# Homogeneous Vapour Condensation of Combustion Products in Boundary Layer Flows

## Numerical Solution of a Thermophysical Model and a Singular Perturbation Approach

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# Motivation and subject

Relatively cold surfaces exposed to hot gases carrying mixtures of suspended particles and condensible vapors produced by combustion are fouled and corroded by condensate deposition

Consider the case of negligibly few particles compared to dilute condensible vapors

## Context

1. Clean hot gas containing condensible vapor is subject to stagnation point boundary layer flow near a cold wall.
2. Very close to the wall, vapor molecules start to nucleate producing the seeds for further condensation of vapor.
3. Wall temperature $T_w$ is fixed and smaller than bulk temperature of the gas $T_\infty$.
4. Far from the wall the vapor has a constant bulk density $c_\infty$

# Delimiting the problem

## In general

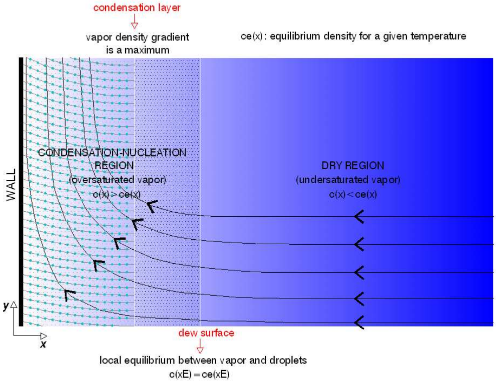
1. Incompressibility of the carrier gas ($800K \leq T_w \leq 1200K$).
2. No dependence of gas density, gas kinematic viscosity $\nu$ and vapor diffusivity $D$ with temperature. Temperature and velocity fields are uncoupled. Temperature field $T(x)$ satisfies a convection-diffusion boundary value problem, and velocity field $u(x)$ satisfies the incompressible Navier-Stokes equations.
3. No Soret effect
4. No Dufour effect

## Specifically

1. Time independence
2. Monodisperse distribution of clusters
3. Clusters move towards the wall due to the gas flow and termophoresis. Thermophoretical velocity in the direction of decreasing temperature is $-\alpha\nu\frac{\nabla\tilde{T}(\tilde{x})}{\tilde{T}(\tilde{x})}$ with $\alpha$ assumed to be constant.
4. Vapor is so dilute that temperature and velocity fields are not affected by the nucleation-condensation process

# Model description

## A stagnation point boundary layer flow is considered




Condensation layer $(x = x_{\mathcal{F}})$ is detached from the dew surface $(x = x_{\mathcal{E}})$

At the dew surface nucleation and condensation are both possible, but condensation cannot proceed unless a previous nucleation has created droplets

# Temperature $T$ and velocity $u$

## Non-dimensional equations

$$P_r u T'' = T'$$

$B.C.: \; T(x=0) = T_w/T_\infty; \; T(x=\infty) = 1$

$$u''' + uu'' + 1 - (u')^2 = 0$$

$B.C.: \; u(x=0) = u'(x=0) = 0; \; u'(x=\infty) = 1$

$[x] = \sqrt{\dfrac{\nu}{\gamma}}$; $\gamma$: strain rate of flow; $[u] = \sqrt{\gamma\nu}$; $[T] = T_\infty = 1713\ K$

Units for nondimensionalization

## Non-dimensional equations

$$c'' + S_c\, u\, c' = \left[ A c^2 n_{cr} \exp\left(\frac{-\sigma^3}{2\eta^2}\right) + B(c - c_e)\rho T^{1/2} n^{2/3} H_n \right] H_c$$

$$\eta = \ln\left(\frac{c}{c_e}\right)$$

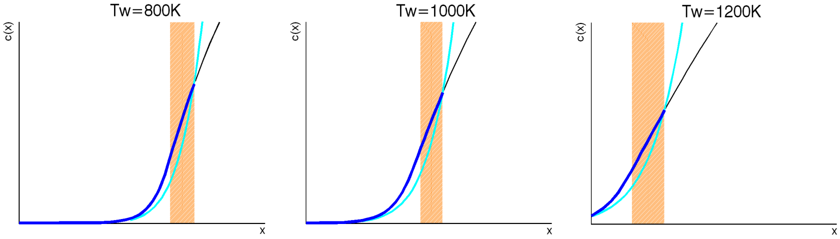
$$U\rho' + \alpha\left(\frac{T'}{T}\right)'\rho = -Lc^2 \exp\left(\frac{-\sigma^3}{2\eta^2}\right) H_c$$

$$Un' = -N(c - c_e) T^{1/2} n^{2/3} H_n H_c$$

B.C.: $c(x=0) = c_e(x=0)$; $c(x=\infty) = 1$; $\rho(x \geq x_E) = 0$; $n(x \geq x_E) = 1$

