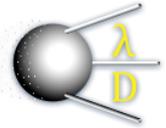




Investigation of Transient Gas Phase Column Density Due to Droplet Evaporation

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ATV Edoardo Amaldi Approaches ISS



ESA/NASA/Don Pettit



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

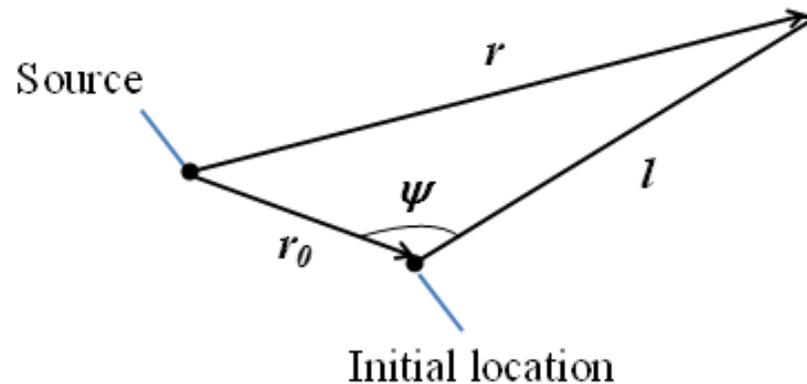
- Develop analytical CND expressions associated with spherically-symmetric, radially evaporating droplets in isolation
 - Instantaneous evaporation
 - Finite-period, constant-temperature
 - Identify ways to account for motion, changes in evaporation rate with size and temperature



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

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

- 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

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



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:

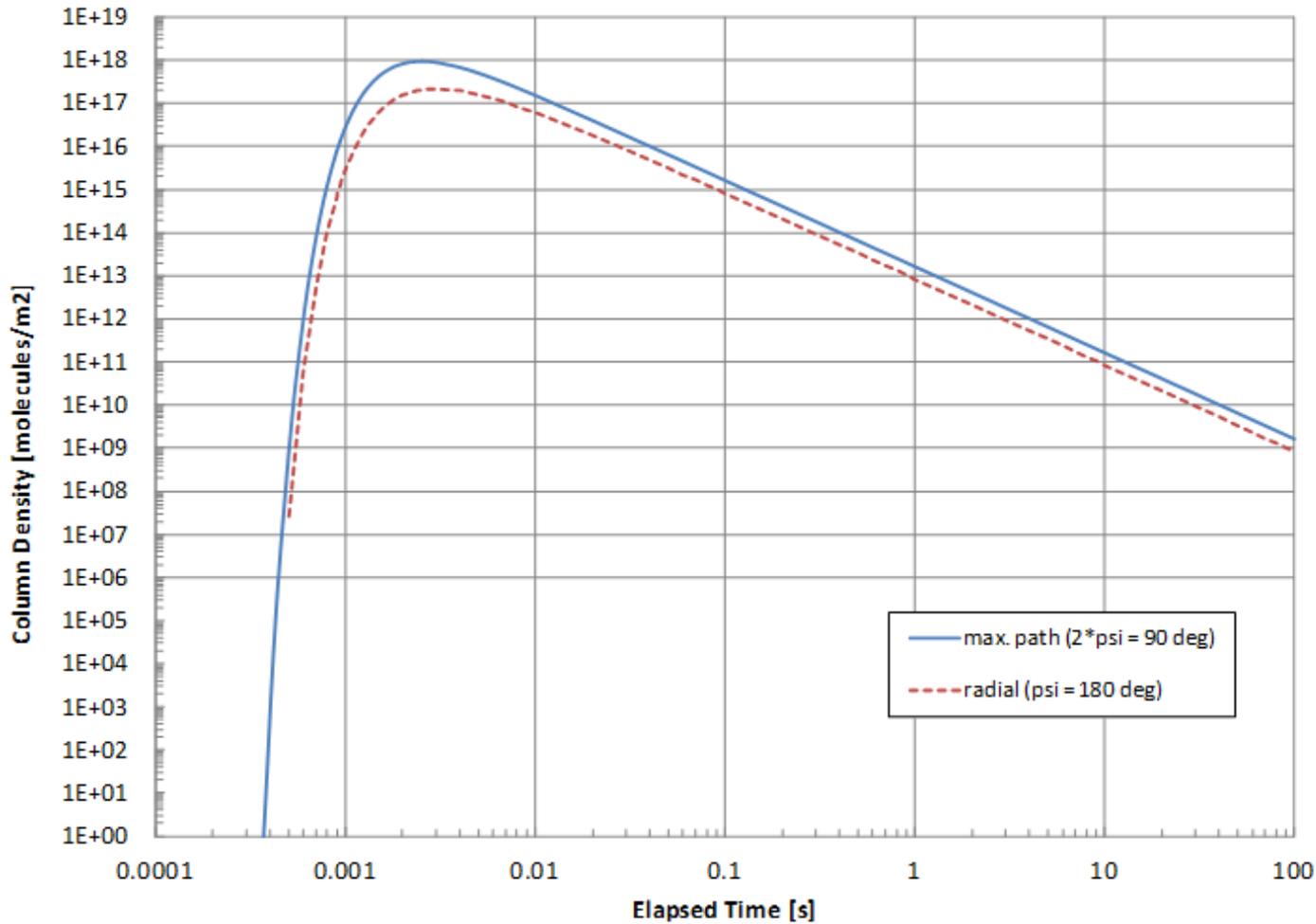
$$(t, \sigma_{\max})_{\text{peak}} = \left(\beta r_0, \frac{N}{\pi e r_0^2} \right)$$

