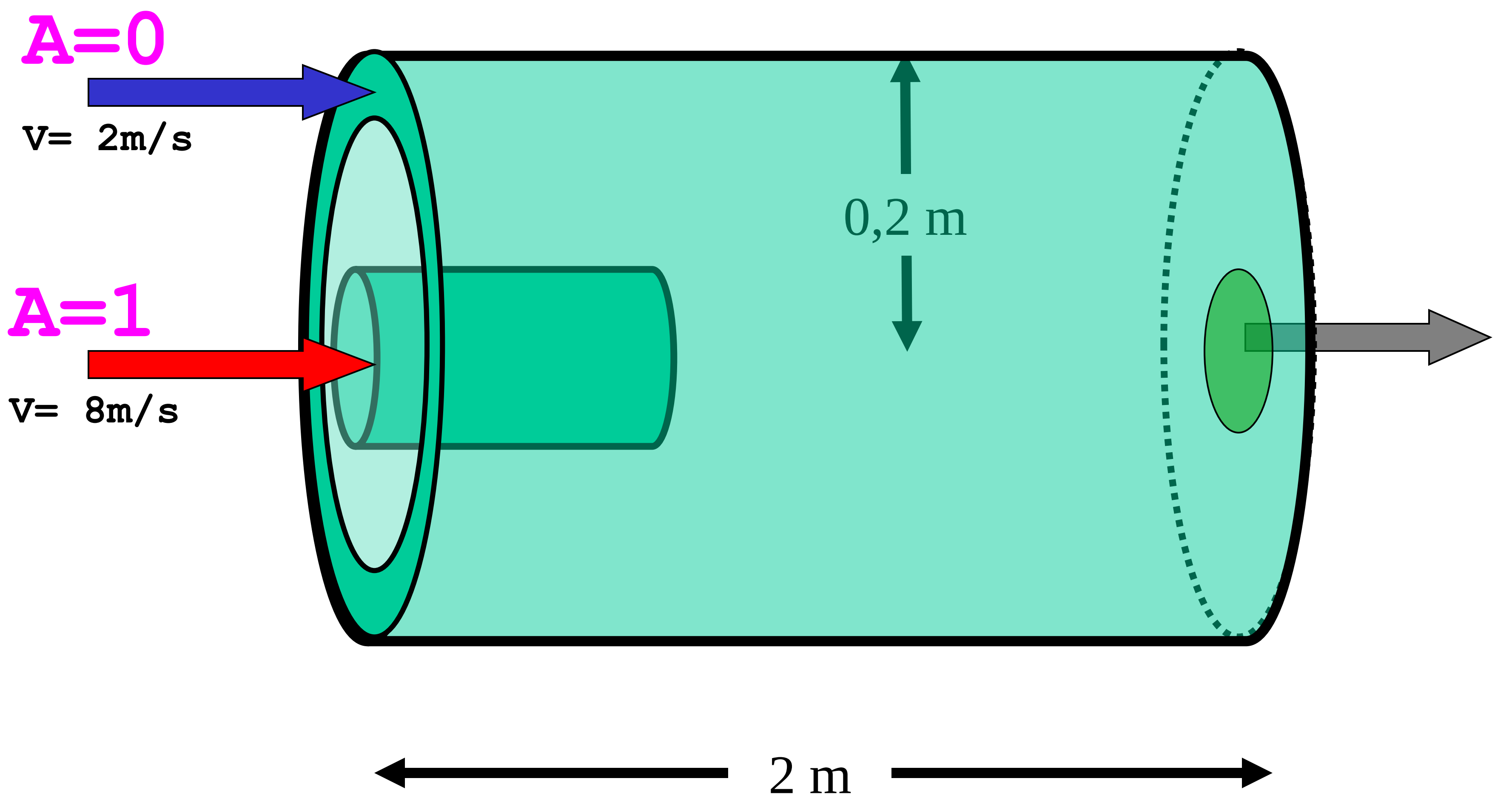
viscosidade turbulenta

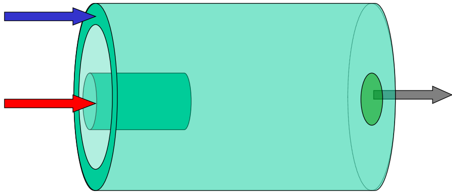



33
EPKE
0
25
TEMPERATURA
80
1
k = - 1
CONCENTRAÇÃO
0
r = 1 c_A^2
~0,43
k = + 1
r = 1 c_A
~0,3

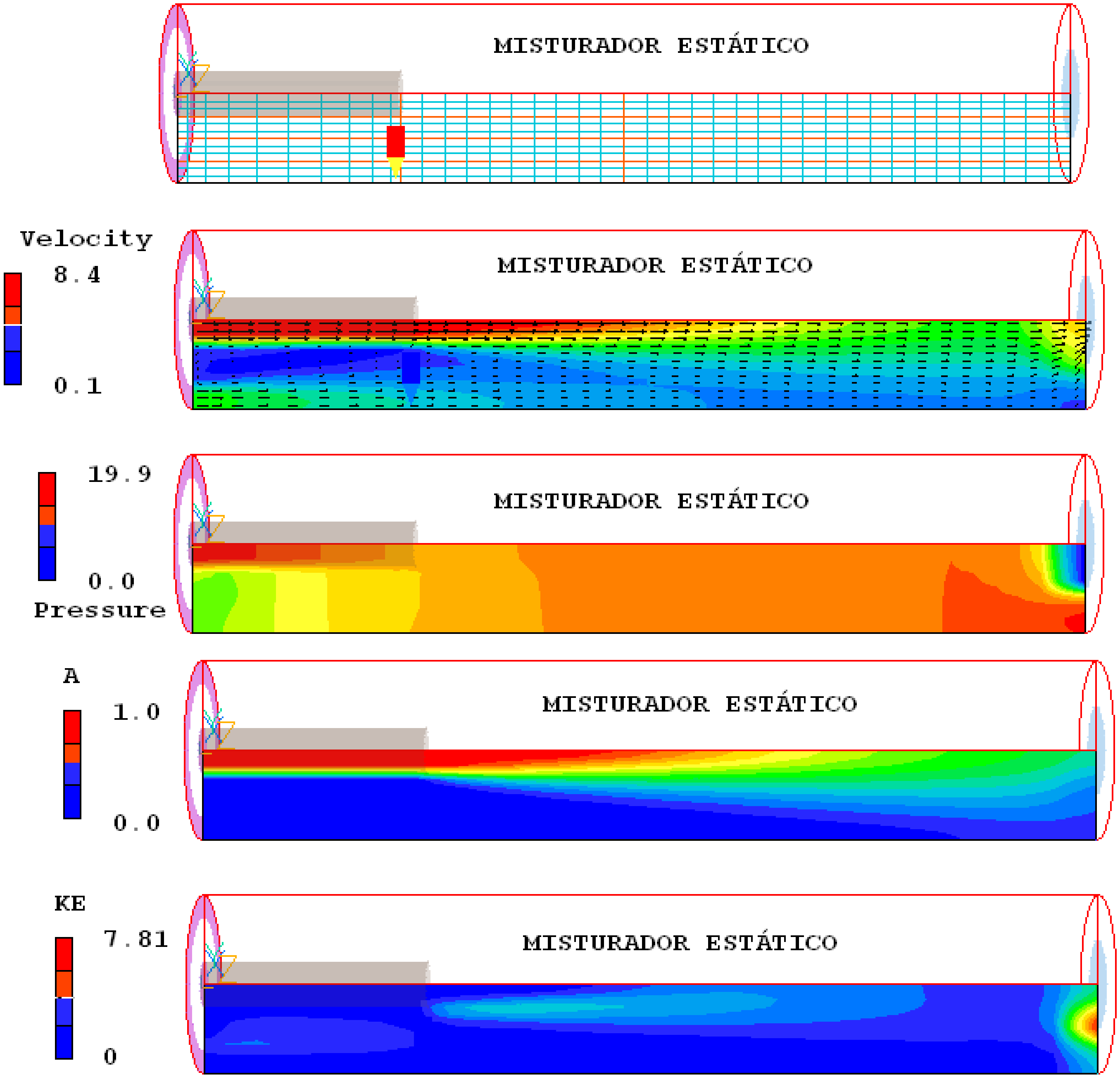


Caso 1

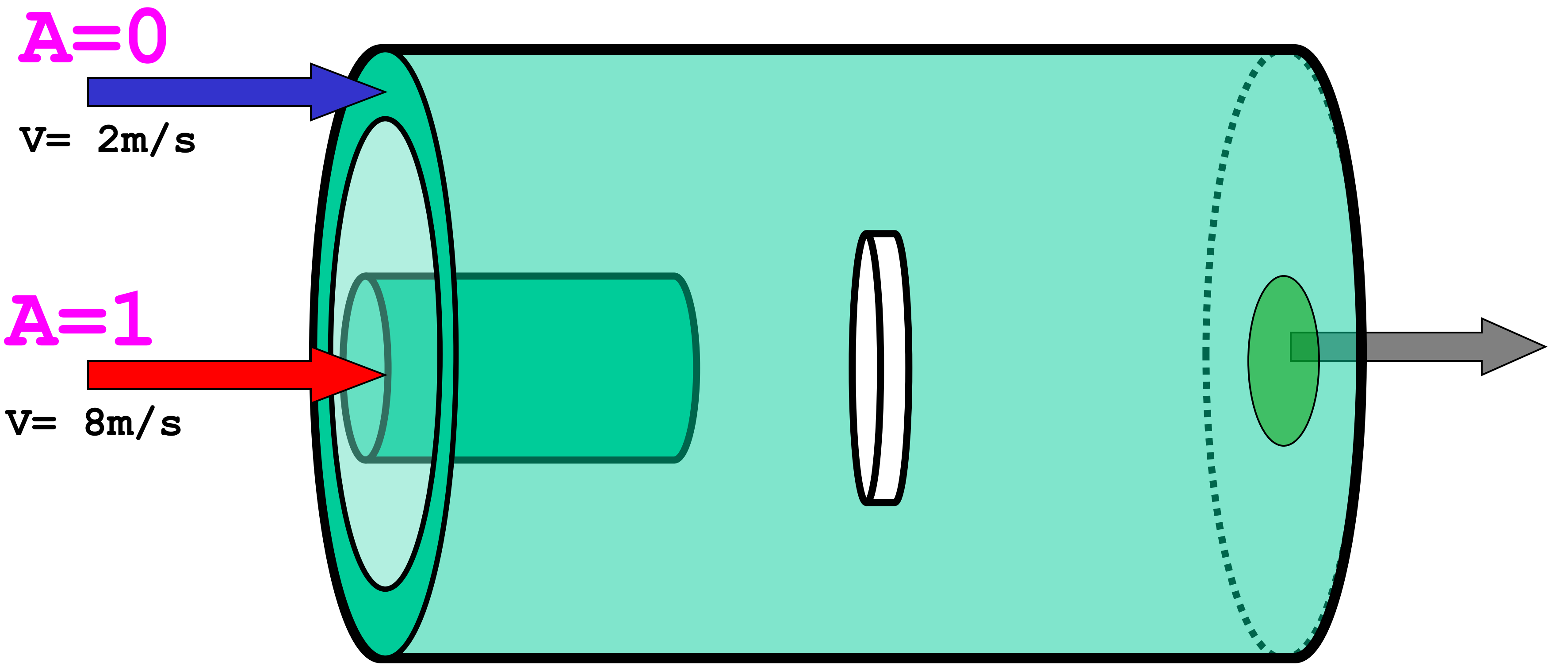


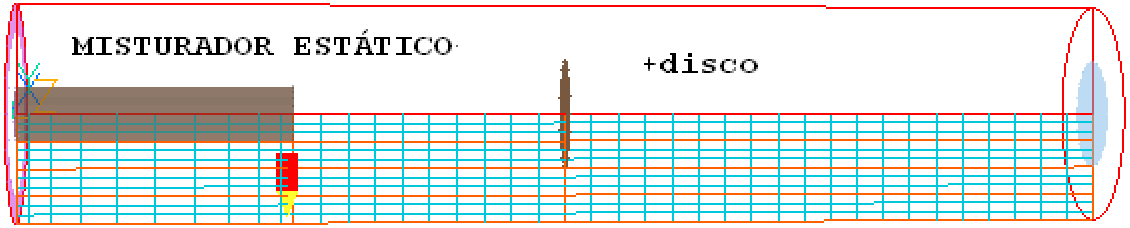


Caso 1

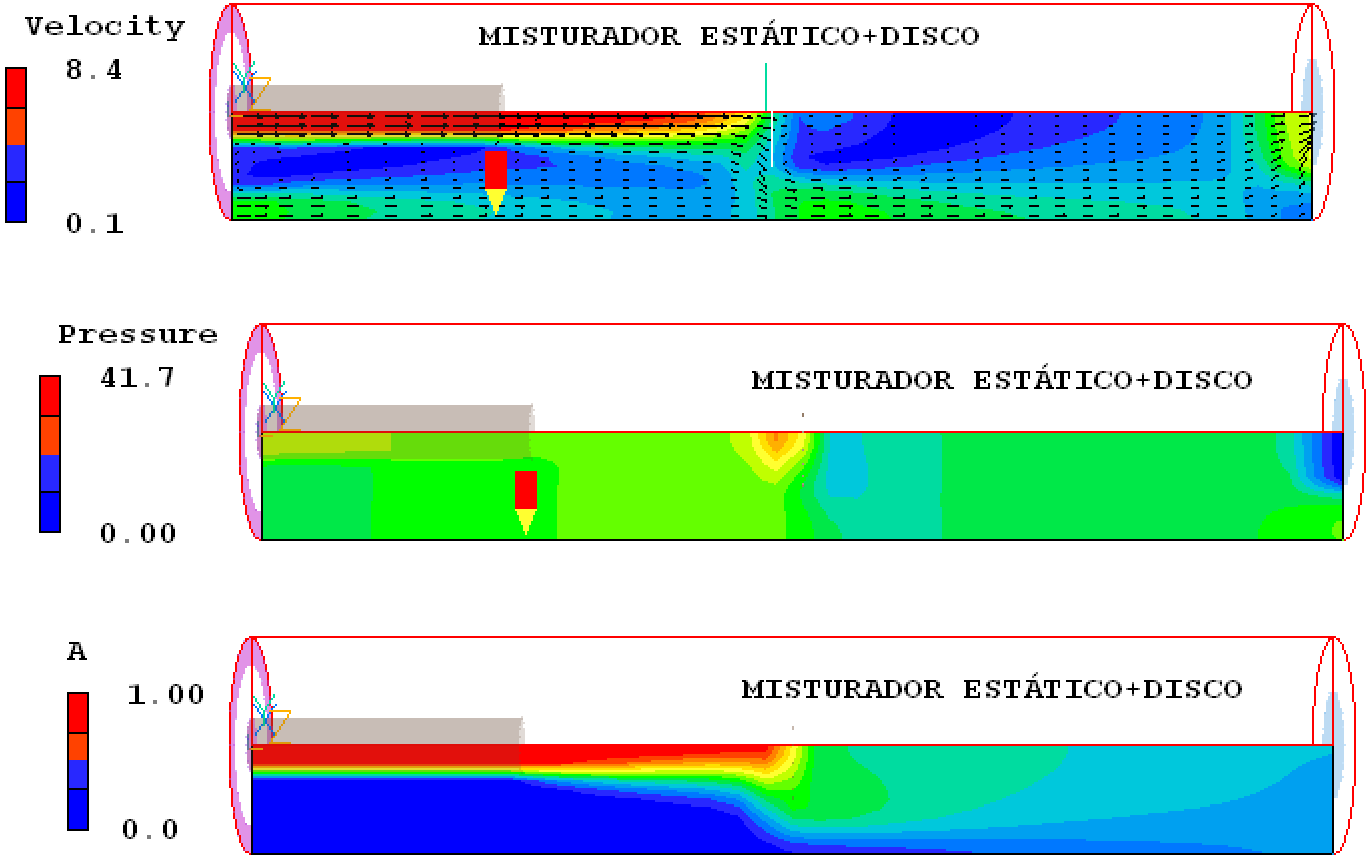

MISTURADOR ESTÁTICO
Velocity
8.4
0.1
MISTURADOR ESTÁTICO
19.9
0.0
Pressure
MISTURADOR ESTÁTICO
A
1.0
0.0
MISTURADOR ESTÁTICO
KE
7.81
0
MISTURADOR ESTÁTICO

Caso 2

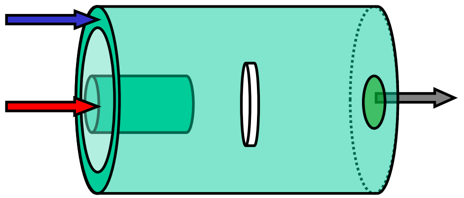




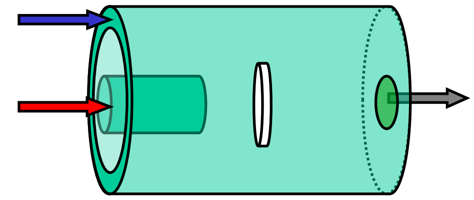
MISTURADOR ESTÁTICO
+disco



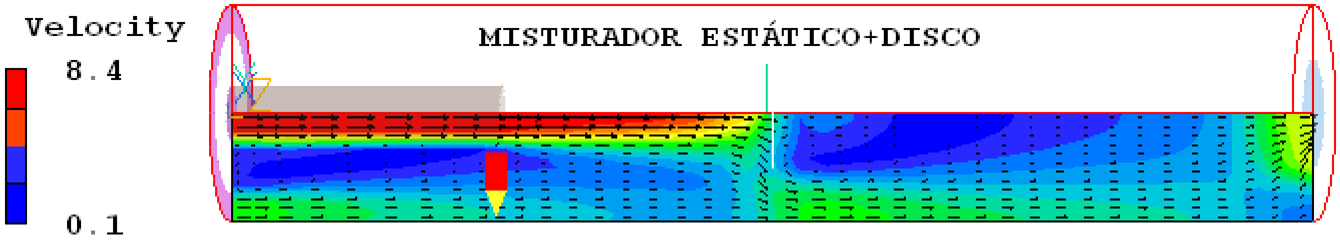
Velocity
8.4
0.1
MISTURADOR ESTÁTICO+DISCO
Pressure
41.7
0.00
MISTURADOR ESTÁTICO+DISCO
A
1.00
0.0
MISTURADOR ESTÁTICO+DISCO

