Thermal Plasma Modeling

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Outline:
1. Introduction to thermal plasmas
2. Generation of thermal plasmas
3. Equilibrium relations
4. Thermodynamic and transport functions
5. Conservation equations and solution methods
6. Non-equilibrium and turbulence
7. Examples of recent calculations
8. Electrode regions
9. Conclusions

1. Introduction to thermal plasmas

- a plasma is called “thermal” if it is partially in Local Thermal Equilibrium (LTE)
- a thermal plasma is typically at pressures above 0.1 atmospheres
- collision processes dominate
- high degrees of ionization (5 to 100%)
- high electron densities (typically >10^{22} m^{-3})
- continuum approach is used for description

Thermal plasmas are widely used for processing
- high energy fluxes in controlled environment
- high fluxes of reactant species
Thermal Plasma Characteristics and Processing Paths

Example of pressure effect on equilibrium condition

- If $p \downarrow$, $n \downarrow$ and collision number $\downarrow$

Behavior of electron temperature ($T_e$) and heavy-particle temperature ($T_h$) in an arc plasma.
Example of non-equilibrium in “thermal plasma”

Anode region of high intensity arc

\[ T_e \approx 12 \text{ kK} \]
\[ n_e \approx 10^{22}-10^{23} \text{ m}^{-3} \]

- extent of regions and all plasma characteristics strongly dependent on macroscopic fluid flow

2. Generation of thermal plasmas

- electric arcs - most widely used method
  - Joule heating of gas by passing current through it
  - requires electrodes
  - characteristics strongly depending on fluid dynamics
  - different configurations require different modeling approaches

- radio frequency induction discharges
  - no electrodes needed
  - larger plasma volume generated
  - lower gas heating efficiency
  - more sensitive to process variations

- laser, shockwave, etc.

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Discharges are characterized by their voltage - current relation

Region 1 and 2:
Non-self sustained discharge, electrons are generated by external means

Region 3:
Glow discharge: sufficient ionizing collisions to sustain discharge

Region 4:
Abnormal glow - increasing voltage

Region 5: arc: after breakdown strong increase in current density, decrease in voltage, ionization mechanism changes, cathode electron emission mechanism changes, cathode fall only ~10 V

Different regions of electric arc

Cathode region:
I. Cathode fall, 10^{-3} mm
   - ions are accelerated towards cathode
II. Cathode boundary layer, 1 to few mm
   - widening of arc, lower current density

Column region
III. Arc column, electric field, temperature determined by interaction with surroundings

Anode region
IV. Anode boundary layer, 1 to 2 mm
   - arc constricts because of axial heat loss
V. Anode fall, 10^{-3} mm
   - electrons driven towards anode
   - positive for constricted attachment, negative for diffuse attachment
Different thermal plasma generator configurations

Transferred Arc Plasma Generator

- arcing between one electrode (usually cathode) and metal workpiece
- high heat flux, low gas flow
- high energy transfer efficiency to solid

Temperature profiles in transferred arc plasma reactor
Different thermal plasma generator configurations

Non-Transfered Plasma Generator

- plasma generation confined to torch
- high bulk gas heating efficiency
- wider heat flux distribution with lower peak values

Temperature distribution in a plasma jet
[Boffa and Pfender, 1968]

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Arc instabilities

Arcs are usually unstable

- MHD instabilities can lead to arc extinction
- shear layer instabilities result in cold gas entrainment
- anode attachment instability results in continuous power fluctuation
- electron heating instability can result in arc constriction in anode region

Stabilization mechanisms:

- wall stabilization provides stabilizing radial gradients
- convection stabilization with parallel cold flow
- jet stabilization

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Example of anode attachment instability in plasma torch

3. THERMODYNAMIC EQUILIBRIUM RELATIONS

Maxwellian Velocity Distribution (most probable distribution):

\[
\frac{dN(v)}{N} = \frac{4\pi v^2 dv}{(2\pi kT/m)^{3/2}} \exp(-mv^2 / 2kT)
\]

Average Velocity:

\[
\bar{v} = \left(\frac{8kT/\pi m}{m}\right)^{1/2}
\]

Average Kinetic Energy:

\[
\bar{v}^2 = 3kT/m
\]

Definition of Temperature:

\[
\frac{3}{2}kT = \frac{1}{2}mv^2
\]

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Maxwellian velocity distribution for two different temperatures

![Graph showing Maxwellian velocity distribution for two different temperatures](image)