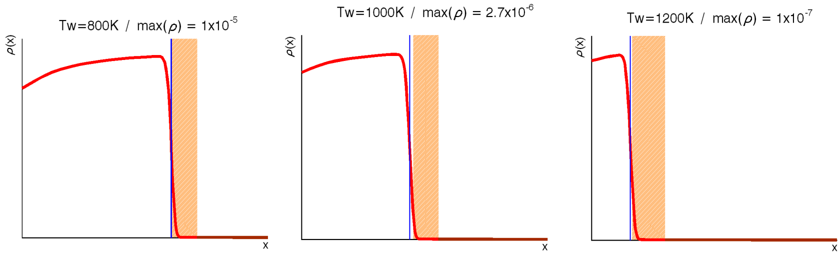
$[c] = c_\infty = 1.9 \times 10^{13}\ cm^3$; $[n] = 1$; $[\rho] = c_\infty$

Units for nondimensionalization




- Left boundary of the orange strip represents the condensation layer or inflexion point, $x = x_F$
- Right boundary of the orange strip represents the dew surface or equilibrium point, $x = x_E$
- The whole strip represents the zone of increasing nucleation process

The maximum wall temperature at which there is a condensation layer is $1293K$




The blue line represents the maximum of the nucleation rate

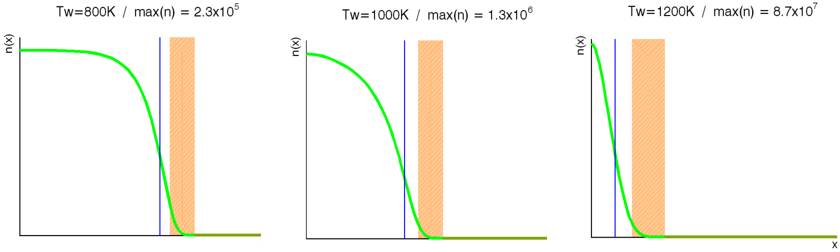
For $T_w = 800K$ the inflexion point and the blue line coincide, which means that nucleation is the most important process for that wall temperature

For $T_w = 1000K$ the gap between the blue line and the orange strip is maximum so nucleation and condensation processes are equally active

For $T_w = 1200K$ the gap diminishes because an intense condensation compensates a weaker nucleation

# Number of molecules per droplet. Results for different Tw

## (Corresponding to sodium sulphate vapors)




The blue line represents the maximum of the growth rate

The gap between the blue line and the orange strip decreases with the wall temperature, which means that condensation process also becomes weaker.

# Singular perturbation approach

## Equations for $c$, $n$ and $\rho$

$$c'' + S_c\, u\, c' = \left[ \cancel{A c^2 n_{cr} \exp\left(\frac{-\sigma^3}{2\eta^2}\right)} + B(c - c_e)\rho T^{1/2} n^{2/3} H_n \right] H_c$$

$$A c^2 n_{cr} \exp\left(\frac{-\sigma^3}{2\eta^2}\right) \ll B(c - c_e)\rho T^{1/2} n^{2/3}$$

$$U n' = -N(c - c_e) T^{1/2} n^{2/3} H_n H_c$$

$$U\rho' + \alpha \left(\frac{T'}{T}\right)' \rho = -L c^2 \exp\left(\frac{-\sigma^3}{2\eta^2}\right) H_c$$