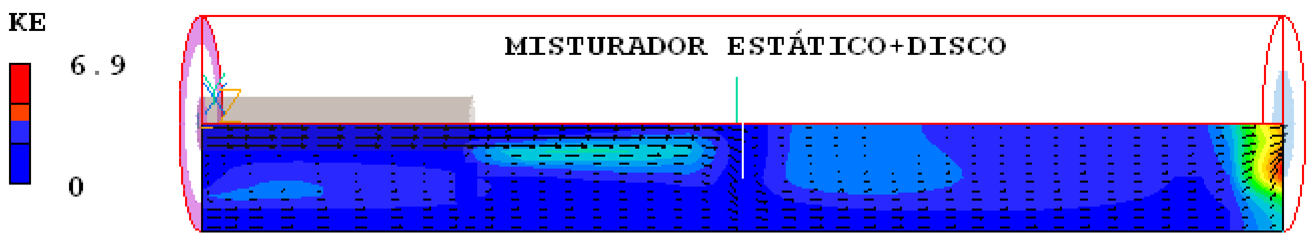


Caso 2



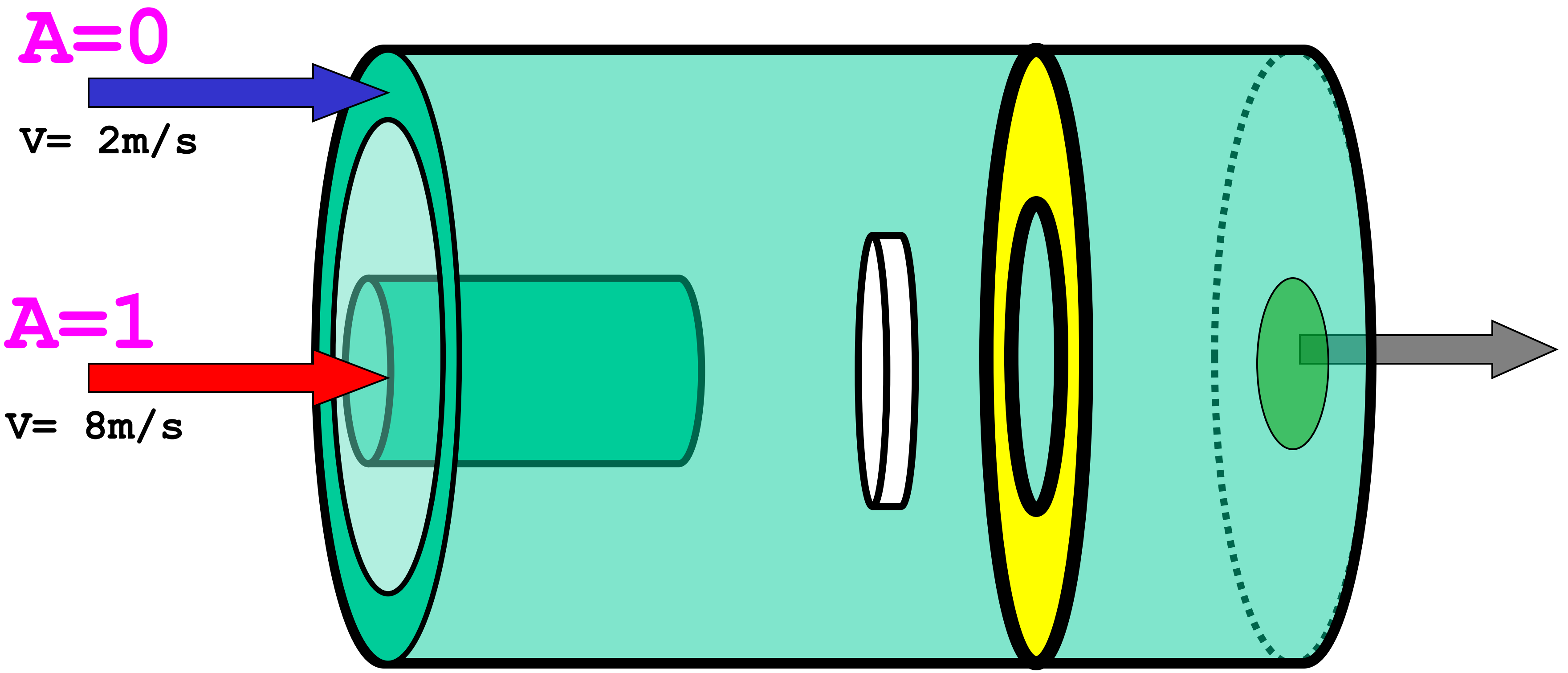
Caso 2

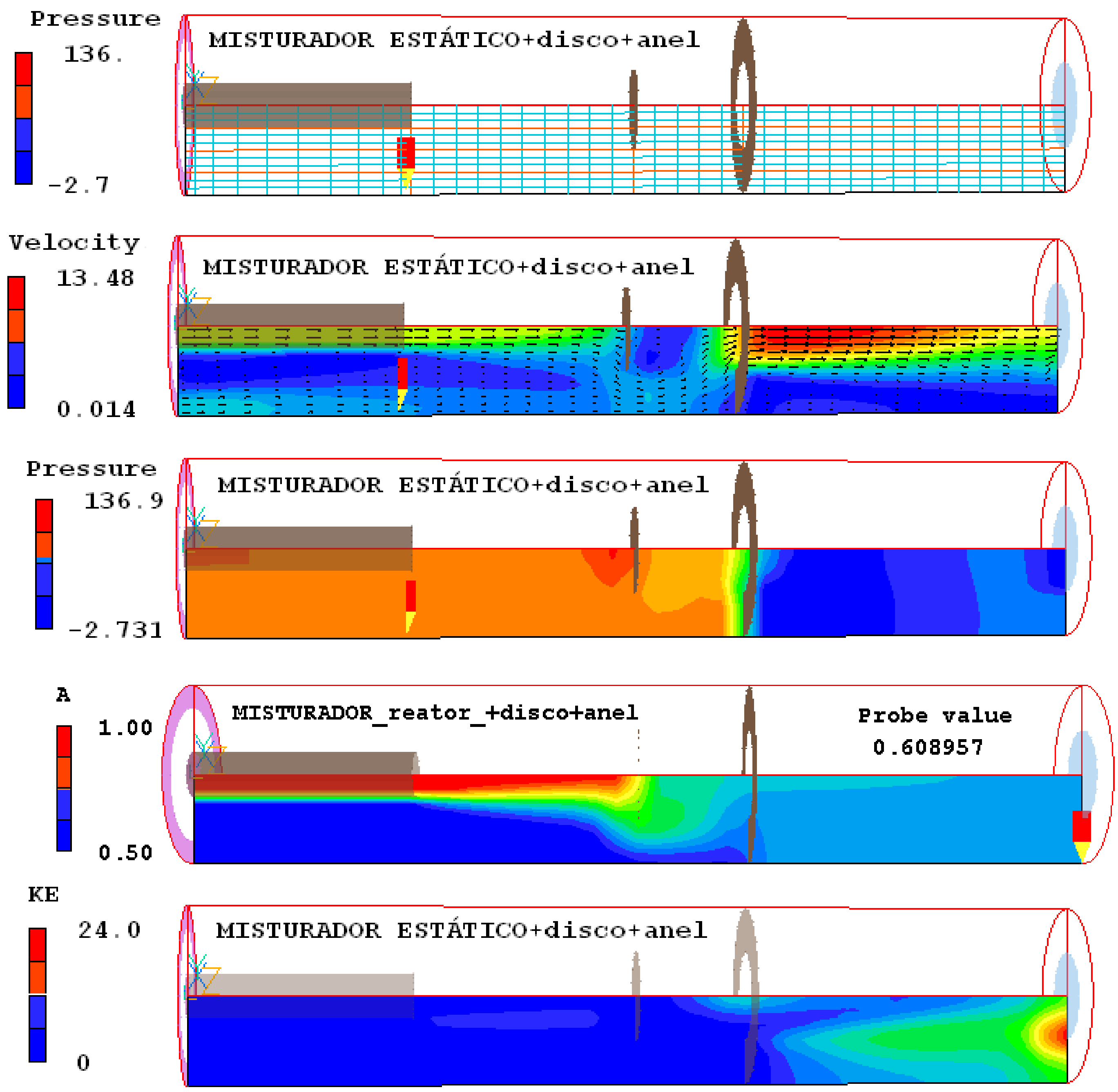

Velocity
8.4
0.1
MISTURADOR ESTÁTICO+DISCO

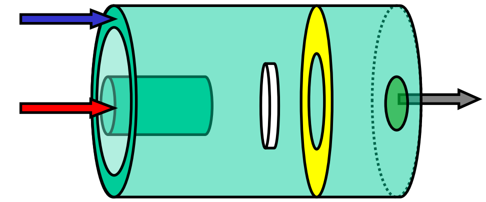

KE
6.9
0
MISTURADOR ESTÁTICO+DISCO


EP
134.
0
MISTURADOR ESTÁTICO+DISCO

Caso 3

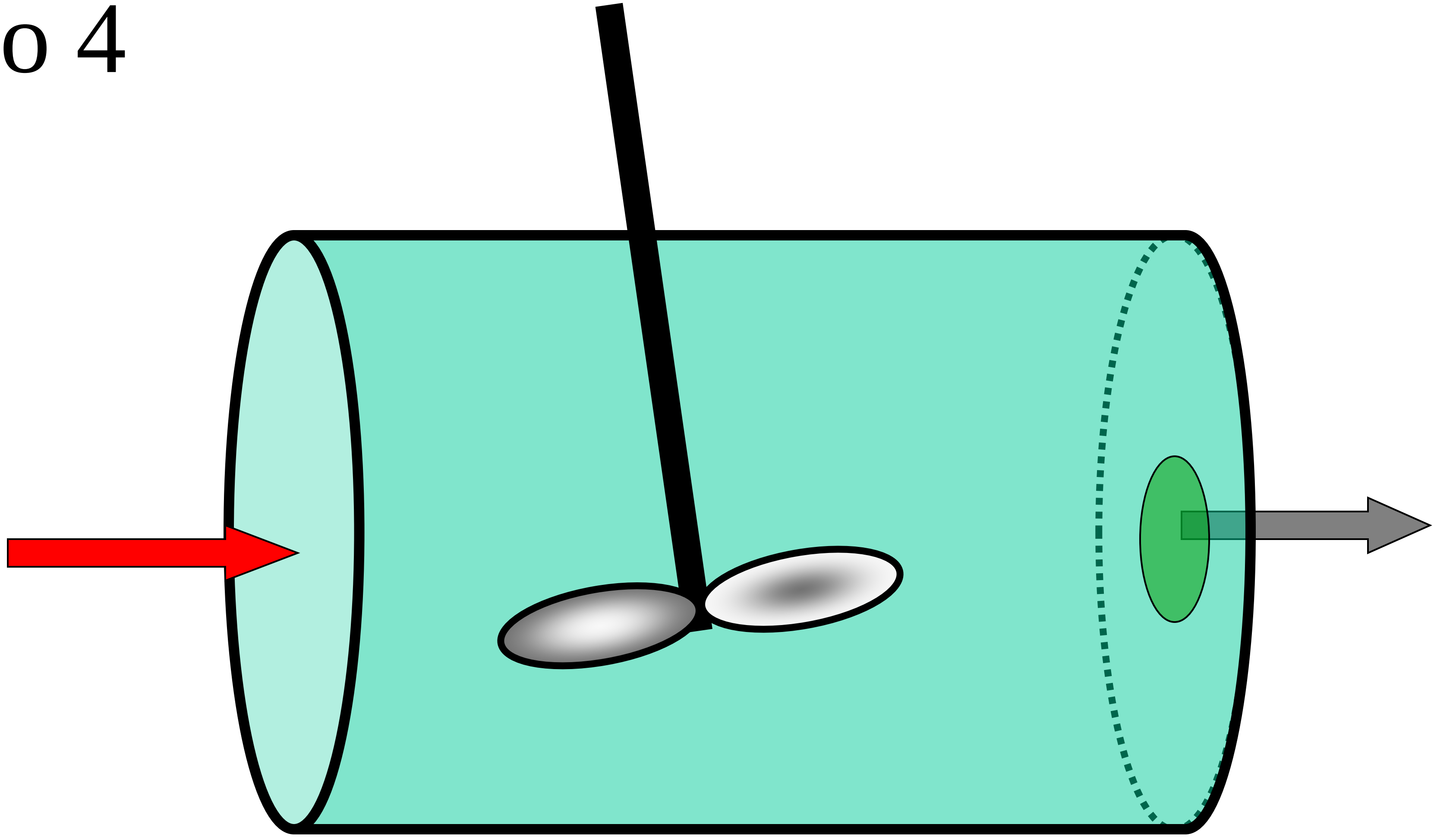



Pressure
136.
-2.7
MISTURADOR ESTÁTICO+disco+anel
Velocity
13.48
0.014
MISTURADOR ESTÁTICO+disco+anel
Pressure
136.9
-2.731
MISTURADOR ESTÁTICO+disco+anel
A
1.00
0.50
MISTURADOR_reator_+disco+anel
Probe value
0.608957
KE
24.0
0
MISTURADOR ESTÁTICO+disco+anel