**THERMODYNAMIC EQUILIBRIUM RELATIONS**

**Boltzmann Distribution of Excited States**

\[
\frac{n_s}{n} = \frac{g_s}{Z} \exp\left(-\frac{E_s}{kT}\right)
\]

- \(g_s\) = statistical weight of state \(S\)
- \(Z\) = partition function = \(\sum g_r \exp\left(-E_r/kT\right)\)

**Saha Equation (Mass Action Law For Ionization)**

\[
\frac{n_e n_i}{n} = \frac{2 g_i}{Z} \frac{(2\pi m_e kT)^{3/2}}{h^3} \exp\left(-\frac{E_i}{kT}\right)
\]

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THERMODYNAMIC EQUILIBRIUM RELATIONS

Dalton's Law: \( p = p_n + p_e + p_i \)

Perfect Gas Law: \( pV = NkT \)

- Additional requirement: blackbody radiation according to \( T \)
  - seldom obtained in terrestrial plasmas
  - use concept of Local Thermal Equilibrium (LTE)
    all relations applicable except radiation field

- "Thermal Plasmas" are approximating LTE conditions except in boundaries

- Pressure reduction leads to non-equilibrium conditions

DEVIATIONS FROM THERMAL EQUILIBRIUM

- High density, temperature gradients
  - Diffusion faster than equilibration
  - Important in arc fringes, at surfaces

- High electric fields
  - Charge carriers acquire energy faster than they can equilibrate
  - Important in low pressure discharges

- Fast flow velocities
  - Macroscopic motion faster than equilibration
  - "Frozen flow conditions"
  - Important in high velocity jets

Most important deviations
- \( T_e \neq T_h \) because of slow electron-heavy particle equilibration
- Frozen recombination reactions
- Ground state - excited states non-equilibrium

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4. THERMODYNAMIC AND TRANSPORT PROPERTIES
(Boulos, Fauchais and Pfender, 1994)

Difference to normal gases:
• Dissociation, ionization increase energy density
• Electrons lead to higher electrical, thermal conductivities
• Dissociation, ionization increases energy transport
  – Peaks in thermal conductivity
  – $K = K_{tr}^h + K_{tr}^e + K_{in} + K_{react}$
• Viscosity increases because of larger momentum transfer collision cross-section
• Higher radiation transport because of high population of excited states

Thermodynamic and transport properties

Need to determine:
(1) Composition - minimization of Gibb’s free energy
  $G = H - TS$
  Saha equation for ionization reaction of noble gas

(2) Thermodynamic functions using partition function and mixture rules
  - density, enthalpy, specific heat

(3) Transport coefficients using Chapman-Enskog approach for solving Boltzmann equation
  - thermal conductivity, viscosity, electrical conductivity, diffusion coefficient
  - need collision cross sections, interaction potentials or collision integrals

(4) Radiation properties - emission coefficient

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Temperature dependence of the composition (species number densities) of an argon plasma at atmospheric pressure (starting from one mole of Ar at room temperature)

Temperature dependence of the composition (species number densities) of a nitrogen plasma at atmospheric pressure (starting from one mole of N\textsubscript{2} at room temperature)

Temperature dependence of the composition (species number densities) of an Ar - H\textsubscript{2} (20 vol\%) plasma at atmospheric pressure
Partition Function
(sum over all energy states)

\[ Z_t = Z_{tr} \cdot Z_{rot} \cdot Z_{vib} \cdot Z_{el} \cdot Z_{chem} = \frac{V}{h^3} (2\pi mkT)^{3/2} \cdot Z_{el} \cdot Z_{chem} \]

Neglecting rotational and vibrational energy states

\[ Z_{el} = \sum_s g_s \exp\left(-\frac{E_s}{kT}\right) \quad \text{Specific Internal Energy:} \quad U_{int} = RT \left( \frac{\partial \ln Z_t}{\partial T} \right)_V \]

\[ Z_{chem} = \exp\left(-\frac{E_{chem}}{kT}\right) \quad \text{Specific enthalpy} \quad h = u + pv \]

\[ Z_{ion} = \exp\left(-\frac{E_i - \Delta E_i}{kT}\right) \]

\( \Delta E_i \) is reduction of ionization energy due to overlapping energy levels.

\[ p = RT \left( \frac{\ln Z_t}{\partial V} \right)_T \]

\[ h = RT \left[ \left( \frac{\partial \ln Z_t}{\partial T} \right)_V + V \left( \frac{\partial \ln Z_t}{\partial V} \right)_T \right] \]

Enthalpies for various plasmas

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Variation of specific heats with temperature [K.S. Drellishak, 1963]

\[ c_p = \left( \frac{\partial h}{\partial T} \right)_p \]