# Singular perturbation approach

## New equations for $c$, $n$ and $\rho$

$$c'' + S_c\, u\, c' = B \boxed{(c - c_e)} \rho T^{1/2} n^{2/3} H_n H_c$$

$$U n' = -N \boxed{(c - c_e)} T^{1/2} n^{2/3} H_n H_c$$

$$c - c_e \ll c$$

$$U\rho' + \alpha \left(\frac{T'}{T}\right)' \rho = -L c^2 \exp\left(\frac{-\sigma^3}{2\eta^2}\right) H_c$$

The problem posed by

**Equation for $\rho$**

$$\chi\left[\rho' + \alpha\left(\frac{T'}{T}\right)'\frac{\rho}{U}\right] = -\frac{c^2}{U}\exp\left(\frac{-\sigma^3}{2\eta^2}\right)H_c$$

$$\chi = \frac{1}{L}$$

**Equations for $C$ and $n$**

$$\varepsilon[C'' + S_c\,u\,C' + c_e'' + S_c\,u\,c_e'] = BC\rho T^{1/2}n^{2/3}H_nH_c$$

$$\varepsilon n' = -\tilde{N}\frac{C}{U}T^{1/2}n^{2/3}H_nH_c$$

$$C = c - c_e;\ \varepsilon = \frac{1}{B};\ \tilde{N} = N\varepsilon = O(1)$$

can be solved using the boundary-layer theory ($\chi$ and $\varepsilon$ are small parameters)

# Singular perturbation approach

Solution can be implemented in two steps:

1. Solution of the equation for $\rho$ for which an initial guess for $c$ and for $x_F$ has to be made.
2. Solution of the system of equations for $C$ and $n$ for which the value of $\rho$ obtained through the former step is to be used.

but...

# Singular perturbation approach

Solution can be implemented in two steps:

1. Solution of the equation for $\rho$ for which an initial guess for $c$ and for $x_F$ has to be made.
2. Solution of the system of equations for $C$ and $n$ for which the value of $\rho$ obtained through the former step is to be used.

but...

**...because of the exponential-logarithmic dependance on $c$, $\rho$ is very sensitive to the value of $c$**

How to obtain a sufficiently good guess for $c$ in order to achieve convergence?

# Equations for $\rho$

$\rho$ is written as a composite of an outer and an inner solution:

Outer equation

$$\rho'_{out} + \alpha \left( \frac{T'}{T} \right)' \frac{\rho_{out}}{U} = 0$$

Inner equation

$$\frac{d\tilde{\rho}_{in}}{dX} + \frac{c_{\mathcal{F}}^2}{U_{\mathcal{F}}} \exp\left( \frac{-\sigma^3}{2\eta^2} \right) = 0$$

$$\tilde{\rho}_{in} = \frac{\rho_{in}}{\gamma}; \quad X = \frac{(x - x_{\mathcal{F}})}{\delta}$$

$$\frac{\gamma}{\delta} = \frac{1}{\chi}$$

$$c_{\mathcal{F}} = c(x_{\mathcal{F}}); \quad U_{\mathcal{F}} = U(x_{\mathcal{F}})$$

To zeroth-order $\rho$ becomes:

$$\rho = \rho_{out} + \rho_{in} - \rho_{match}$$

Outer equations

$$c_e'' + S_c\, u\, c_e' = \tilde{C}_{out}\,\rho T^{1/2}\tilde{n}_{out}^{2/3}$$

$$\tilde{n}'_{out} = -\frac{\tilde{N}\tilde{C}_{out}T^{1/2}\tilde{n}_{out}^{2/3}}{U}$$

$$\tilde{C}_{out} = \frac{C_{out}}{\varepsilon};\quad \tilde{n}_{out} = n$$

Inner equations

$$\left(\frac{d^2\tilde{C}_{in}}{dX^2}\right)^3 + (c_e'')^3 = \left(\frac{d\tilde{C}_{in}}{dX}\right)^2 \tilde{C}_{in}^3 T^{3/2} q^2 \frac{\tilde{\rho}_{in}}{\rho_{\mathcal{M}}}$$

$$\frac{d^2\tilde{C}_{in}}{dX^2} + c_e'' = \left(\frac{d\tilde{C}_{in}}{dX}\right)^{2/3} \tilde{C}_{in} T^{1/2} q^{2/3} \left(\frac{\tilde{\rho}_{in}}{\rho_{\mathcal{M}}}\right)^{1/3}$$