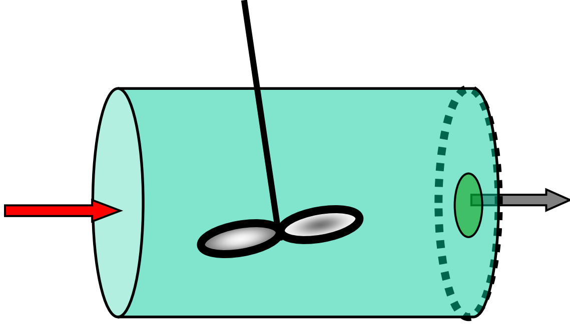
Caso 3

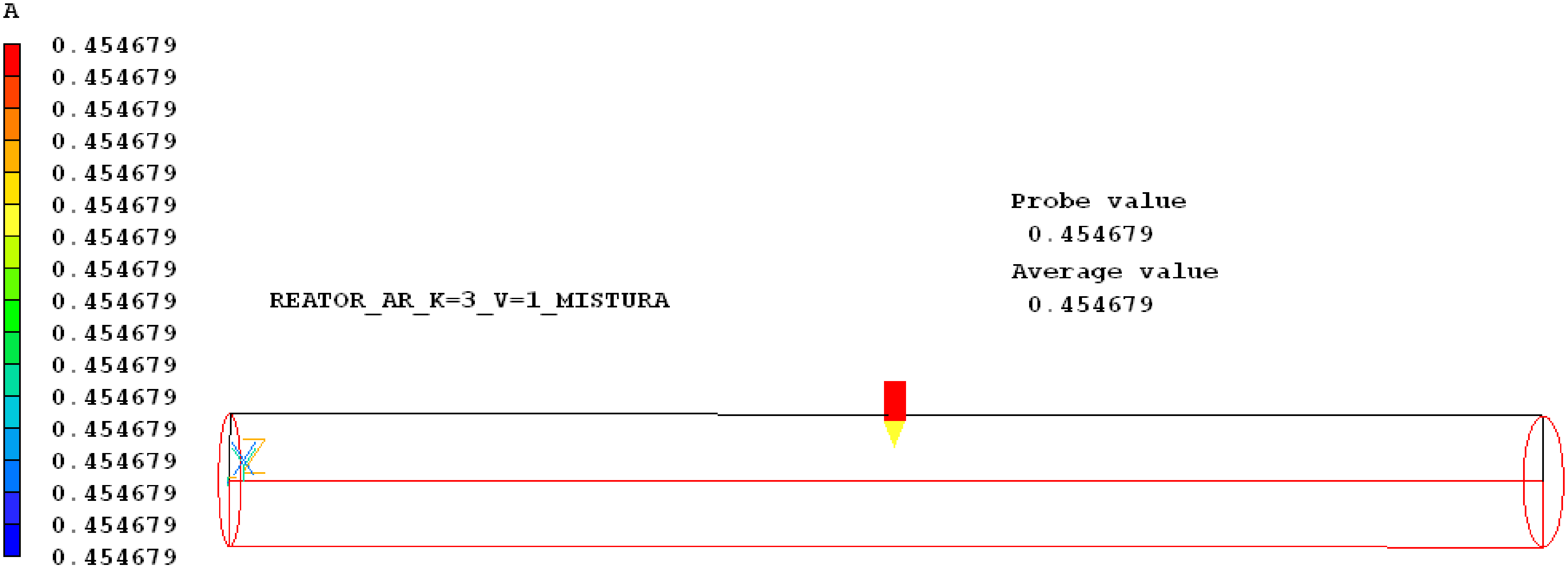
Caso 4



CFSTR

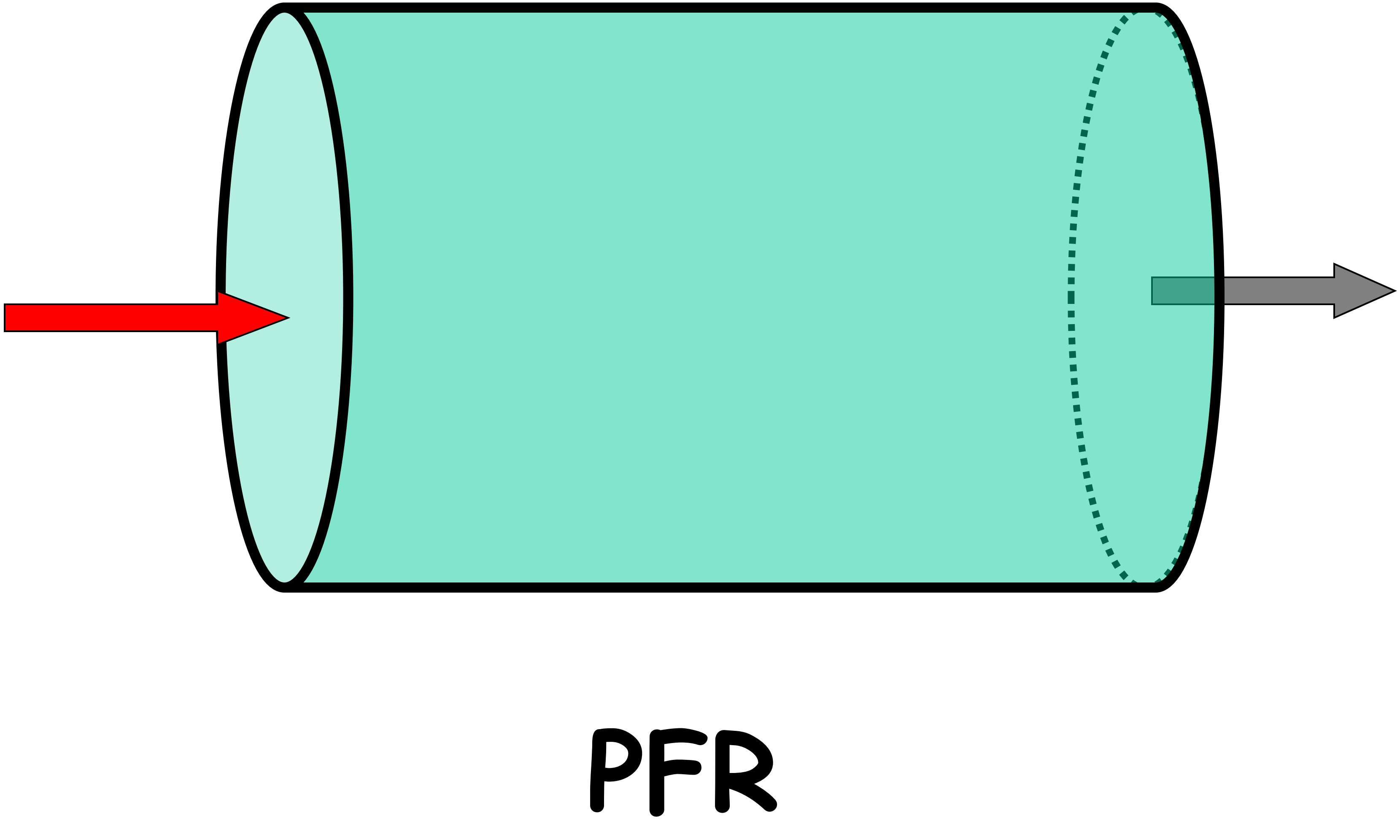
Caso 4




A
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
0.454679
REATOR_AR_K=3_V=1_MISTURA
Probe value
0.454679
Average value
0.454679