Thermal Conductivity

Heat flux

\[ q = -K \frac{dT}{dz} \]

\( K \) = thermal conductivity

from simplified kinetic theory

\[ K = \frac{1}{3} n \bar{V} c_v \ell = \frac{2 c_v}{3 \sigma} \sqrt{\frac{kT}{\pi m}} \]

\( n \) = number density of particles
\( \bar{V} \) = average thermal velocity
\( c_v \) = specific heat at constant volume
\( \ell \) = mean free path
\( \sigma \) = collision cross section for momentum transfer

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Thermal Conductivity

For reacting gases, e.g. with dissociation, ionization, transport of reaction energy must be considered

$$K = K_{tr}^h + K_{tr}^e + K_{react} + K_{int}$$

$K_{tr}^h$, $K_{tr}^e$ = translational thermal conductivities of heavy particles and electrons, respectively

$K_{react}$ = reactive contribution to thermal conductivity

$K_{int}$ = internal energy transport of atoms (i.e. excited states)

Contributions to the thermal conductivity of a nitrogen plasma

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Thermal conductivities of H₂-Ar mixtures

Electrical conductivity of various gases

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Viscosity

Simplified kinetic theory

\[ \mu = \frac{1}{3} n \cdot m \cdot \bar{v} \cdot \ell = \frac{1}{3} \sqrt{\frac{8}{\pi}} \frac{\sqrt{mkT}}{\sigma} \]

only valid for low degrees of ionization

- \( n \) = particle density
- \( m \) = particle mass
- \( \bar{v} \) = average thermal velocity
- \( \ell \) = mean free path
- \( \sigma \) = total momentum transfer cross section

Viscosity

For neutral atoms (low temperatures)

\[ \sigma_{H-H} < \sigma_{He-He} < \sigma_{N-N} < \sigma_{Ar-Ar} \]

For appreciable ionization (\( x_i > 0.03 \))

i.e. \( T > 10,000 \) K for Ar, H\(_2\), N\(_2\) and \( T > 17,000 \) K for He

long range Coulomb forces become important, then \( \mu \) decreases with increasing \( T \)
5. Conservation equations and solution methods

- conservation of mass, momentum and energy
- typically used with boundary layer assumptions
  - axial gradients $\ll$ radial gradients
- derived for arc column region
- description of electrode regions require modification of approach
Formulation for LTE

**Fluid** (conservation eqns.) +

**Electromagnetic** (Maxwell’s eqns.) +

**Thermodynamic & Transport Properties**

1. Total mass: \[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \]

2. Mass averaged momentum: \[ \rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) = -\nabla p - \nabla \cdot \tau + j \times B \]

3. Total thermal energy: \[ \rho C_p \left( \frac{\partial T}{\partial t} + u \cdot \nabla T \right) = \nabla \cdot (k \nabla T) + j \cdot (\sigma \mathbf{E}^\prime - \mathbf{U}_r) + \frac{\varepsilon}{2} \frac{k_B}{e} j \cdot \nabla T \]

4. Current conservation: \[ \nabla \cdot (\sigma \nabla \phi) = 0 \]

5. Ampere’s law: \[ \nabla^2 A = -\mu_0 j \]

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**Conservation equations for steady state, 2-dimensional arc, with boundary layer assumptions**

**MASS CONSERVATION** \[ \frac{\partial}{\partial z} (\rho u) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v) = 0 \]

**MOMENTUM CONSERVATION** \[ \rho \left( \frac{\partial u}{\partial z} + v \frac{\partial u}{\partial r} \right) = -\frac{\partial p}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu \frac{\partial u}{\partial r} \right) + j_r B_\theta \]

**ENERGY CONSERVATION** \[ \rho \left( \frac{\partial h}{\partial z} + v \frac{\partial h}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\kappa}{C_p} \frac{\partial h}{\partial r} \right) + \sigma \mathbf{E}_z^2 - P_r \]

**OHM’S LAW** \[ I = 2\pi \mathbf{E}_z \int_0^R \sigma r dr \]

**PERFECT GAS LAW** \[ p = \sum_r n_r kT \]

fully developed: \[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\kappa}{C_p} \frac{\partial h}{\partial r} \right) + \sigma \mathbf{E}_z^2 - P_r = 0 \]

