Investigation of Transient Gas Phase Column Density Due to Droplet Evaporation

Michael Woronowicz

KBR, Inc.

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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 (CH_4) 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

Introduction (continued)

- 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 ($d \ll 1$ mm) cannot sustain mass flow rates associated with steady density fields

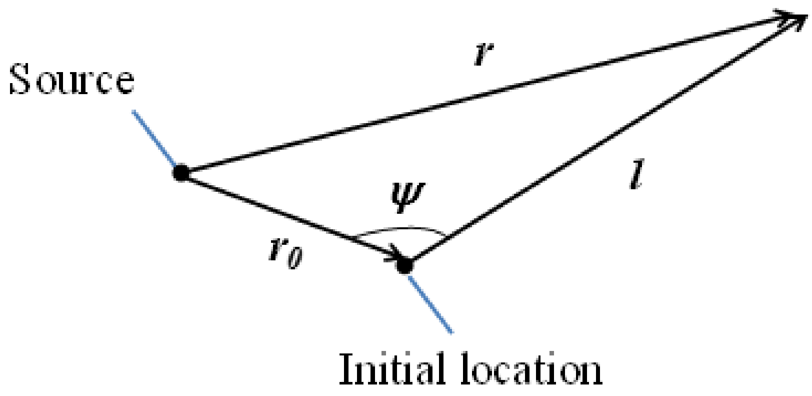
Objective

- 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, σ)

- 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

$$\xi \equiv \frac{\beta}{t}; \qquad \alpha_0 \equiv \xi\, r_0$$

- 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

$$\sigma\left(r_0,\psi,t\right) = \frac{N\beta^2}{2\pi t^2} e^{-\alpha_0^2 \sin^2\psi}\left[1 + \operatorname{erf}\left(\alpha_0\cos\psi\right)\right]$$

Instant. Evap.—Comments

- 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:

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

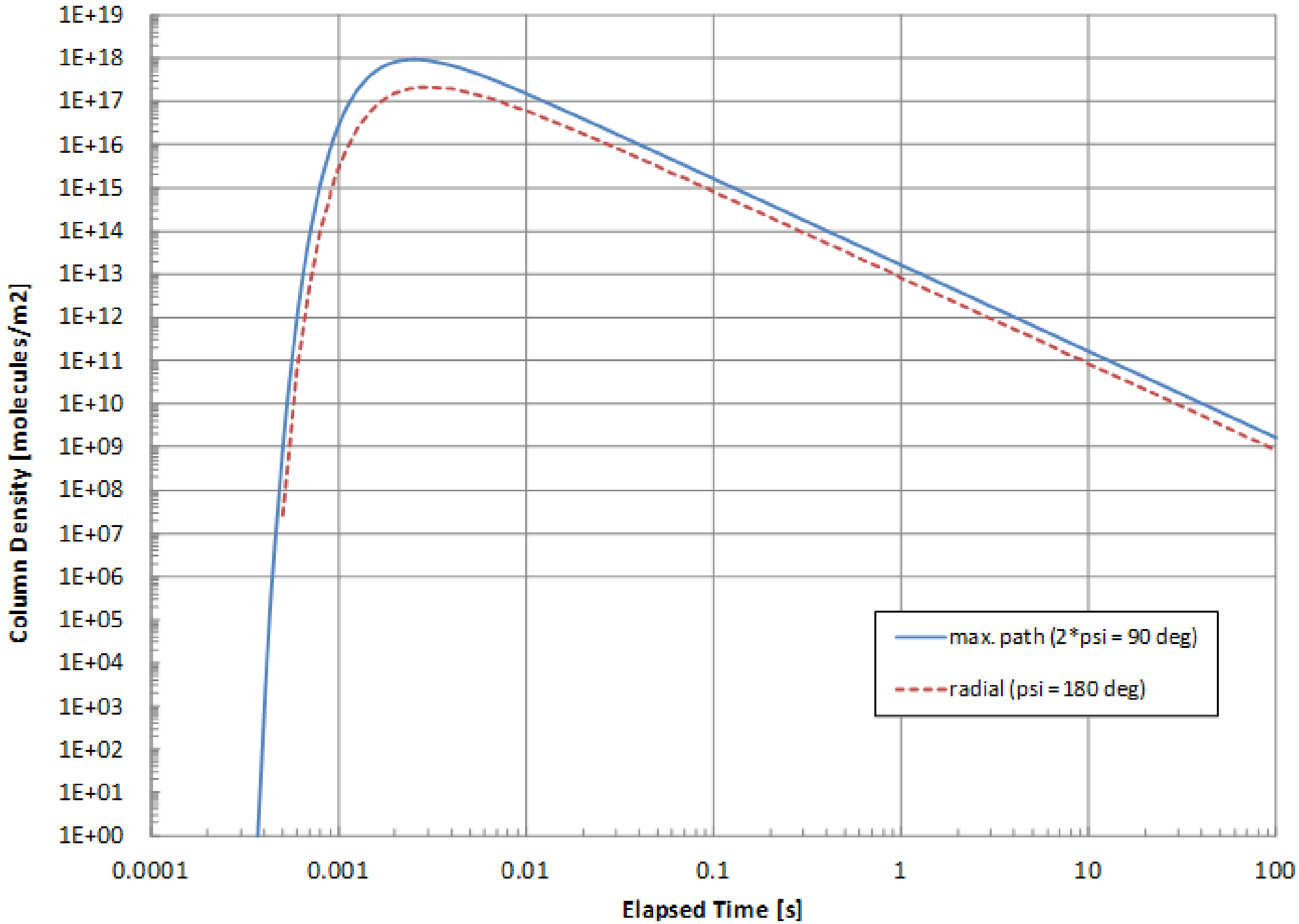
- Conditions for peak column density along this path:

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

- General condition for peak influence:

$$\left(1 - \alpha_0^2 \sin^2\psi\right)\left[1 + \mathrm{erf}\left(\alpha_0 \cos\psi\right)\right] = -\frac{\alpha_0 \cos\psi}{\sqrt{\pi}} e^{-\alpha_0^2 \cos^2\psi}$$

Inst. Evap., *d* = 1 mm CH_4 @ 150 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

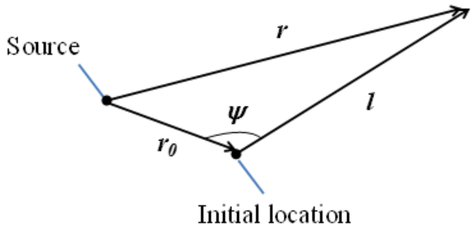
$$n(r, t \to \infty) \to \frac{\dot{N}}{\pi r^2 \sqrt{8\pi R T}}$$

- 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 $L \equiv l/r_0$:

$$\sigma\left(t \le t_f\right) = \frac{\dot{N}\beta}{2\pi\sqrt{\pi}\,r_0} e^{-\alpha_0^2} \int_0^\infty \frac{e^{-\alpha_0^2\left(L^2 - 2L\cos\psi\right)}}{1 + L^2 - 2L\cos\psi}\, dL$$



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

$$\sigma_\perp\left(t \le t_f\right) = \frac{\dot{N}\beta}{2\pi\sqrt{\pi}\,r_0} e^{-\alpha_0^2} \int_0^\infty \frac{e^{-\alpha_0^2 L^2}}{1 + L^2}\, dL = \frac{\dot{N}\beta}{2\pi\sqrt{\pi}\,r_0} e^{-\alpha_0^2}\, I_\perp$$

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

$$I_\perp = \int_0^{\pi/2} e^{-\alpha_0^2 \tan^2\eta}\, d\eta$$

Right-Angle Case—Soln. Approach

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

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

- 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 α_0 is a function of elapsed "on" time $t \leq t_f$