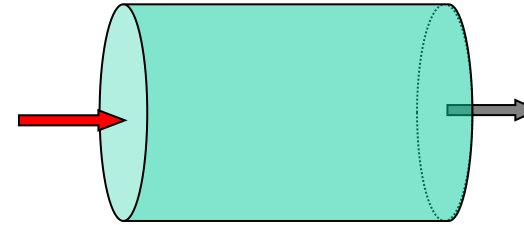
CFSTR

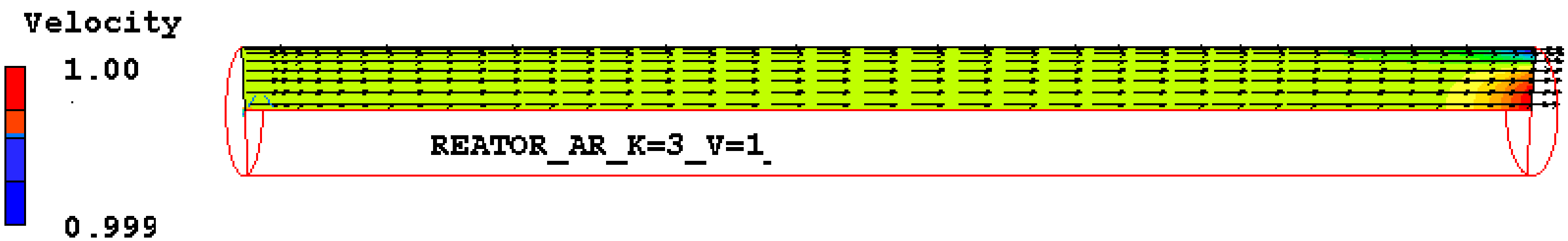
Caso 5

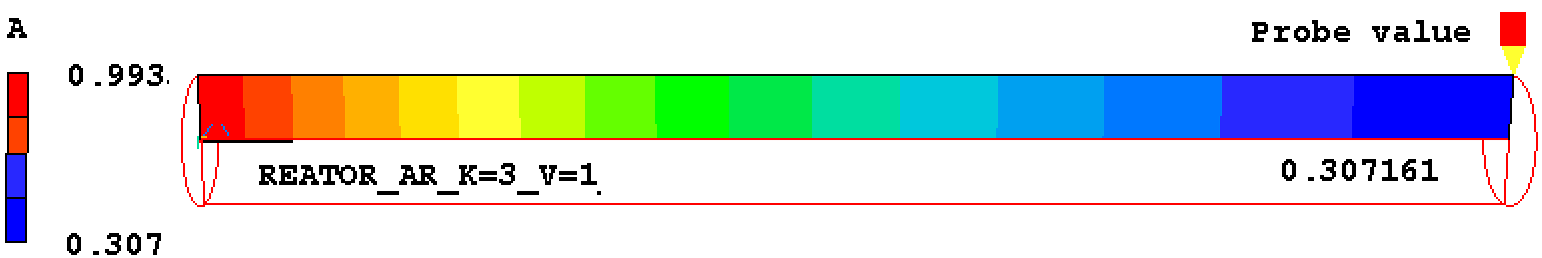


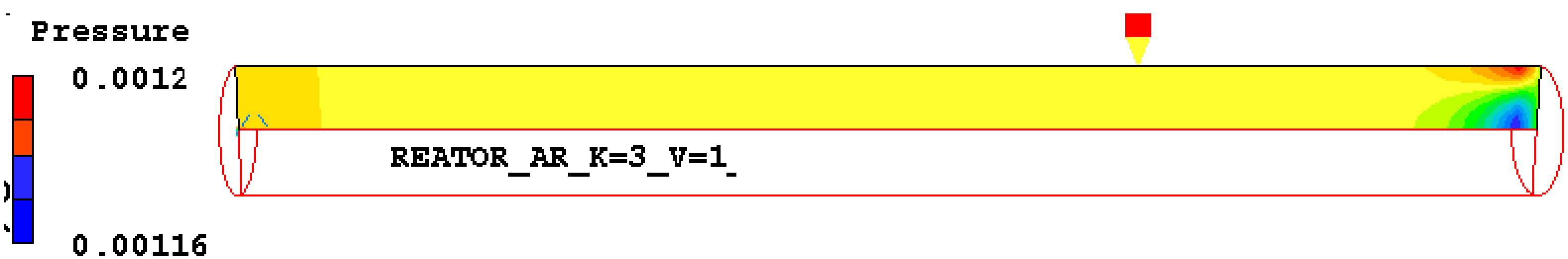
Caso 5

PFR




Velocity
1.00
0.999
REATOR_AR_K=3_V=1


A
0.993
0.307
Probe value
REATOR_AR_K=3_V=1
0.307161

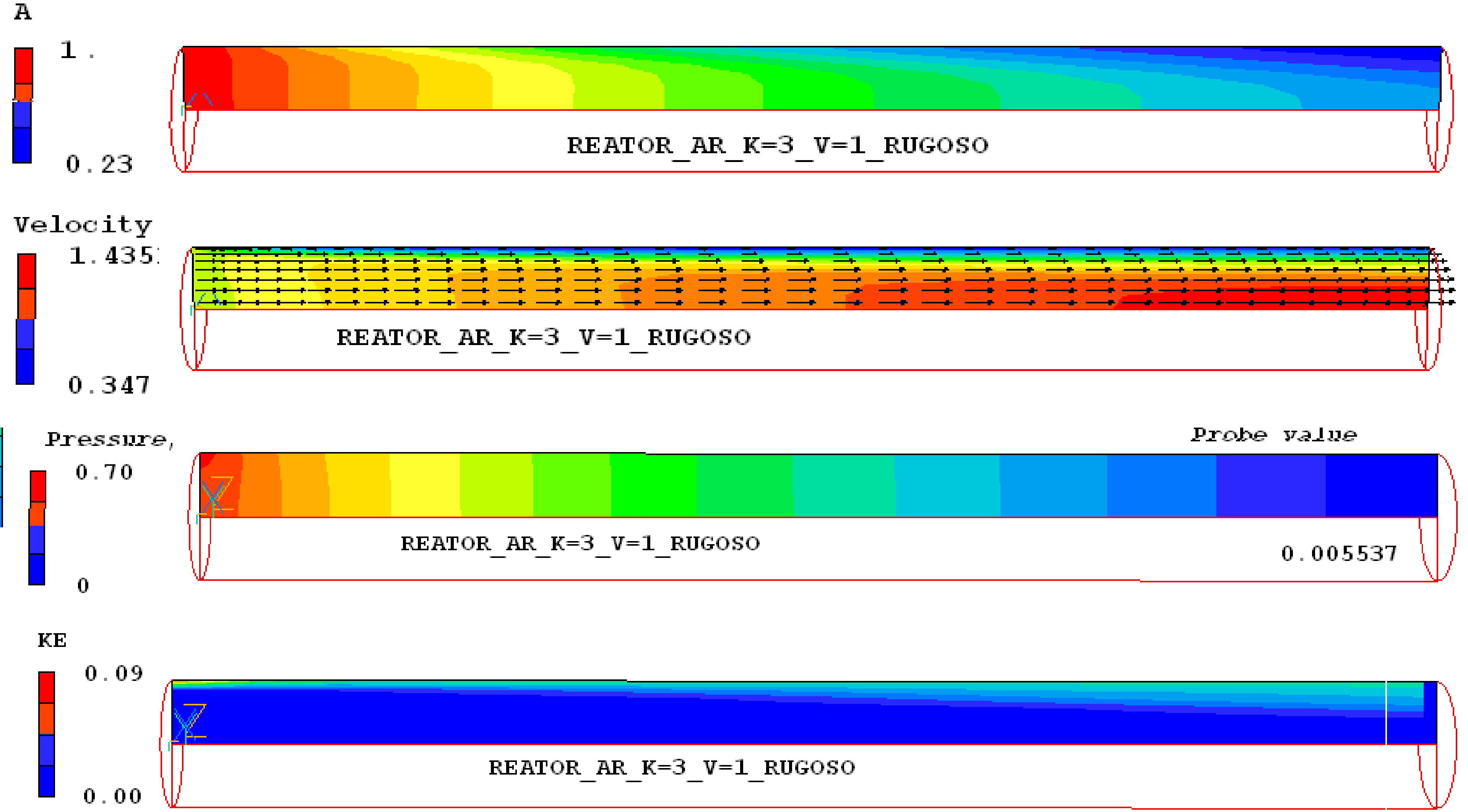

Pressure
0.0012
0.00116
REATOR_AR_K=3_V=1

Caso 6

PFR com atrito na parede

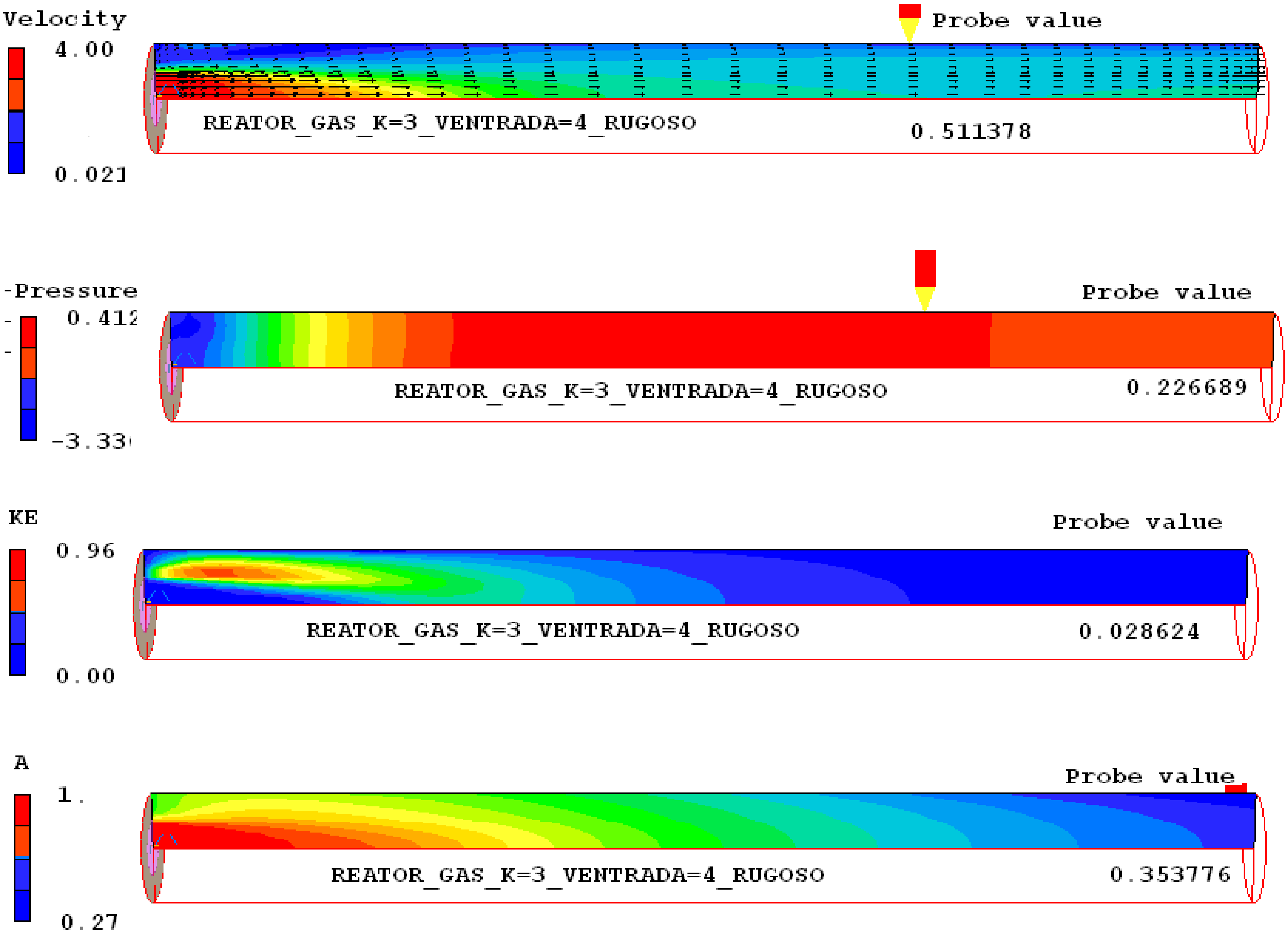
