UNIVERSITY OF NEBRASKA-LINCOLN

Physics & Astronomy

Gas surface interaction

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Gas-Surface Interaction

- In physics, the Boltzmann equation or Boltzmann transport equation (BTE) describes the statistical behavior of a thermodynamic system not in thermodynamic equilibrium.
- To solve the Boltzmann equation, we need to specify boundary conditions for the velocity distribution function at solid surfaces. Thus, we need to know how incident molecules interact with a solid surface.

Model of gas-surface interaction

The interaction of molecules and the surface

- ✓ can be adsorbed,
- ✓ move around the surface
- ✓ or undergo chemical reaction with the surface molecules.

Treat collisions as instantaneous and local

Accurate modeling of gas surface interaction is very complicated due to lack of complete knowledge of surface properties (surface finish, cleanliness, adsorbed gas layers, etc.) and due to lack of accurate surface interaction potentials.

Maxwell Model of Gas-Surface Interaction

- Maxwell suggested a simplified model using two types of interactions that bound the problem: specular and diffuse.
- A parameter σ is defined to represent the fraction of diffuse reflections and 1-σ is the fraction of specular reflections. The parameter is called [tangential momentum] accommodation coefficient.

Specular Reflection

Specular reflection is mirror like reflection. Specular reflection happens for

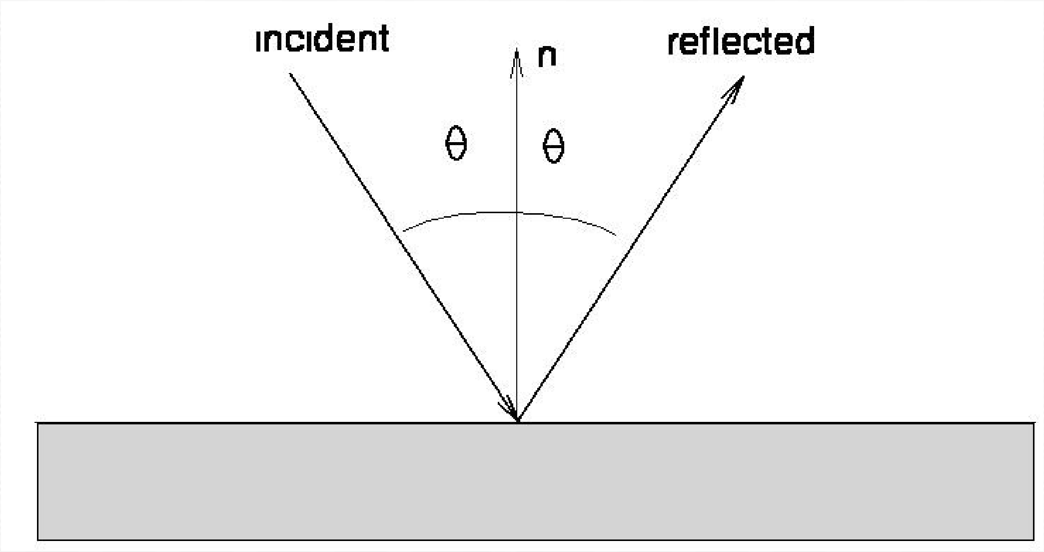
- ✓ Smooth metal surface that has been outgassed through exposure to high vacuum and temperatures (baked surface)
- ✓ The ratio of molecular weights of the gas to that of the surface molecules is small in comparison to unity
- ✓ The translational energy of molecules relative to the surface is larger than several electron volts

1 eV=1.6E-19 J. Thus, for N_2 (m = 4.65E-26 kg) V>3.7 km/s

Specular Reflection

Fluxes for specularly reflected molecules:

- ✓ $N = N_i + N_r = 0$ – No net molecular flux (impermeability condition)
- ✓ $p_r = p_i$ or $p = 2p_i$ – Net normal momentum flux
- ✓ $\tau_r = -\tau_i$ τ – No net shear
- ✓ $q_{i,tr} = -q_{r,tr}$ or $q = 0$ – No net translational energy flux

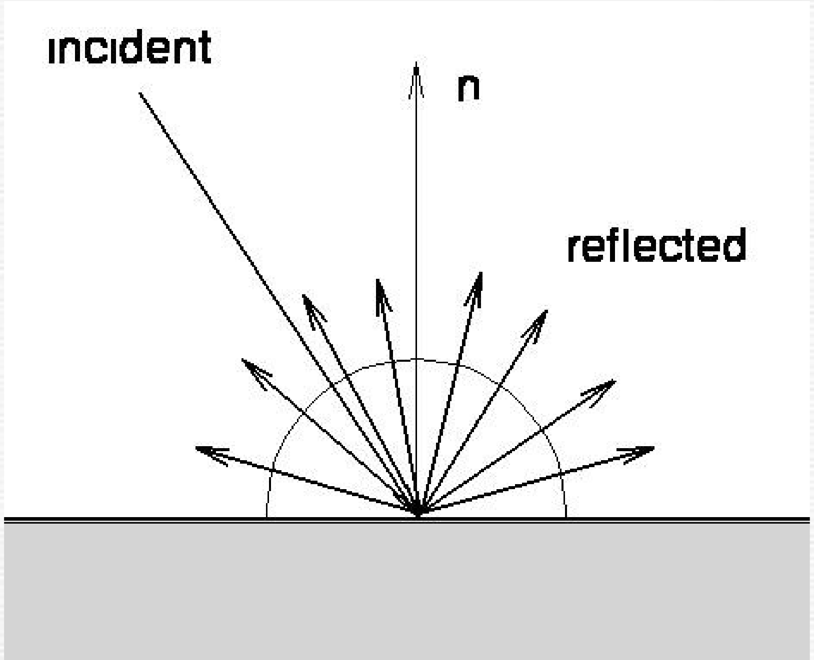


Diffuse Reflection

- Velocity of reflected molecule is independent of incident velocity. Reflected molecules have a half-range Maxwellian distribution corresponding to the wall temperature and velocity.
- Fully accommodated diffuse reflections are typical for microscopically rough surfaces and low-speed flows at common temperatures.

$$f_r(\vec{v}) = \left(\frac{\beta_w}{\pi^{3/2}} e^{-\beta_w \overrightarrow{v^2}}\right) \quad \text{For } (\vec{v}, \vec{n}) > 0$$

Where $\beta_w = \frac{1}{\sqrt{2RT_w}}$ $\vec{n}$ is the normal of the surface



Diffuse Reflection (cont)

Calculate fluxes for diffuse reflection. Impermeability condition gives $N_r = -N_i$. The reflected molecule flux is then (Bird Eq. (4.22) for stationary gas)

$$N_r = -\frac{n_w}{4}\sqrt{\frac{8}{\pi} R T_w}$$

Thus $$n_w = n_\infty \sqrt{\frac{T_\infty}{T_w}} \left(e^{-s^2 \cos 2\theta} + \sqrt{\pi}\, s \cos\theta\right)$$

Diffuse Reflection (cont)

Normal momentum flux for reflected molecules is (Bird's Eq. (4.25) for stationary gas):

$$p_r = \frac{n_w m R T_w}{2} = \frac{\rho_w R T_w}{2} = \frac{p_w}{2}$$

Parallel momentum flux for reflected molecules is zero (Bird's Eq. (4.26) for stationary gas):

$$\tau_r = 0$$

Maxwell Model of Gas-Surface Interaction

- Specular Reflection and diffuse Reflection
- Maxwell accommodation coefficient
- ✓ σ is the fraction of diffuse reflections
- ✓ 1-σ is the fraction of specular reflections.

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Thank you for your time!