Properties of $H(\eta)$

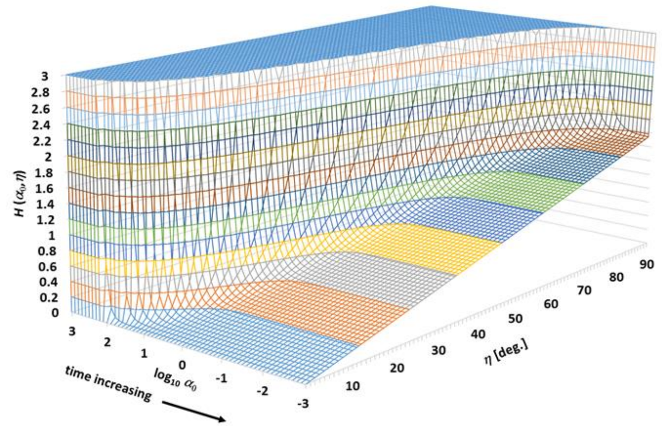
- Grows like $H \approx \eta$ for small α_0
- For large α_0 it rises like

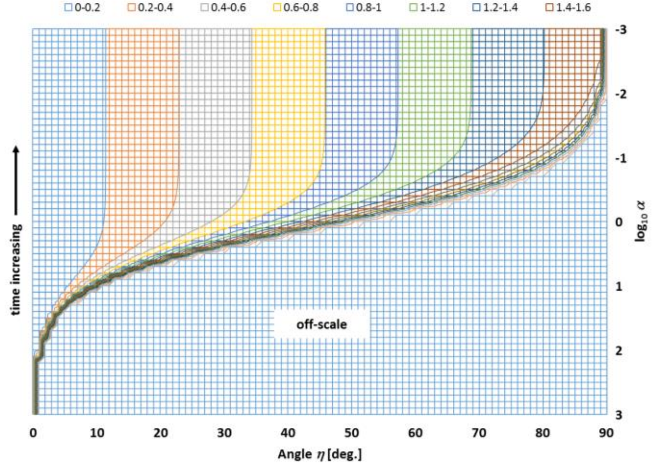
$$H \approx \exp\left(\alpha_0^2 \sec^2 \eta\right)$$