- General condition for peak influence:

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



Inst. Evap., $d = 1$ mm CH_4 @ 150 K





Finite Evaporation Period

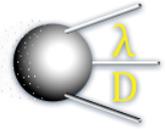
- Instantaneous limit may be considered a conservative approximation producing worst case peak CND values
 - May underpredict the time to decay to some value if the peak violates the ISS constraint on intensity

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

- Produces the correct steady limit for Narasimha's model

$$n(r, t \rightarrow \infty) \rightarrow \frac{\dot{N}}{\pi r^2 \sqrt{8\pi RT}}$$

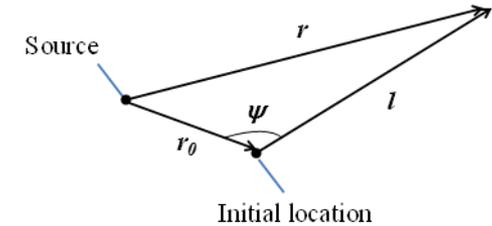
- Can use integral to produce a square wave response
 - Constant evaporation rate not precise due to thermal effects
 - Held fixed here in order to compare to instantaneous case



Finite Period—Right-Angle Case

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

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



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

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

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

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

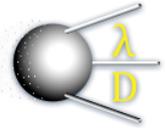
- Function $H(\zeta)$ is the solution to

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

- 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 $H(\eta)$

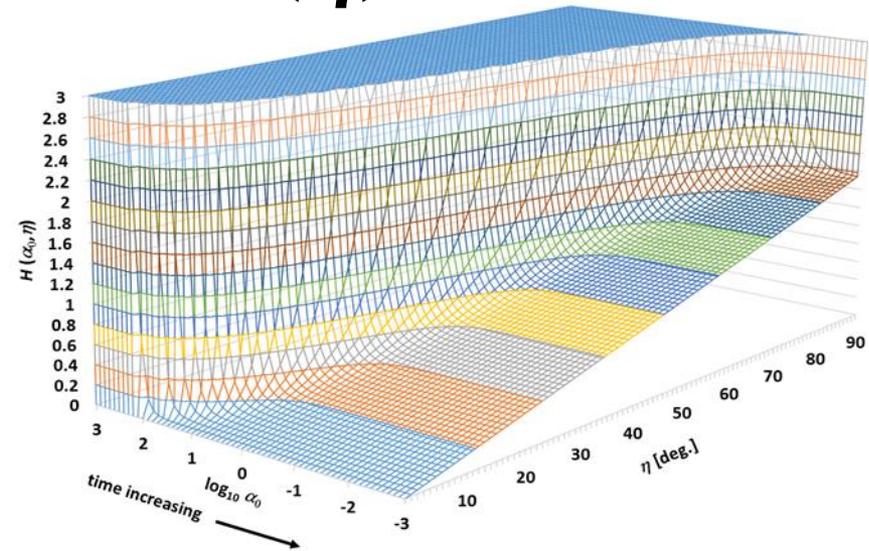
- Grows like $H \approx \eta$ for small α_0
- For large α_0 it rises like

