Investigation of Transient Gas Phase Column Density Due to Droplet Evaporation

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Introduction

• Plans call for performing the Robotic Refueling Mission—Phase 3 (RRM3) experiment at the International Space Station (ISS)
  – A simulated cryogenic propellant (CH₄) will be transferred between two dewars
  – After each metered transfer, the transferred cryogen will be vented to space via sublimation or evaporation

• Providers of externally-mounted scientific payloads at ISS are required to evaluate column number density (CND, σ) associated with various gas releases and demonstrate that they fall below some maximum requirement
  – Must be considerate of other payloads
  – Since this includes unknown future additions, becomes a search for maximum CND along any path
For this particular configuration, cryogen venting may include a few fine, rapidly-evaporating liquid droplets along with the vapor.

Venting rates and temperatures ~150 K indicate these droplets ($d << 1$ mm) cannot sustain mass flow rates associated with steady density fields.
Objective

- Develop analytical CND expressions associated with spherically-symmetric, radially evaporating droplets in isolation
  - Instantaneous evaporation
  - Finite-period, constant-temperature
  - Identify ways to account for motion, changes in evaporation rate with size and temperature
Column Number Density (CND, $\sigma$)

- Integrated effect of molecules encountered across a prescribed path $l$
  - Number density $n$ varies across path; when unbounded,

$$\sigma = \int_{0}^{\infty} n \, dl$$
Instantaneous Evaporation

- Model spherically-symmetric expansion of $N$ molecules with no bulk radial velocity from a point source
  - thermal expansion only

- Use number density $n$ solution due to Narasimha

\[ n(r, t) = \frac{N \beta^3}{\pi \sqrt{\pi} t^3} e^{-\frac{\beta^2 r^2}{t^2}} \]

  - Elapsed time $t$, radius $r$, $\beta \equiv$ inverse of most probable speed $\sqrt{2RT}$
Instantaneous Evaporation Solution

• Substituting variables

\[ \xi = \frac{\beta}{t}; \quad \alpha_0 = \xi r_0 \]

• Applying the Law of Cosines to relate \( r \) to path length \( l \)

\[
\sigma = \frac{N \beta^3}{\pi \sqrt{\pi} t^3} \int_0^\infty \exp \left[ -\xi^2 \left( r_0^2 + l^2 - 2lr_0 \cos \psi \right) \right] dl
\]

• The solution becomes

\[
\sigma (r_0, \psi , t) = \frac{N \beta^2}{2 \pi t^2} e^{-\alpha_0^2 \sin^2 \psi} \left[ 1 + \text{erf} (\alpha_0 \cos \psi) \right]
\]
Radial path occurs when $\psi = \pi$, right-angle path occurs when $\psi = \pi/2$

- Maximum CND passing through $r_0$ given by twice the right-angle path:

$$\sigma_{\text{max}} = 2 \sigma_\perp = \frac{N \beta^2}{\pi t^2} e^{-\alpha_0^2}$$

Conditions for peak column density along this path:

$$(t, \sigma_{\text{max}})_{\text{peak}} = \left(\beta r_0, \frac{N}{\pi e r_0^2}\right)$$

General condition for peak influence:

$$\left(1 - \alpha_0^2 \sin^2 \psi \right) \left[1 + \text{erf} \left( \alpha_0 \cos \psi \right) \right] = -\frac{\alpha_0 \cos \psi}{\sqrt{\pi}} e^{-\alpha_0^2 \cos^2 \psi}$$
Inst. Evap., $d = 1 \text{ mm CH}_4 @ 150 \text{ K}$
Finite Evaporation Period

- Instantaneous limit may be considered a conservative approximation producing worst case peak CND values
  - May underpredict the time to decay to some value if the peak violates the ISS constraint on intensity

\[
n(r, t) = \int_0^t \frac{\dot{N} \beta^3}{\pi \sqrt{\pi} t^3} e^{-\frac{\beta^2 r^2}{t^2}} dt = \frac{\dot{N} \beta}{2\pi \sqrt{\pi} r^2} e^{-\frac{\beta^2 r^2}{t^2}}
\]

  - Produces the correct steady limit for Narasimha’s model

\[
n(r, t \to \infty) \to \frac{\dot{N}}{\pi r^2 \sqrt{8\pi RT}}
\]

- Can use integral to produce a square wave response
  - Constant evaporation rate not precise due to thermal effects
  - Held fixed here in order to compare to instantaneous case
Finite Period—Right-Angle Case

- Applying Law of Cosines for relating $r$ to $l$ and introducing $L \equiv l/r_0$:

$$
\sigma \left( t \leq t_f \right) = \frac{N \beta}{2 \pi \sqrt{\pi} r_0} e^{-\alpha^2_0} \int_0^\infty \frac{e^{-\alpha^2_0 (L^2 - 2L \cos \psi)}}{1 + L^2 - 2L \cos \psi} dL
$$