$$\frac{d^3\tilde{Y}}{dX^3} + \frac{\tilde{N}(c_e'' + Sc\, u\, c_e')T^{1/2}}{3U} = \left(\frac{\tilde{Y}}{\tilde{N}}\right)^2 \frac{d\tilde{Y}}{dX} T^{1/2} \frac{\tilde{\rho}_{in}}{\rho_{\mathcal{M}}}$$

$$Y = -n_{in}^{1/3}$$

$$\tilde{\rho}_{in} = \frac{\rho_{in}}{\gamma};\quad \tilde{C}_{in} = \frac{C}{\varsigma};\quad \tilde{Y} = \frac{Y}{\mu};\quad X = \frac{(x - x_{\mathcal{F}})}{\delta}$$

$$\zeta = \frac{1}{B\rho_{\mathcal{M}}N^2};\quad \delta = (\zeta\chi)^{1/9};\quad \gamma = \frac{\delta}{\chi};\quad \varsigma = \delta^2;\quad \mu = \frac{\delta^3}{\varepsilon}$$

$$q = \left(\frac{1}{U}\right)_{\mathcal{F}} - (x - x_{\mathcal{F}})\left(\frac{U'}{U^2}\right)_{\mathcal{F}}$$

$C$ is also written as a composite of an outer and an inner solution. To zeroth-order $C$ becomes:

$$C = C_{out} + C_{in} - C_{match}$$

# Solving the equations for $C$ and $n$

1. Solve equation for $n_{in}$
2. Solve equations for $n_{out}$ and $C_{out}$

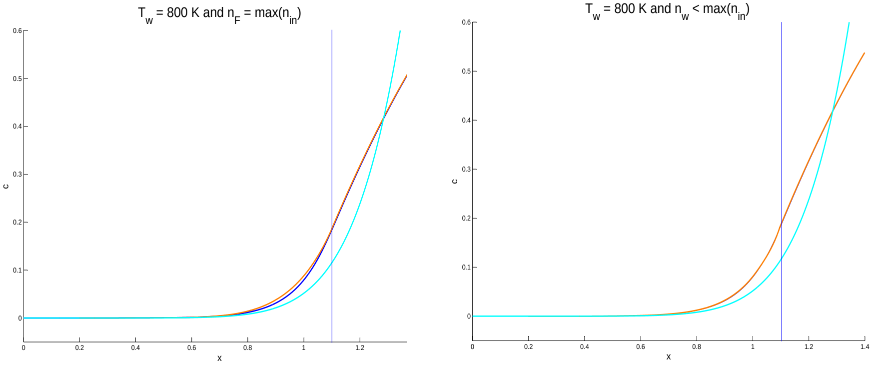
$$C_{out} = \frac{\dfrac{(c_e'' + S_c\, u\, c_e')}{T^{1/2}\rho}}{\left[n_{\mathcal{F}} + \tilde{N}\displaystyle\int_x^{x_{\mathcal{F}}} \dfrac{(c_e'' + S_c\, u\, c_e')dx}{\rho U}\right]^{2/3}}\, \varepsilon$$

but $n_{\mathcal{F}}$ is unknown

3. Make an initial guess $n_{\mathcal{F}} = \lim(n_{in})$ as $X \to \infty = \max(n_{in})$
4. Solve equation for $C_{in}$
5. Composite solution $C = C_{out} + C_{in} - C_{match}$

# Singular perturbation approach. Vapor density

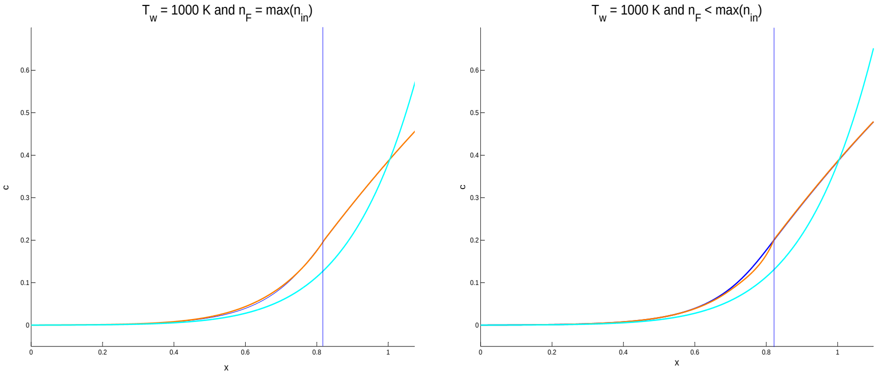
## Results for Tw=800 K




The blue line indicates the location of the inflexion point $(x = x_{\mathcal{F}})$