Caso 6

PFR com atrito na parede



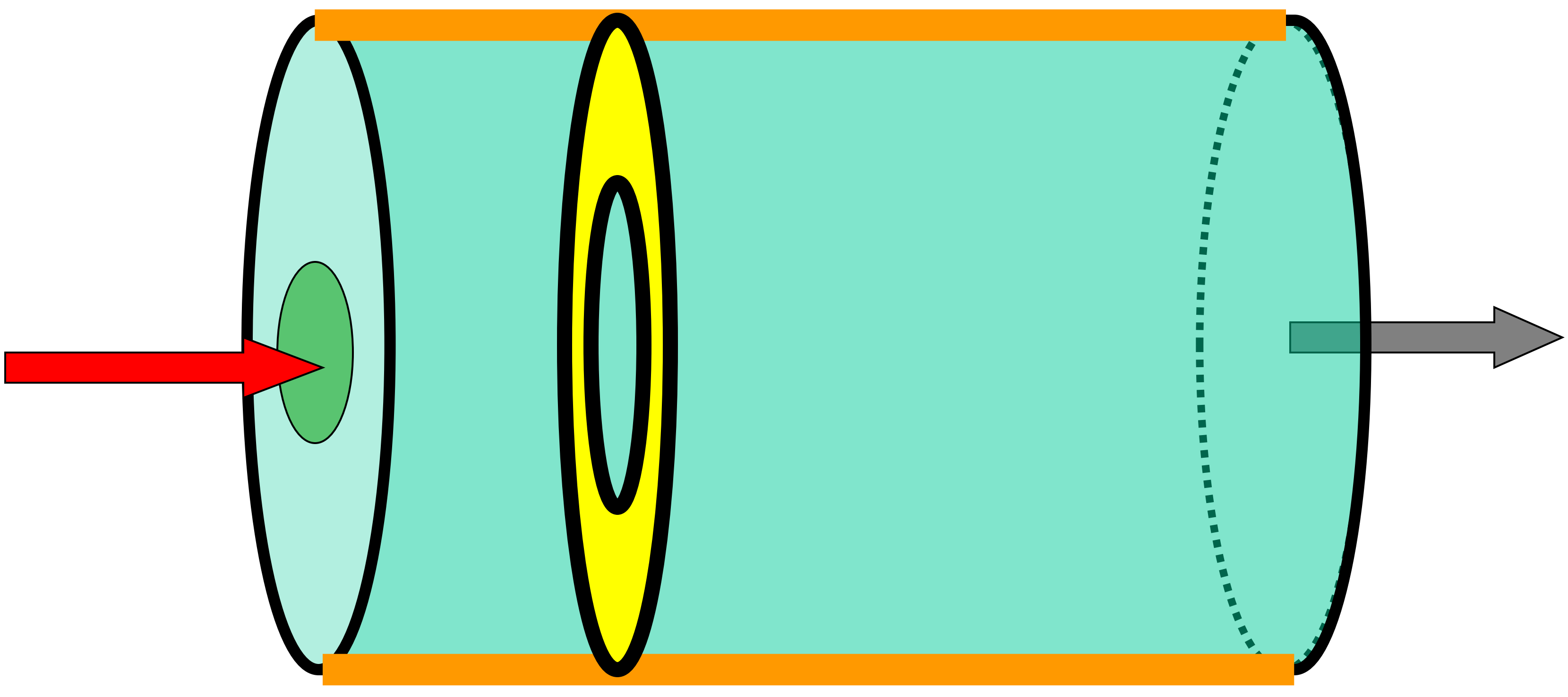
Caso 7

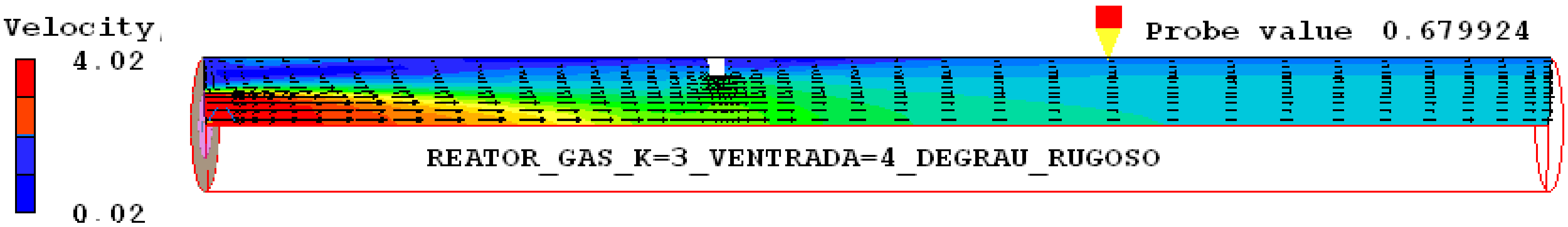
rugoso

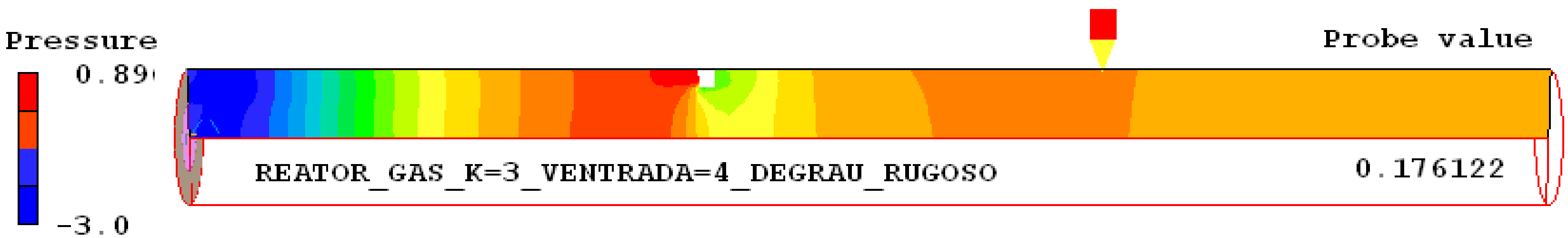

Velocity
4.00
0.021
Probe value
REATOR_GAS_K=3_VENTRADA=4_RUGOSO
0.511378
-Pressure
0.412
-3.33
Probe value
REATOR_GAS_K=3_VENTRADA=4_RUGOSO
0.226689
KE
0.96
0.00
Probe value
REATOR_GAS_K=3_VENTRADA=4_RUGOSO
0.028624
A
1.
0.27
Probe value
REATOR_GAS_K=3_VENTRADA=4_RUGOSO
0.353776

