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A flow and transport model for low-temperature gaseous nitrocarburizing of stainless steels

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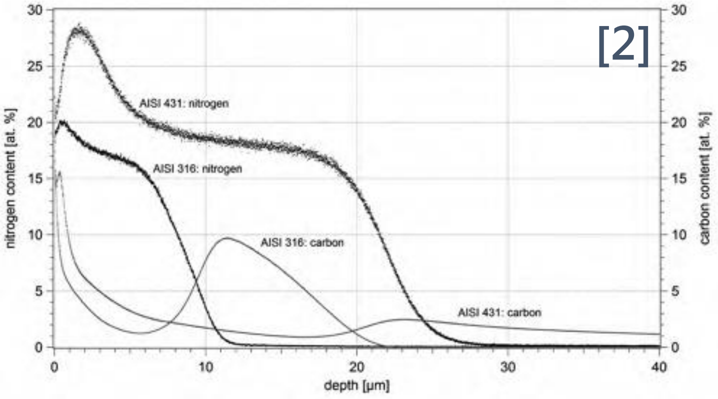
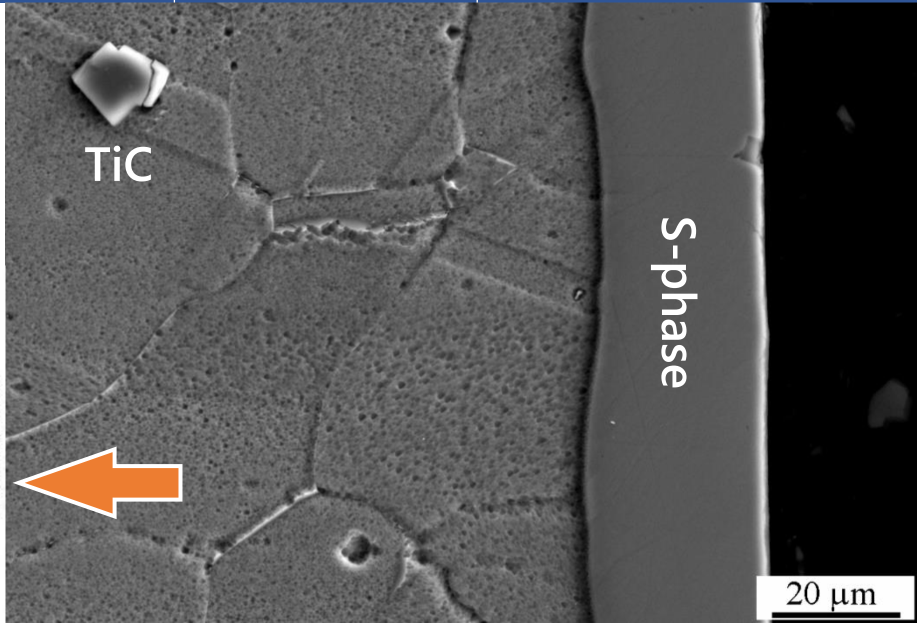
Austenitic Stainless Steel

DIN	1.4301	1.4305	1.4404	1.4541	1.4571
AISI	304	303	316L	321	316Ti

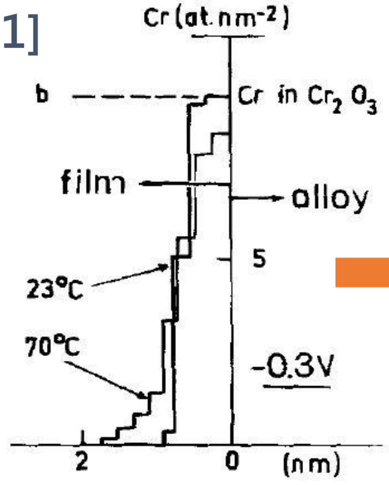




Nitrocarburized 316Ti alloy

Passive Film

[1]



Antipassivation

$\boxed{C_2H_2} > CO > C_2H_4 > C_4H_{10} > C_3H_8 > CO_2$

+

NH_3 and H_2

+

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[1] Lorang, G., et al. *J. Electrochem. Soc.* 141.12 (1994): 3347-3356.