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

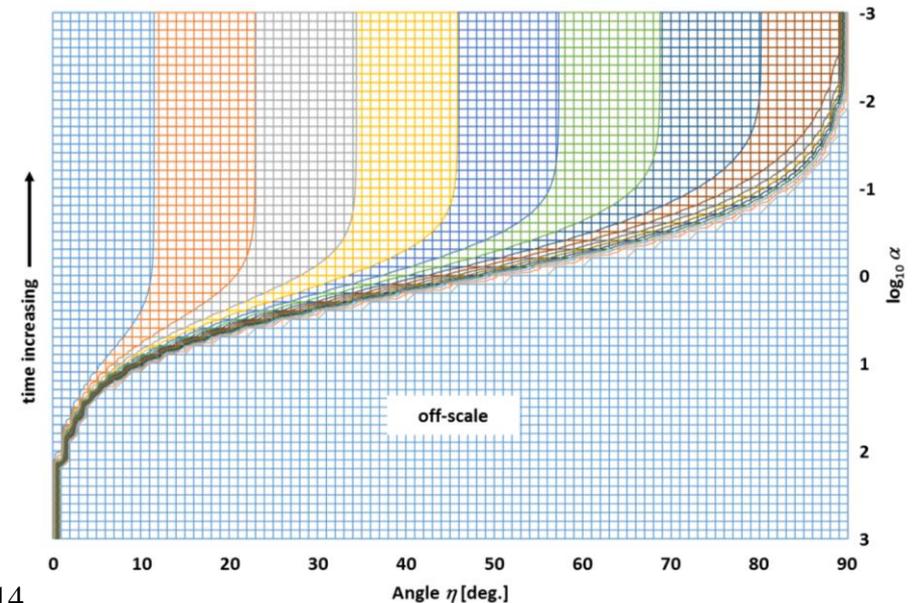
- Crossover characterized by $\alpha_0 \approx 1$, or