Caso 7

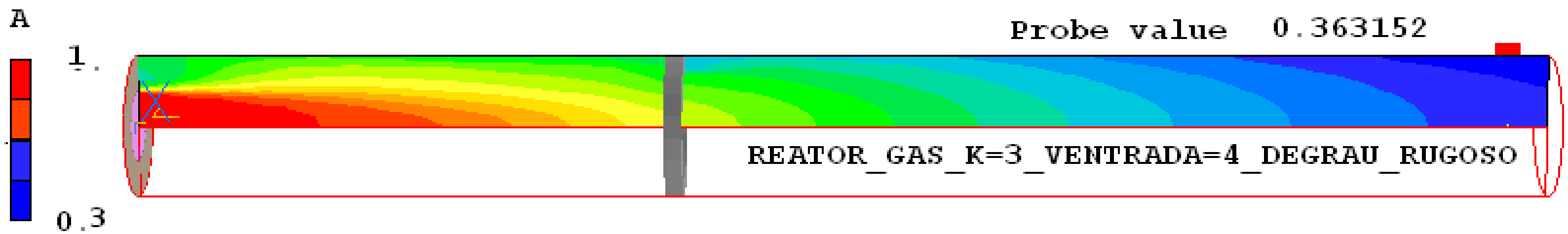
Caso 8

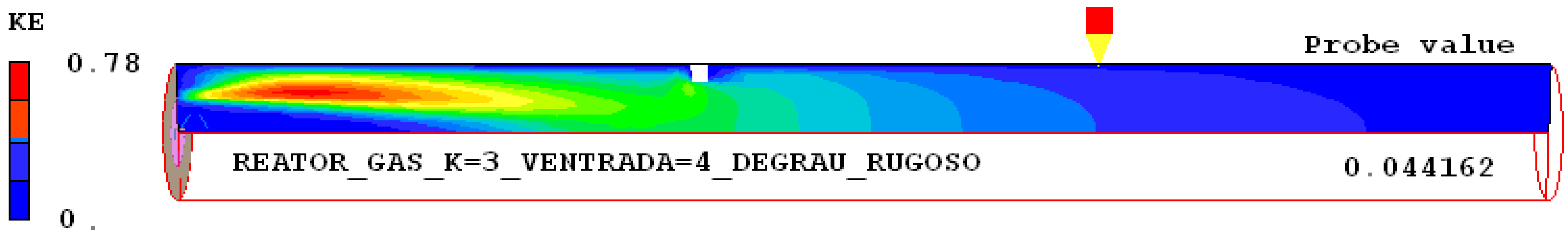



Velocity
4.02
0.02
Probe value 0.679924
REATOR_GAS_K=3_VENTRADA=4_DEGRAU_RUGOSO

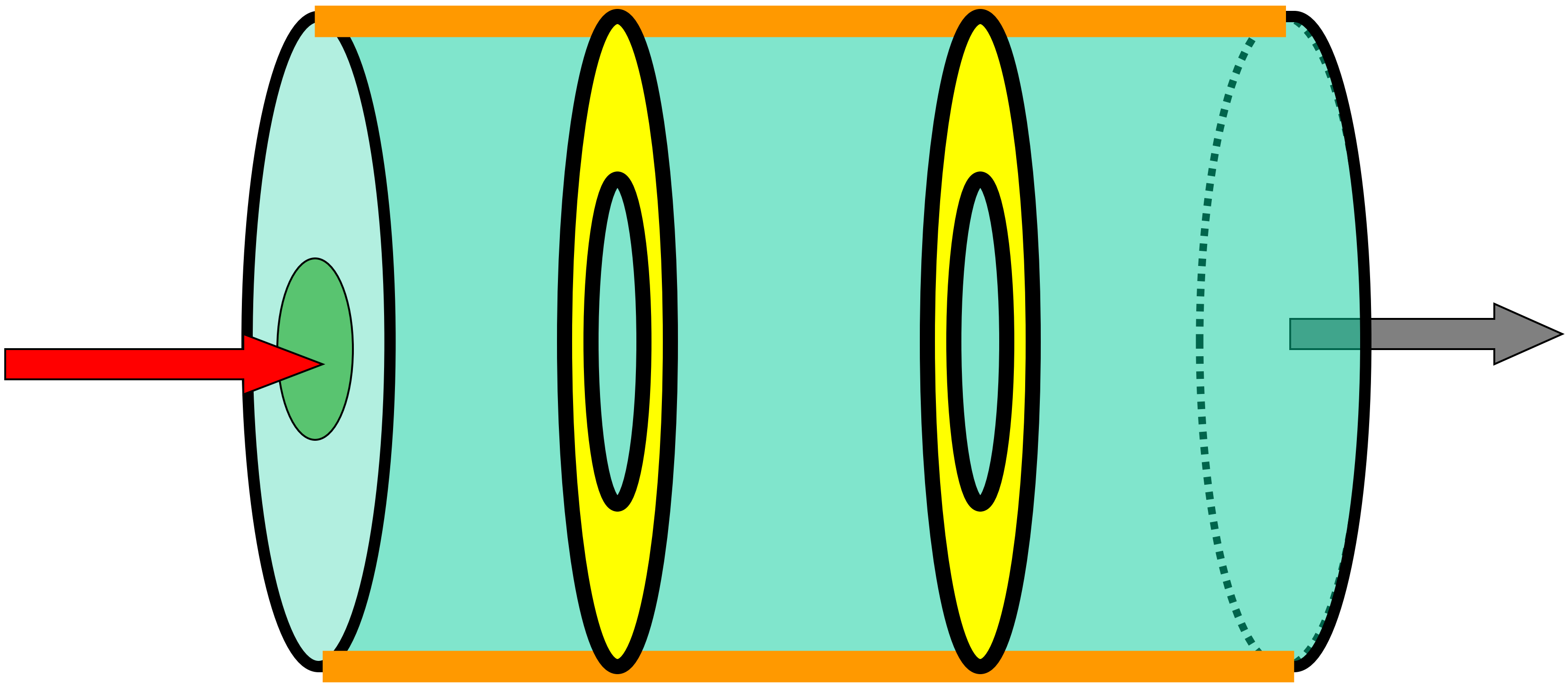

Pressure
0.89
-3.0
Probe value
REATOR_GAS_K=3_VENTRADA=4_DEGRAU_RUGOSO
0.176122

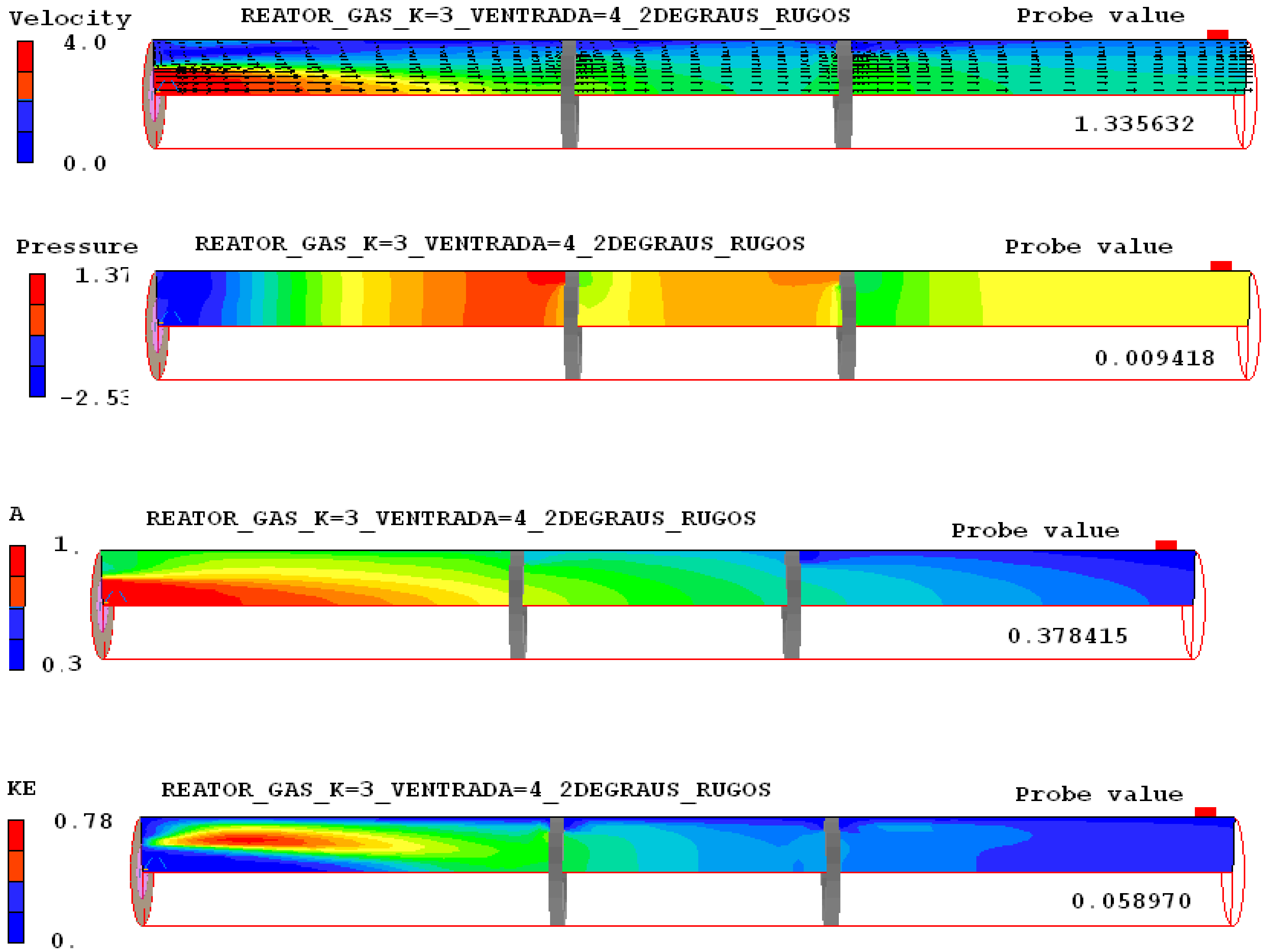
Caso 8


A
1.
0.3
Probe value 0.363152
REATOR_GAS_K=3_VENTRADA=4_DEGRAU_RUGOSO


KE
0.78
0.
Probe value
REATOR_GAS_K=3_VENTRADA=4_DEGRAU_RUGOSO
0.044162

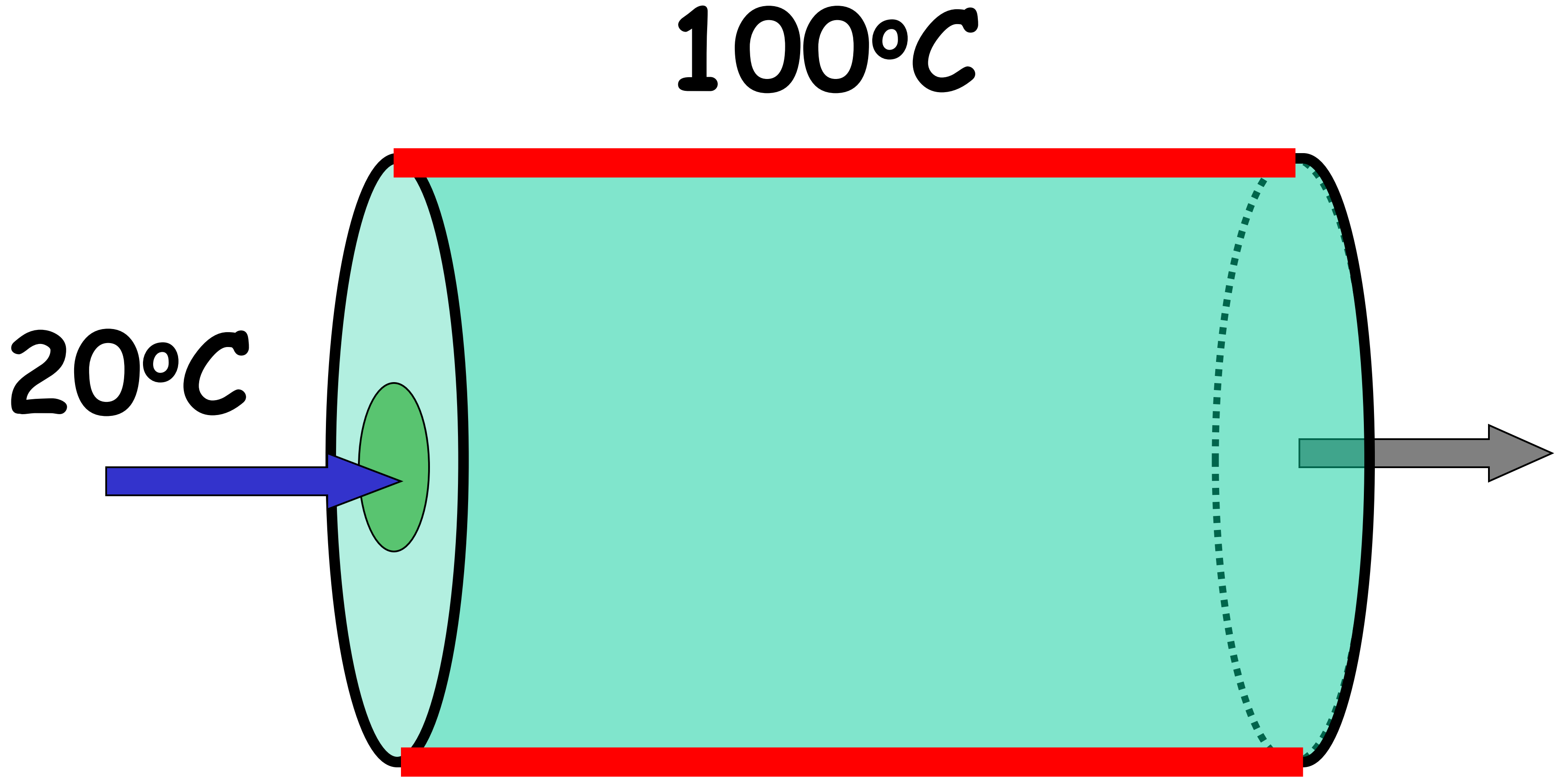
Caso 9



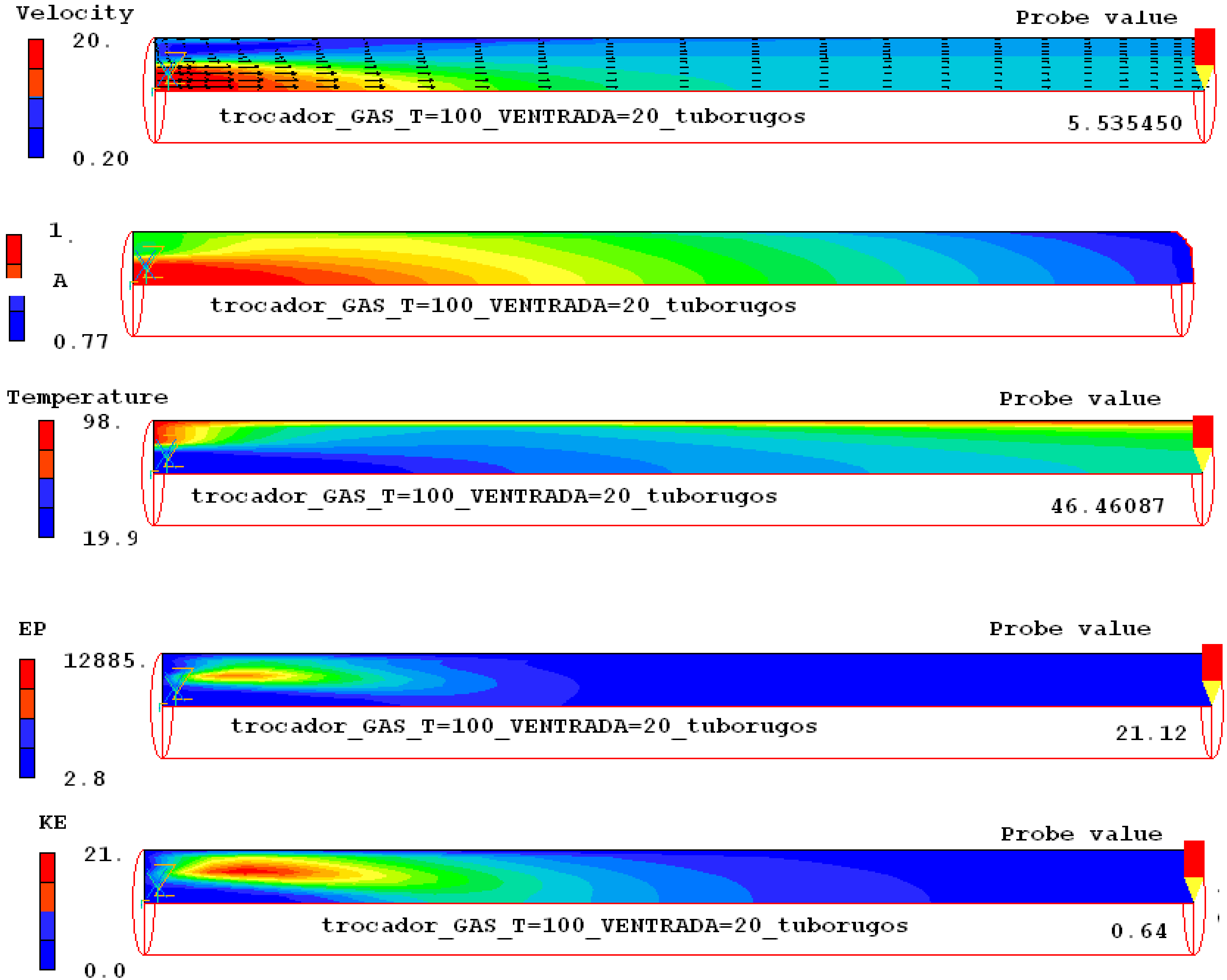

Velocity
4.0
0.0
REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS_RUGOS
Probe value
1.335632
Pressure
1.37
-2.53
REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS_RUGOS
Probe value
0.009418
A
1.
0.3
REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS_RUGOS
Probe value
0.378415
KE
0.78
0.
REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS_RUGOS
Probe value
0.058970

Caso 9

Caso 10

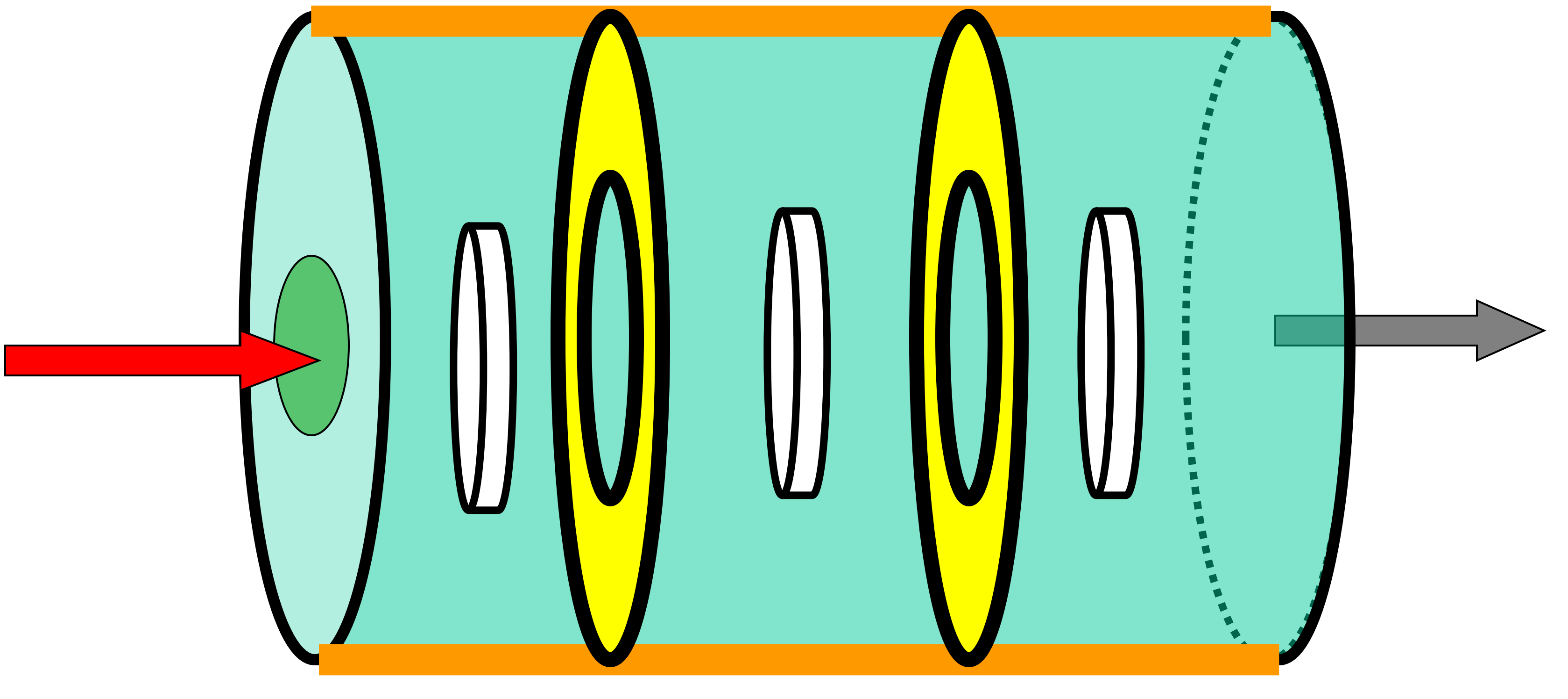


Rugosa & Quente

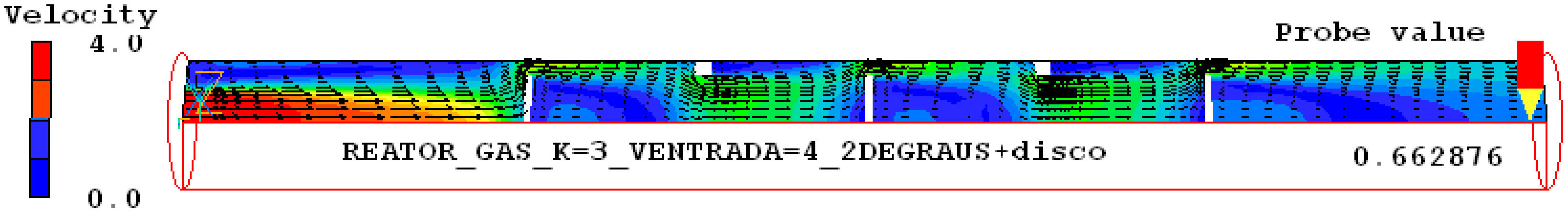

Velocity
20.
0.20
Probe value
trocador_GAS_T=100_VENTRADA=20_tuborugos
5.535450
1.
A
0.77
trocador_GAS_T=100_VENTRADA=20_tuborugos
Temperature
98.
19.9
Probe value
trocador_GAS_T=100_VENTRADA=20_tuborugos
46.46087
EP
12885.
2.8
Probe value
trocador_GAS_T=100_VENTRADA=20_tuborugos
21.12
KE
21.
0.0
Probe value
trocador_GAS_T=100_VENTRADA=20_tuborugos
0.64