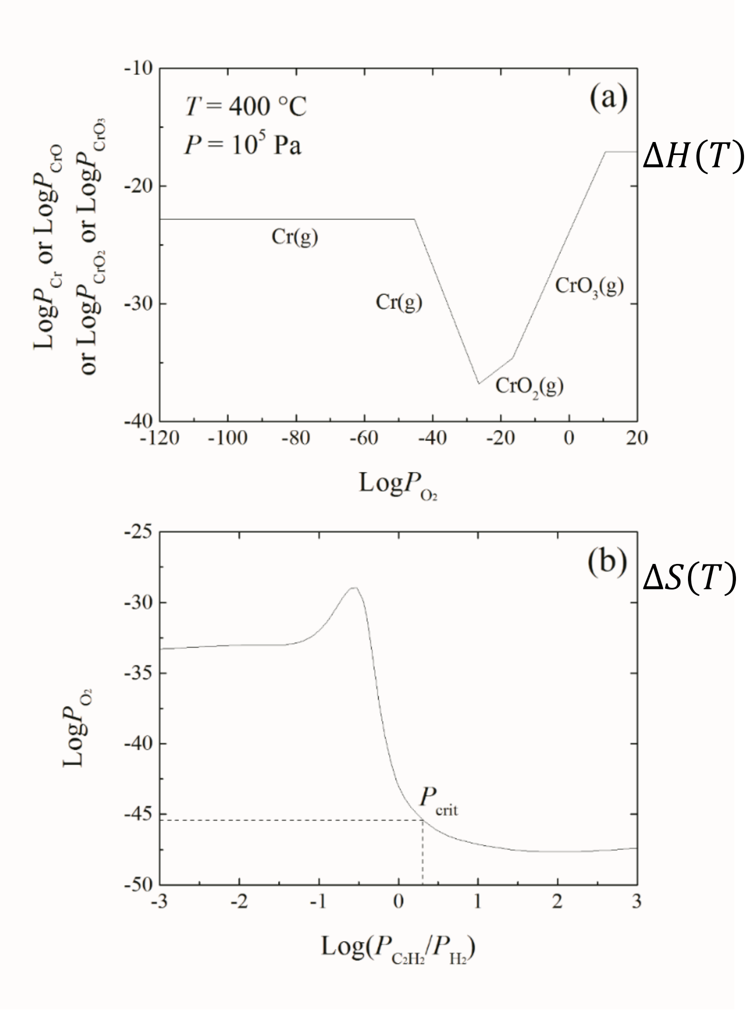
[2] Christiansen, T. L. and Somers, M. A, *HTM*, 66(2011)2:109-115