# Singular perturbation approach. Vapor density

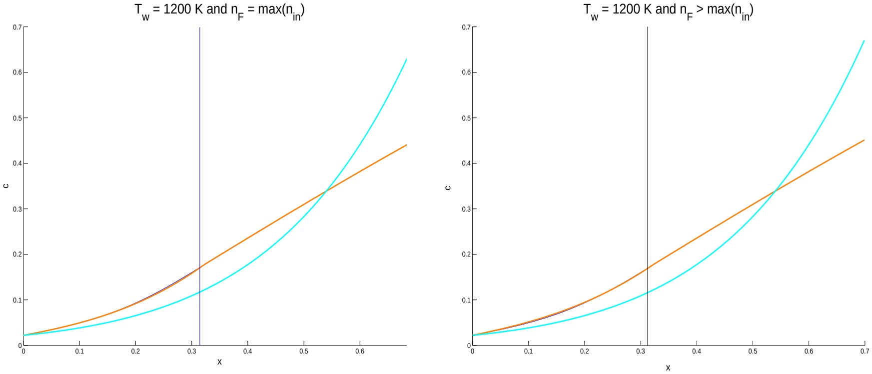
## Results for Tw=1000 K




The blue line indicates the location of the inflexion point ($x = x_{\mathcal{F}}$)

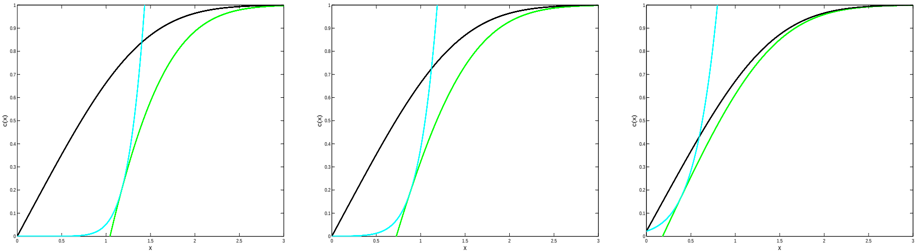
# Singular perturbation approach. Vapor density

## Results for Tw=1200 K




The blue line indicates the location of the inflexion point ($x = x_{\mathcal{F}}$)

# Singular perturbation approach: guessing $c(x)$



The cyan curve represents $c_e(x)$ as given by the Clausius-Clapeyron relation

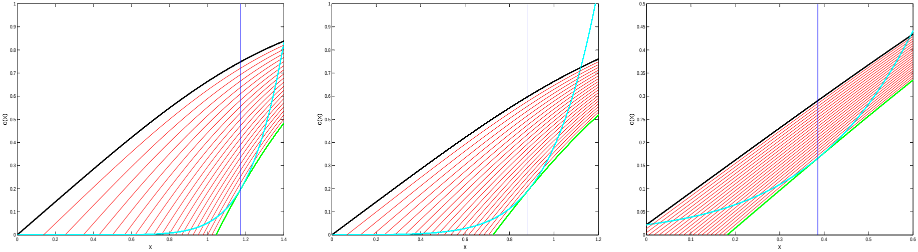
The black curve ($c_s$) and the green curve ($c_0$) are two solutions of:

$$c'' + S_c\, u\, c' = 0$$

B.C.: $c_s(x=0) = c_e(x=0)$ for the black curve

B.C.: $c_0(x=x_0) = c_e(x=x_0)$; $c_0'(x=x_0) = c_e'(x=x_0)$ for the green curve

The black and the green curves provide upper and lower limits for $c(x)$

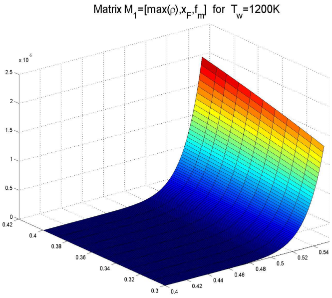


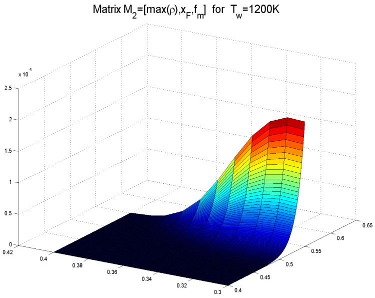

$c(x)$ and $x_{\mathcal{F}}$ are guessed as:

$$c_m(x) = c_0 + (c_0 - c_s) f_m;\ \ 0 < f_m < 1$$

$$0 < x_{\mathcal{F}} < x_0$$

where $x_0$ is the position of the tangency point of $c_e$ and $c_0$




In order to discriminate the best guess for $x_{\mathcal{F}}$ and $f_m$, we proceed as follows:

1. The equation for $\rho$ is solved for each guess $(x_{\mathcal{F}}, f_m)$, applying $c_m = c_m(f_m)$ for calculating $\eta$ in the exponent. A matrix $M_1$ with the maximum values of $\rho(x_{\mathcal{F}}, f_m)$ is obtained.
2. The equation for $\rho$ is solved for each guess $(x_{\mathcal{F}}, f_m)$, taking a Taylor expansion to the $2^{nd}$ order of the exponent around $x = x_{\mathcal{F}}$. The reason for that choice is that the maximum of both, the nucleation rate and the supersaturation, occurs very closely to $x_{\mathcal{F}}$. A matrix $M_2$ with the maximum values of $\rho(x_{\mathcal{F}}, f_m)$ is obtained.

# Obtaining $x_{\mathcal{F}}$ and $f_m$

1. ...
2. ...
3. For each guess $f_m$ the value of $x_{\mathcal{F}}$ for which the condition $M_1 = M_2$ holds, is obtained. These values $x_{\mathcal{F}_{\mathcal{M}}}$ are the best estimations for $x_{\mathcal{F}}$.
4. With the former values the vector $\rho_{\mathcal{M}} = \rho(x_{\mathcal{F}_{\mathcal{M}}}, f_m)$ is obtained.
5. Now the equation for $n(x)$ has to be integrated for each guess $(x_{\mathcal{F}}, f_m)$:

$$n = \frac{1}{3}\left[\int \frac{(c_m - c_e)T^{1/2}}{U} dx\right]^3$$

   for obtaining the matrix $M_3 = [\max(n), x_{\mathcal{F}}, f_m]$ and then, the vector $n_{\mathcal{M}} = M_3(x_{\mathcal{F}_{\mathcal{M}}}, f_m)$.
6. Eventually the product $\rho_{\mathcal{M}}.n_{\mathcal{M}}$ is obtained. This product represents the maximum density of molecules that could condense at a point.
7. It is assumed that this maximum is of the same order that the bulk vapor density. In the limit $\rho_{\mathcal{M}}.n_{\mathcal{M}} = 1$. This condition leads to definitive values for $x_{\mathcal{F}}$ and $f_m$ with which $c_m$ is obtained and finally equation for $\rho$ can be solved.

# Temperature $T$ and velocity $u$

## Non-dimensional equations

$$P_r u T'' = T'$$

$B.C.: \ T(x=0) = T_w/T_\infty; \ T(x=\infty) = 1$

$$u''' + uu'' + 1 - (u')^2 = 0$$

$B.C.: \ u(x=0) = u'(x=0) = 0; \ u'(x=\infty) = 1$

$-u$ is the non-dimensional velocity along the $x$ axis

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$B.C.: \; u(x=0) = u'(x=0) = 0; \; u'(x=\infty) = 1$

$P_r = \dfrac{\nu}{\kappa} = 0.7$; $\nu$: kinematic viscosity; $\kappa$: thermal diffusivity