- For a right-angle path ($\psi = \pi/2$):

$$
\sigma_\perp \left( t \leq t_f \right) = \frac{N \beta}{2 \pi \sqrt{\pi} r_0} e^{-\alpha^2_0} \int_0^\infty \frac{e^{-\alpha^2_0 L^2}}{1 + L^2} dL = \frac{N \beta}{2 \pi \sqrt{\pi} r_0} e^{-\alpha^2_0} I_\perp
$$

- Let $\eta \equiv \text{Arctan} \ L$, then

$$
I_\perp = \int_0^{\pi/2} e^{-\alpha^2_0 \tan^2 \eta} d\eta
$$
Right-Angle Case—Soln. Approach

- It is possible to solve integral $I$ by introducing function $H$

$$I = \int e^{f(\zeta)} \, d\zeta \quad H(\zeta) \equiv e^{-f(\zeta)} \int e^{f(\zeta)} \, d\zeta$$

- Function $H(\zeta)$ is the solution to

$$\frac{dH}{d\zeta} + H \frac{df}{d\zeta} = 1$$

- For the present application:

$$\frac{dH}{d\eta} - 2\alpha_0^2 \tan \eta \sec^2 \eta \, H = 1$$

- Note $\alpha_0$ is a function of elapsed “on” time $t \leq t_f$
Properties of $H(\eta)$

- Grows like $H \approx \eta$ for small $\alpha_0$
- For large $\alpha_0$ it rises like
  $$H \approx \exp\left(\alpha_0^2 \sec^2 \eta \right)$$
- Crossover characterized by $\alpha_0 \approx 1$, or
  $$t \approx r_0 / \sqrt{2RT}$$
  - CND solution will be a bit smeared out
    - No longer coincides with peak value
    - Indicates transition in $\sigma$ response
      (“knee” in curve)
Finite Period Column Density Example

- Observe behavior for a source taking $N$ molecules, spreading constant introduction rate over $\Delta t$, twice right-angle case
  - Peak occurs shortly after extinction, but a bit quicker than $\Delta t + \beta r_0$
Finite Evap. Period, General Case (Obtuse)

- Return to column number density integral

\[ \sigma (t \leq t_f) = \frac{N \beta}{2\pi \sqrt{\pi} r_0} e^{-\frac{\alpha_0^2}{2}} \int_0^\infty e^{-\frac{\alpha_0^2}{2} \left(L^2 - 2L \cos \psi\right)} dL \]

- let \( \eta = \frac{1}{\sin \psi} \arctan \left( \frac{L - \cos \psi}{\sin \psi} \right) \)

- then \( \sigma (r_0, \psi, t) = \frac{N \beta}{2\pi \sqrt{\pi} r_0} e^{-\frac{\alpha_0^2}{2} \left(1 + \cos^2 \psi\right)} \int_{\eta_0}^{\frac{\pi}{2 \csc \psi}} e^{-\frac{\alpha_0^2}{2} \sin^2 \psi \tan^2 (\eta \sin \psi)} d\eta ; \quad \eta_0 \equiv \left( \psi - \frac{\pi}{2} \right) \csc \psi \)

- or \( \sigma (r_0, \psi, t) = \frac{N \beta}{2\pi \sqrt{\pi} r_0} e^{-\frac{\alpha_0^2}{2} \left(1 + \cos^2 \psi\right)} \int_{\psi - \frac{\pi}{2}}^{\frac{\pi}{2}} e^{-\frac{\alpha_0^2}{2} \tan^2 \gamma} d\gamma ; \quad \gamma \equiv \eta \sin \psi ; \quad \tilde{\alpha}_0 \equiv \alpha_0 \sin \psi \)

- Can solve integral using \( H (\tilde{\alpha}_0, \gamma) \)
Acute Angle $\psi$ Modification

- For optical paths $l$ characterized by $\psi < \pi/2$, the solution may be determined as the difference between
  - the maximum path case where $r_0$ is replaced by $r_\perp = r_0 \sin \psi$
  - Minus a general case solution where $r_0$ is retained but $\psi$ is replaced by $\pi - \psi$

\[
\begin{align*}
\text{Source} & \\
\text{Initial location} & \\
\end{align*}
\]
Variable $T$, Motion Effects

- Investigators observe that droplet or crystal temperatures tend to fall somewhat upon vacuum exposure
  - Affects evaporation rate as well as characteristic wave velocity $1/\beta$

- Droplet motion will also affect column density

- These effects may be approximately compensated for by defining how $r_0$, $\psi$, & $T$ vary with time relative to the optical path
  - Describe numerically as an incremental series of instantaneous releases

- Straightforward but computationally intensive to extend effect of a single droplet to multiple droplets assuming negligible coupling between individual sources
  - Can also compensate for effect of background density on evap. rate
Concluding Remarks

- A number of increasingly complex expressions have been developed to assist investigators in describing the effect of transient single-droplet evaporation on column density along general paths
  - Especially for path of maximum influence for a given separation distance between droplet and line of sight
  - Instantaneous evaporation case produces a useful bounding case

- Column density solutions for droplets evaporating over finite periods were developed
  - Exploration led to discovery of a new mathematical function helping to gain a bit of insight into solution behavior

- Finally, incorporation of further refinements including direct and indirect effects of transient temperature variation and motion were briefly discussed
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