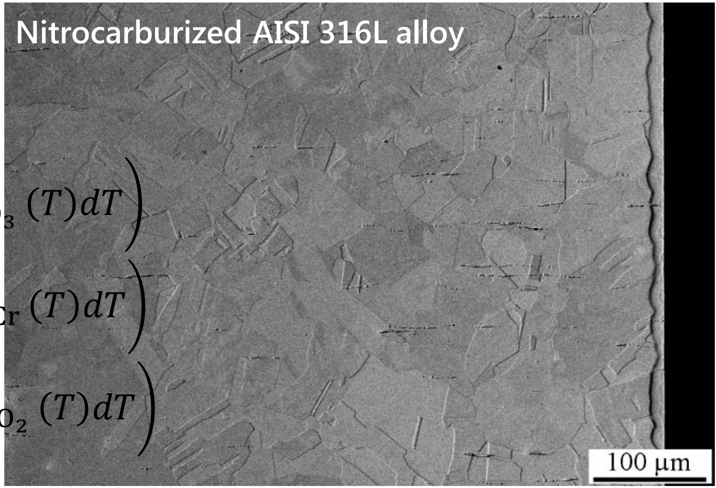
P_{Crit}

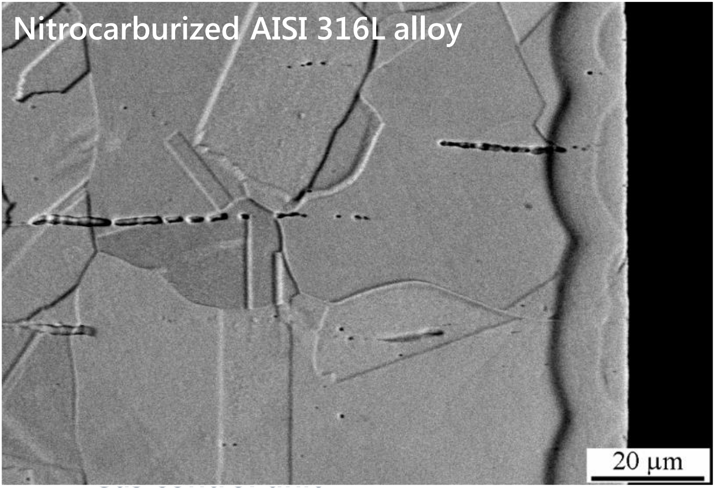
$$\Delta G(T) = \Delta H(T) - T\Delta S(T)$$
$$= -2.303RT\log K(T)$$

$$\Delta H(T) = \left(\Delta H^{O}_{f\mathrm{Cr_2O_3}} + \int_{298.15}^{T} C_{P\mathrm{Cr_2O_3}}(T)dT\right) - 2\left(\Delta H^{O}_{f\mathrm{Cr}} + \int_{298.15}^{T} C_{P\mathrm{Cr}}(T)dT\right) - \frac{3}{2}\left(\Delta H^{O}_{f\mathrm{O_2}} + \int_{298.15}^{T} C_{P\mathrm{O_2}}(T)dT\right)$$

$$\Delta S(T) = \left(\Delta S^{O}_{f\mathrm{Cr_2O_3}} + \int_{298.15}^{T} \frac{C_{P\mathrm{Cr_2O_3}}}{T}\right.$$
$$- 2\left(\Delta S^{O}_{f\mathrm{Cr}} + \int_{298.15}^{T} C_{PC}\right.$$
$$- \frac{3}{2}\left(\Delta S^{O}_{f\mathrm{O_2}} + \int_{298.15}^{T} C_{PC}\right.$$