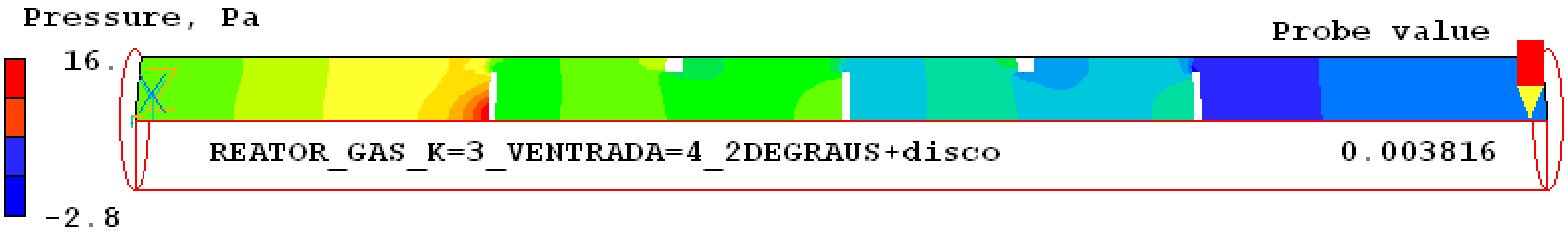
Caso 10

Caso 11

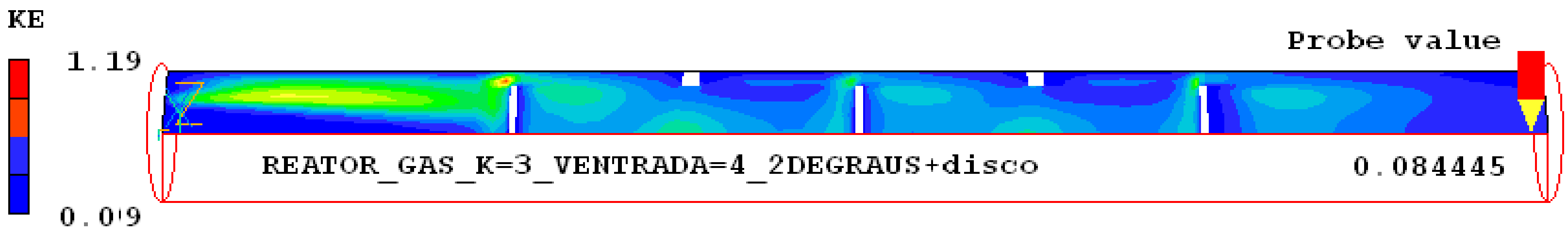


Caso 11

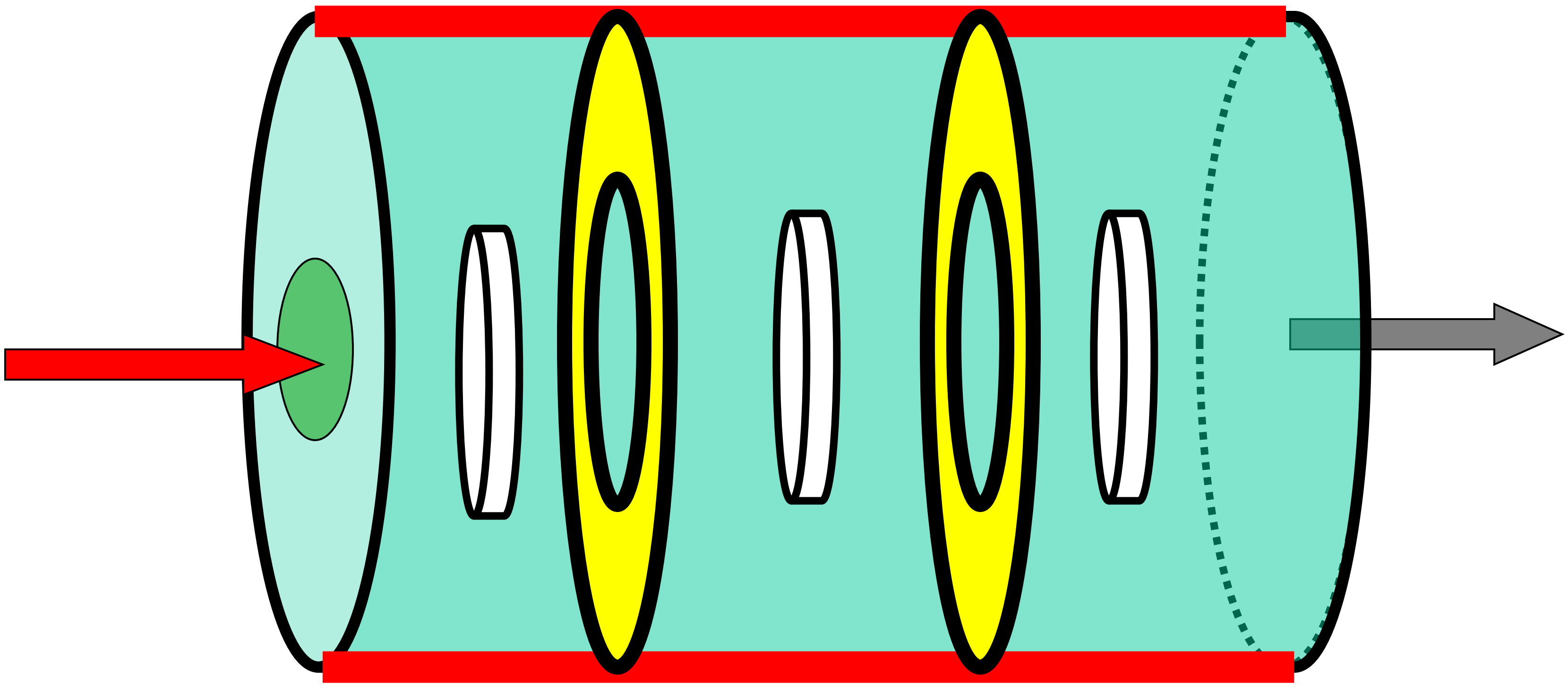

Velocity
4.0
0.0
Probe value
REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS+disco
0.662876


Pressure, Pa
16.
-2.8
Probe value
REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS+disco
0.003816

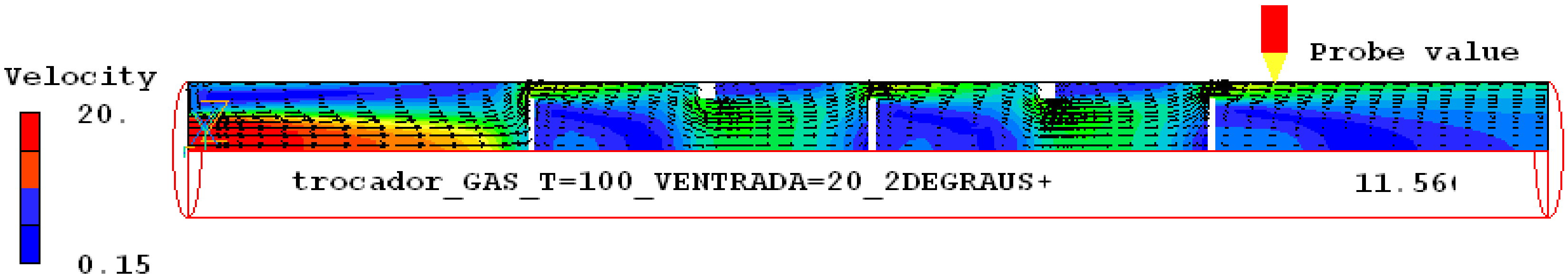

REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS+disco

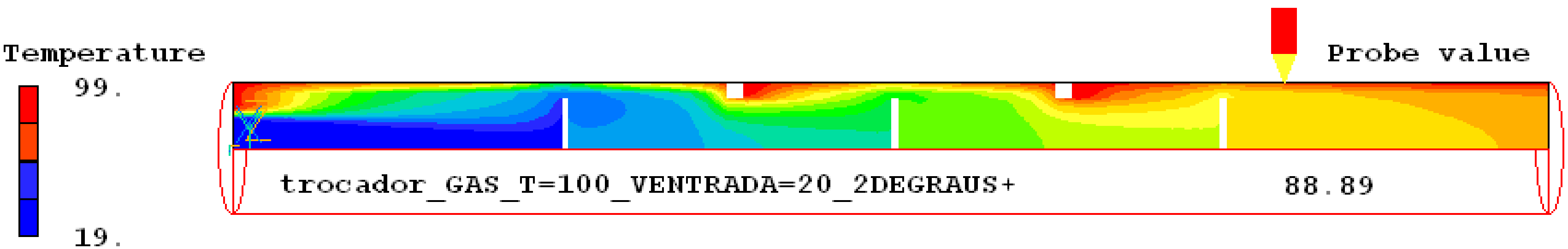

KE
1.19
0.09
Probe value
REATOR_GAS_K=3_VENTRADA=4_2DEGRAUS+disco
0.084445

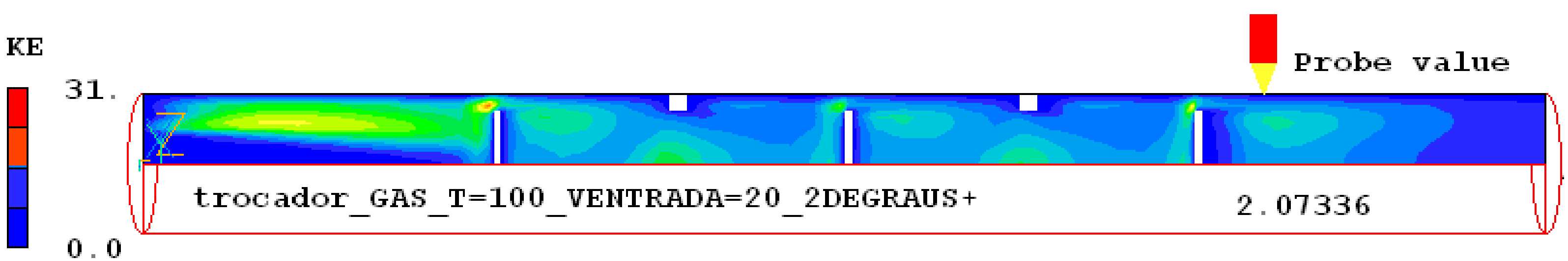
Caso 12



Rugosa & Quente


Probe value
Velocity
20.
0.15
trocador_GAS_T=100_VENTRADA=20_2DEGRAUS+
11.56


Probe value
Temperature
99.
19.
trocador_GAS_T=100_VENTRADA=20_2DEGRAUS+
88.89


Probe value
KE
31.
0.0
trocador_GAS_T=100_VENTRADA=20_2DEGRAUS+
2.07336

Caso 12