## Non-dimensional equations

$$c'' + S_c\, u\, c' = \left[ A c^2 n_{cr} \exp\left(\frac{-\sigma^3}{2\eta^2}\right) + B(c - c_e)\rho T^{1/2} n^{2/3} H_n \right] H_c$$

$$\eta = \ln\left(\frac{c}{c_e}\right)$$

$$U\rho' + \alpha\left(\frac{T'}{T}\right)'\rho = -Lc^2 \exp\left(\frac{-\sigma^3}{2\eta^2}\right) H_c$$

$$Un' = -N(c - c_e) T^{1/2} n^{2/3} H_n H_c$$

B.C.: $c(x=0) = c_e(x=0)$; $c(x=\infty) = 1$; $\rho(x \geq x_E) = 0$; $n(x \geq x_E) = 1$

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$$A = \frac{c_\infty [x]^2}{D} \tilde{v} \sqrt{\frac{2\tilde{\omega}}{\pi \tilde{m}_v}}; \quad L = \frac{A}{S_c}; \quad S_c = \frac{\nu}{D};$$

Parameters associated to nucleation

## Non-dimensional equations

$$c'' + S_c\, u\, c' = \left[ A c^2 n_{cr} \exp\left( \frac{-\sigma^3}{2\eta^2} \right) + B(c - c_e)\rho T^{1/2} n^{2/3} H_n \right] H_c$$

$$\eta = \ln\left( \frac{c}{c_e} \right)$$

$$U\rho' + \alpha \left( \frac{T'}{T} \right)' \rho = -L c^2 \exp\left( \frac{-\sigma^3}{2\eta^2} \right) H_c$$

$$U n' = -N(c - c_e) T^{1/2} n^{2/3} H_n H_c$$

B.C.: $c(x=0) = c_e(x=0)$; $c(x=\infty) = 1$; $\rho(x \geq x_E) = 0$; $n(x \geq x_E) = 1$

$$B = \frac{c_\infty [x]^2}{D} \sqrt{\frac{k_B \tilde{T}}{2\pi \tilde{m}_v}} (36\pi \tilde{v}^2)^{1/3}; \quad N = \frac{B}{S_c}; \quad S_c = \frac{\nu}{D};$$

Parameters associated to condensation

## Non-dimensional equations

$$c'' + S_c\, u\, c' = \left[ A c^2 n_{cr} \exp\left(\frac{-\sigma^3}{2\eta^2}\right) + B(c - c_e)\rho T^{1/2} n^{2/3} H_n \right] H_c$$

$$\eta = \ln\left(\frac{c}{c_e}\right)$$

$$U\rho' + \alpha\left(\frac{T'}{T}\right)'\rho = -Lc^2 \exp\left(\frac{-\sigma^3}{2\eta^2}\right) H_c$$

$$Un' = -N(c - c_e)T^{1/2} n^{2/3} H_n H_c$$

B.C.: $c(x=0) = c_e(x=0)$; $c(x=\infty) = 1$; $\rho(x \geq x_E) = 0$; $n(x \geq x_E) = 1$

$U = \left(u + \alpha\frac{T'}{T}\right)$; Velocity of droplets

## Non-dimensional equations

$$c'' + S_c\, u\, c' = \left[ A c^2 n_{cr} \exp\left(\frac{-\sigma^3}{2\eta^2}\right) + B(c - c_e)\rho T^{1/2} n^{2/3} H_n \right] H_c$$

$$\eta = \ln\left(\frac{c}{c_e}\right)$$

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B.C.: $c(x=0) = c_e(x=0)$; $c(x=\infty) = 1$; $\rho(x \geq x_E) = 0$; $n(x \geq x_E) = 1$

$H_n = H(n - n_{cr})$; $H_c = H(c - c_e)$; Heaviside unit step functions

$n_{cr} = K(T\eta)^{-3}$: critical size of nucleus

# Singular perturbation approach

**Equation for $\rho$**

$$U\rho' + \alpha\left(\frac{T'}{T}\right)'\rho = -Lc^2 \exp\left(\frac{-\sigma^3}{2\eta^2}\right)H_c$$

Parameter $L$ is associated to nucleation

may be uncoupled from

**New equations for $C$ and $n$**

$$C'' + S_c\,u\,C' + c_e'' + S_c\,u\,c_e' = BC\rho T^{1/2}n^{2/3}H_nH_c$$

$$Un' = -NCT^{1/2}n^{2/3}H_nH_c$$

$$C = c - c_e$$

Parameters $B$ and $N$ are associated to condensation