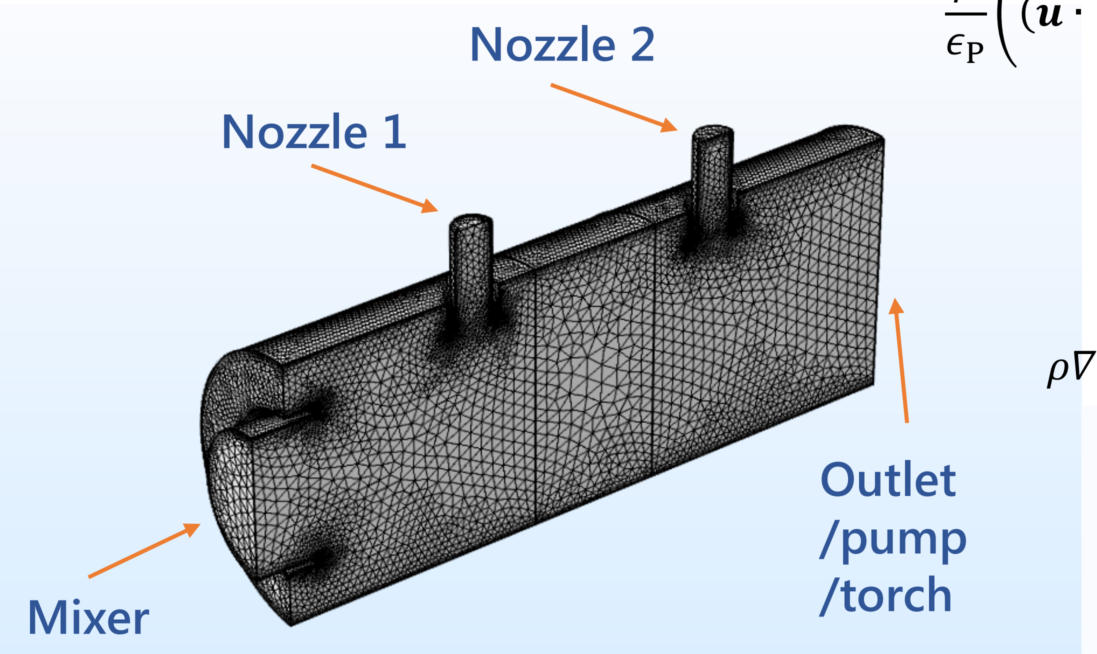






The thermodynamic data for this work were primarily obtained from SpringerMaterials.

Geometry & Meshes

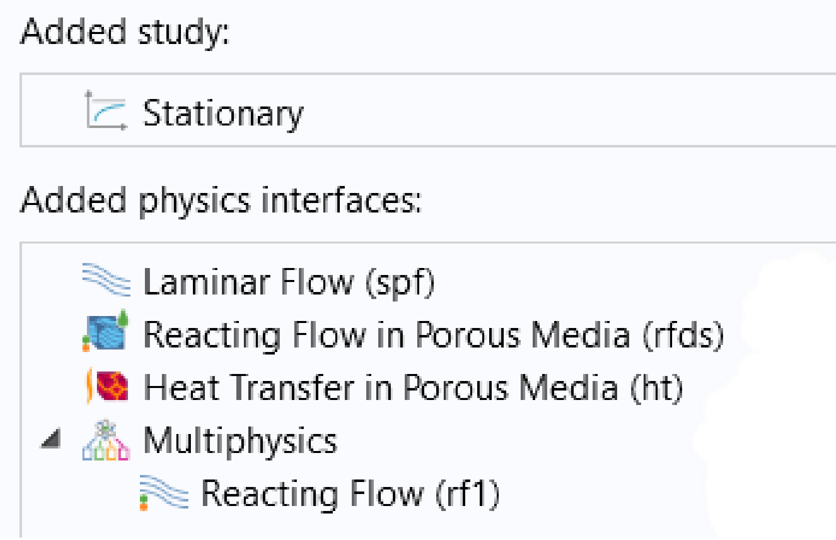


$$\frac{\rho}{\epsilon_{\mathrm{P}}}\left((\boldsymbol{u}\cdot\nabla)\frac{\boldsymbol{u}}{\epsilon_{\mathrm{P}}}\right)$$

$$= \nabla\cdot\left[-pI+\frac{\mu}{\varepsilon_{\mathrm{P}}}\left(\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^{T}\right)-\frac{2\mu}{3\epsilon_{\mathrm{P}}}(\nabla\cdot\boldsymbol{u})\right.$$

$$-\left(\frac{\mu}{\kappa}+\beta_{\mathrm{F}}|\boldsymbol{u}|+\frac{Q_{\mathrm{br}}}{\epsilon_{\mathrm{P}}^{2}}\right)\boldsymbol{u}+\boldsymbol{F}$$

$$\rho\nabla\cdot\boldsymbol{u}=Q_{\mathrm{br}}$$



Added study:

Stationary

Added physics interfaces:

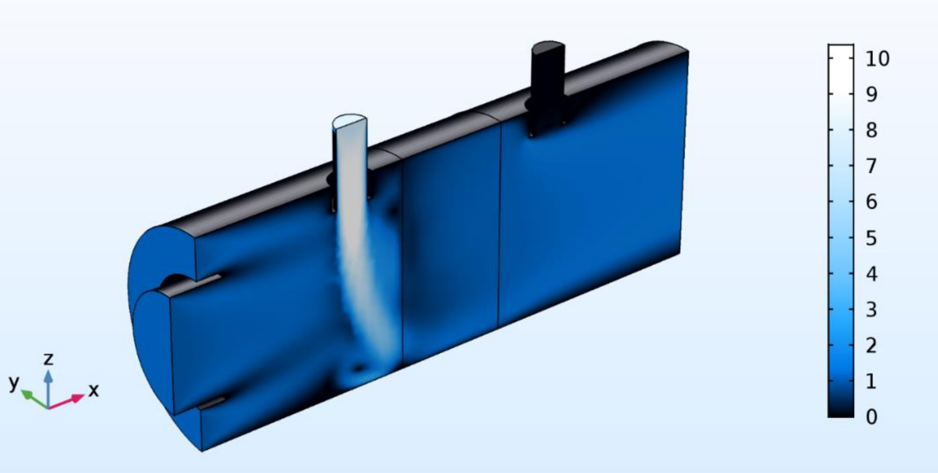
- Laminar Flow (spf)
- Reacting Flow in Porous Media (rfds)
- Heat Transfer in Porous Media (ht)
- Multiphysics
  - Reacting Flow (rf1)

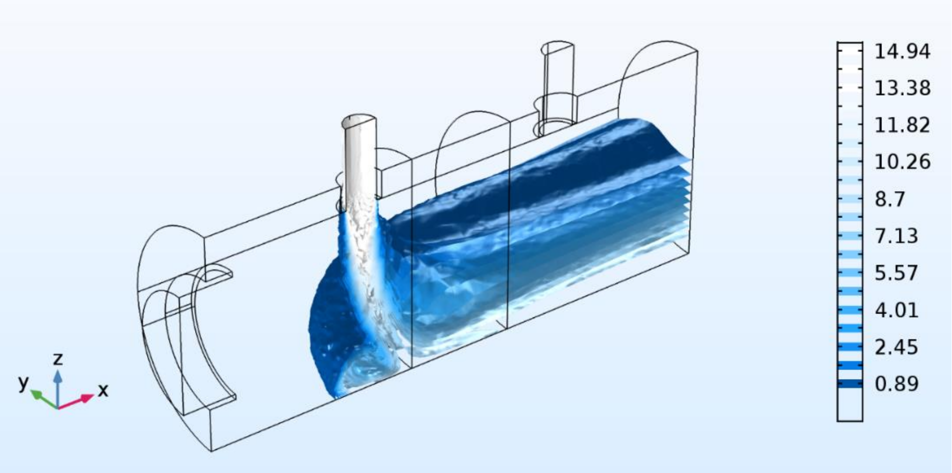
Numeric Models

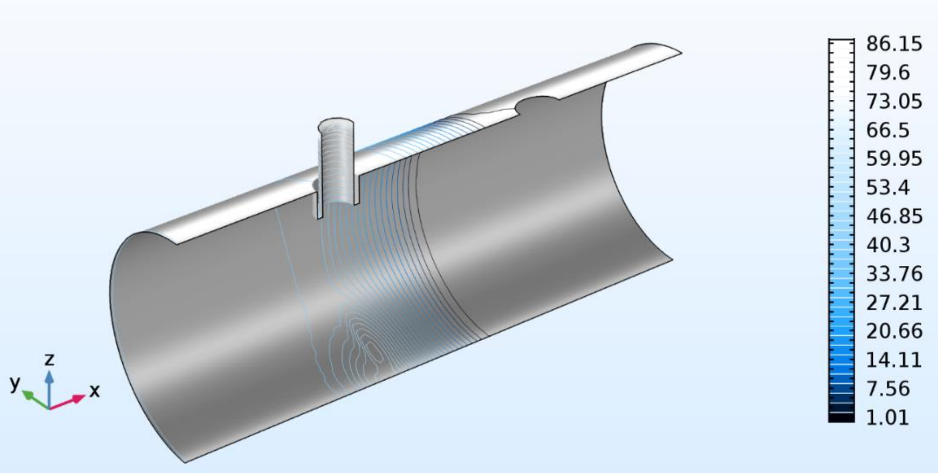
$$\frac{\partial c}{\partial t}+\nabla\cdot(-D\nabla c)+\boldsymbol{u}\cdot\nabla c=R_i$$