- Crossover characterized by $\alpha_0 \approx 1$, or

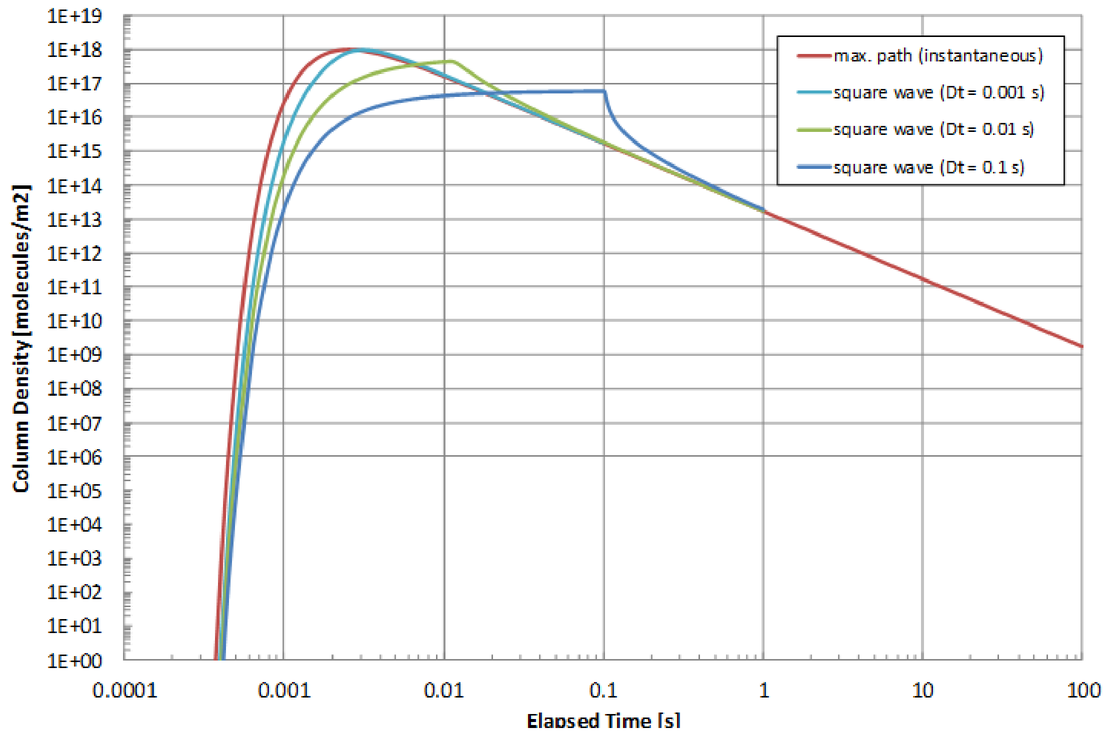
$$t \approx r_0 / \sqrt{2RT}$$

  - CND solution will be a bit smeared out
    - No longer coincides with peak value
    - Indicates transition in σ response ("knee" in curve)





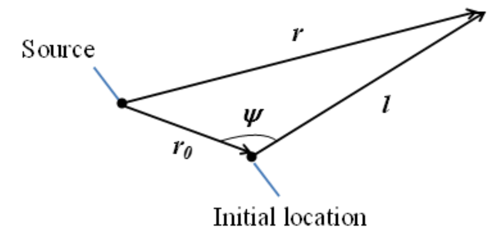
Finite Period Column Density Example



- Observe behavior for a source taking N molecules, spreading constant introduction rate over Δt, 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



$$\sigma\left(t \le t_f\right) = \frac{\dot{N}\,\beta}{2\pi\sqrt{\pi}\,r_0}\, e^{-\alpha_0^2} \int_0^{\infty} \frac{e^{-\alpha_0^2\left(L^2 - 2L\cos\psi\right)}}{1 + L^2 - 2L\cos\psi}\, dL$$

– let $\eta \equiv \frac{1}{\sin\psi}\,\mathrm{Arctan}\left(\frac{L - \cos\psi}{\sin\psi}\right)$

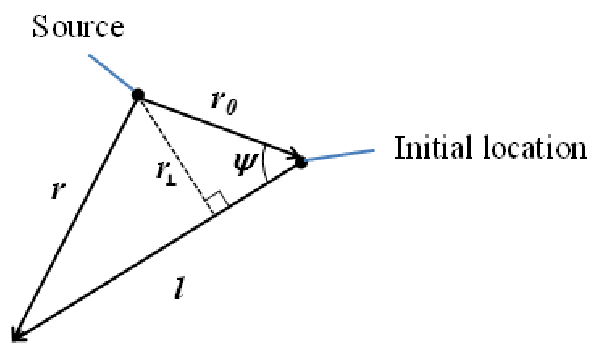
– then $\sigma\left(r_0, \psi, t\right) = \frac{\dot{N}\,\beta}{2\pi\sqrt{\pi}\,r_0}\, e^{-\alpha_0^2\left(1+\cos^2\psi\right)} \int_{\eta_0}^{\frac{\pi}{2}\csc\psi} e^{-\alpha_0^2 \sin^2\psi\, \tan^2\left(\eta\sin\psi\right)}\, d\eta\ ; \qquad \eta_0 \equiv \left(\psi - \frac{\pi}{2}\right)\csc\psi$

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

- Can solve integral using $H\left(\tilde{\alpha}_0, \gamma\right)$

Acute Angle ψ 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 ψ is replaced by $\pi - \psi$



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, ψ, & 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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