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

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

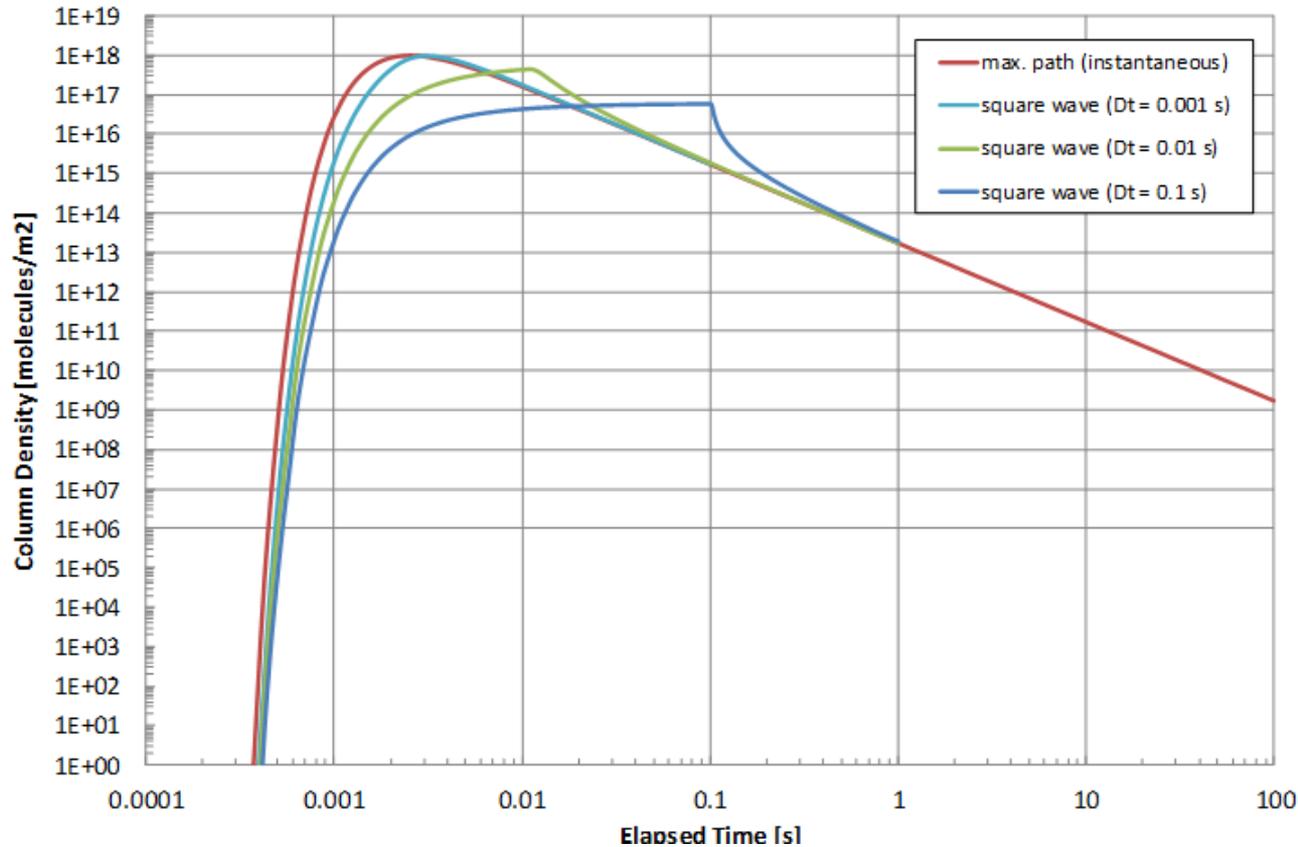


■ 0-0.2
 ■ 0.2-0.4
 ■ 0.4-0.6
 ■ 0.6-0.8
 ■ 0.8-1
 ■ 1-1.2
 ■ 1.2-1.4
 ■ 1.4-1.6





Finite Period Column Density Example

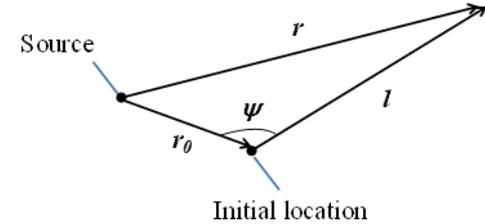


- Observe behavior for a source taking N molecules, spreading constant introduction rate over Δt , twice right-angle case
 - Peak occurs shortly after extinction, but a bit quicker than $\Delta t + \beta r_0$



Finite Evap. Period, General Case

- Return to column number density integral



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

– let

$$\eta \equiv \frac{1}{\sin \psi} \text{Arctan} \left(\frac{L - \cos \psi}{\sin \psi} \right)$$

– then

$$\sigma(r_0, \psi, t) = \frac{\dot{N} \beta}{2\pi \sqrt{\pi} r_0} e^{-\alpha_0^2(1 + \cos^2 \psi)} \int_0^{\frac{\pi}{2} \csc \psi} e^{-\alpha_0^2 \sin^2 \psi \tan^2(\eta \sin \psi)} d\eta ; \quad \eta_0 \equiv \left(\psi - \frac{\pi}{2} \right) \csc \psi$$

– or

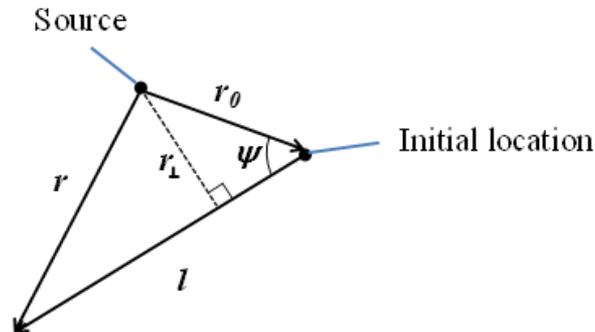
$$\sigma(r_0, \psi, t) = \frac{\dot{N} \beta}{2\pi \sqrt{\pi} r_0} \frac{e^{-\alpha_0^2(1 + \cos^2 \psi)}}{\sin \psi} \int_{\psi - \frac{\pi}{2}}^{\frac{\pi}{2}} e^{-\tilde{\alpha}_0^2 \tan^2 \gamma} d\gamma ; \quad \gamma \equiv \eta \sin \psi ; \quad \tilde{\alpha}_0 \equiv \alpha_0 \sin \psi$$

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



Acute Angle 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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