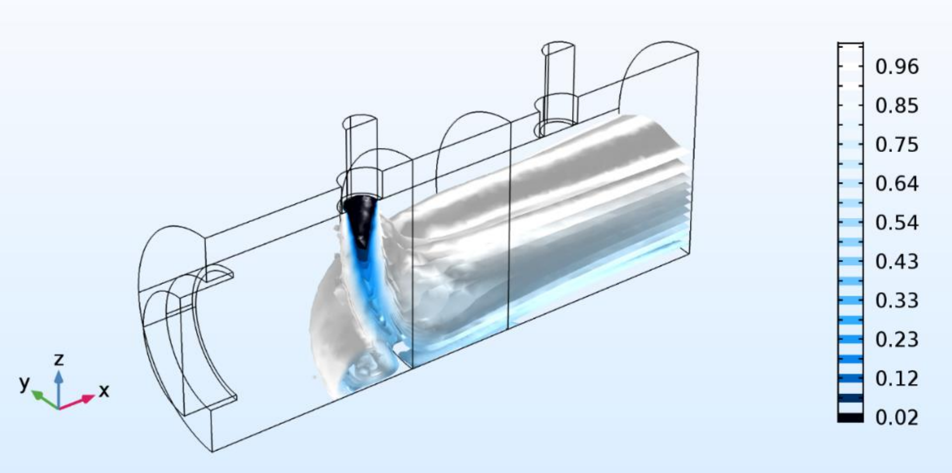
$$\rho C_P\left(\frac{\partial T}{\partial t}+\boldsymbol{u}\cdot\nabla T\right)=\nabla\cdot(\kappa\nabla T)$$

$$\rho\left(\frac{\partial\boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)=-\nabla p+\nabla\cdot\left(\mu\left(\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^{T}\right)\right)\qquad\nabla\cdot\boldsymbol{u}=0$$


Surface: Velocity magnitude (m/s)


Isosurface: Concentration (mol/m^3)


Surface: 1 (1) Contour: Pressure (Pa)

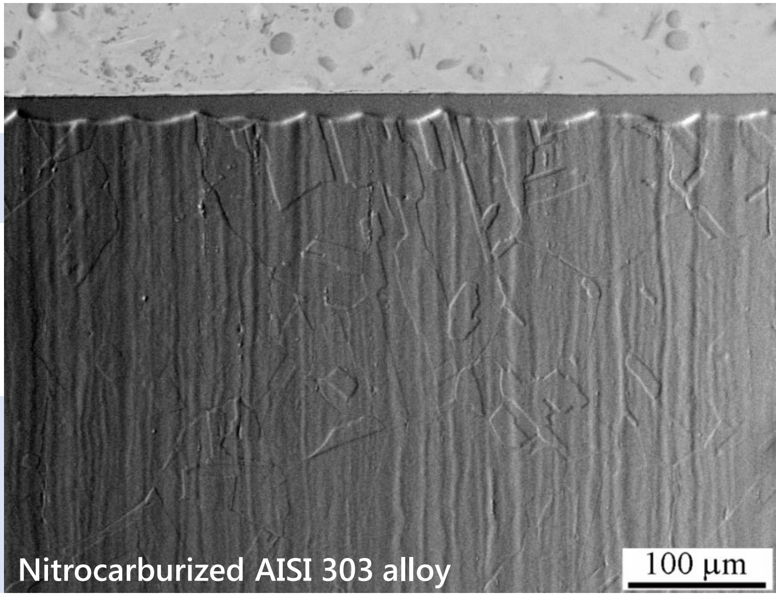

Isosurface: Concentration (mol/m^3)

I. With simple physical modules, fluid flow and transport inside the furnace cell can be evaluated.

II. The purge and pulse cycles can be better controlled.

III. The applicable process parameters can be converted from thermodynamic calculations via numeric simulations.

IV. COMSOL Multiphysics® is a powerful tool to understand thermochemical processes in the heat treatment industry.



Thank you for your attention!

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AiF Forschungsnetzwerk Mittelstand

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