Elenbaas-Heller
### Nomenclature

- $n_s$: Number density of atoms in energy state $s$
- $n$: Total number density of atoms
- $n_e, n_i$: Number densities of electrons, ions, respectively
- $E_s$: Energy of the state $s$
- $E_i$: Ionization energy
- $k, k_s$: Boltzmann constant
- $h$: Planck's constant
- $m_e$: Electron mass
- $p, p_e, p_i$: Partial processes of neutrals, electrons, ions, respectively
- $p$: Total pressure
- $V$: System volume
- $N$: Total number of atoms, ions, electrons in system
- $T, T_e, T_i$: Equilibrium temperature, electron and heavy particle temperature, respectively
- $v$: Velocity of atom, ion or electron
- $\rho$: Density
- $u$: Velocity, axial velocity
- $v$: Radial velocity component
- $\mu$: Viscosity
- $\tau$: Stress tensor
- $j$: Current density
- $B$: Magnetic induction
- $c_p$: Specific heat at constant pressure
- $\kappa$: Total thermal conductivity
- $E^i$: Electric field
- $U_r, P$: Volumetric radiation loss

### Discretization Methods

- System of equations (cons. mass, mom., energy, etc.) written as: $\mathcal{R}(Y) = 0$
- Formulate problem for $Y_h$, the discrete counterpart of $Y$ (vector of unknowns)
- Most common, weighted residual methods with local support:

  - **Finite Differences**
    
    \[
    \mathcal{R}(Y_h) = 0, \quad \int_{\Omega} \mathcal{R}(Y_h) d\Omega = 0
    \]
    
    - ** Finite Volumes**
      
      \[
      \int_{\Omega} \mathcal{R}(Y_h) d\Omega = 0
      \]
    
    - **Finite Elements**
      
      \[
      \int_{\Omega} W_h \mathcal{R}(Y_h) d\Omega = 0
      \]

  - If implemented correctly, all methods perform \~ same
  - Challenge for all methods: multi-scale and multi-physics problems

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Example: Temperature distribution from Elenbaas-Heller equation

**GAS = Argon; RADIUS = 2.0 mm**

<table>
<thead>
<tr>
<th>Current (A)</th>
<th>100</th>
<th>200</th>
<th>300</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power (KW/m)</td>
<td>150</td>
<td>370</td>
<td>760</td>
</tr>
<tr>
<td>Wall heat flux (W/m²)</td>
<td>9.50E + 6</td>
<td>2.50E + 7</td>
<td>5.20E + 7</td>
</tr>
</tbody>
</table>

Example: Temperature distribution from Elenbaas-Heller equation

**GAS = Hydrogen; RADIUS = 2.0 mm**

<table>
<thead>
<tr>
<th>Current (A)</th>
<th>100</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Power (KW/m)</td>
<td>410</td>
<td>750</td>
<td>1030</td>
</tr>
<tr>
<td>Wall heat flux (W/m²)</td>
<td>3.00E + 7</td>
<td>5.70E + 7</td>
<td>7.50E + 7</td>
</tr>
</tbody>
</table>
Importance of magnetic effects

interaction of self magnetic field with radial current density results in pressure gradient, flow acceleration (e.g. cathode jet)

- Cathode arc attachment has smaller diameter than arc
- Current density gradient generates pressure gradient

\[ \Delta p(r, z) = \int_r^R j(r, z)B(r, z)dr \]

\[ = \int_r^R j(r, z) \left[ \frac{\mu_0}{r} \int_0^r j(r', z)dr' \right] \]

for \( j(r, z) = \frac{I}{\pi R^2} \)

\[ \Delta p(r, z) = \frac{\mu_0 I j(z)}{4\pi} \left( 1 - \frac{r^2}{R^2} \right) \]

maximum velocities of \( 10^2 \) to \( 10^3 \) m/s

Energy transport by radiation

- radiation is important transport mechanism at plasma temperatures
  - emission and absorption
  - line radiation and continuum

- correct treatment requires determination of absorption in every volume element of irradiation from entire plasma
  - solution of radiation transfer equation
  - for large number of wavelength intervals

- different modeling approaches with simplifying assumptions exist
  - assume optically thin, only emission is counted at calculated \( T \) integrated over all wavelengths
  - use net emission coefficient based on simplified plasma geometry, integrated over all wavelengths

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Argon emission coefficients at 1 atm.

Spectral emission coefficient

Total net emission coefficient, L=optical path length

Menart, 1996

6. Non-equilibrium and turbulence

Modeling non-equilibrium conditions requires

- two energy conservation equations, one each for electrons and for heavy species
  - assuming electrons have $T_e$, all heavy species $T_h$
  - need momentum transfer cross section $Q_{eh}$

\[
\rho \frac{\partial h_h}{\partial t} + \rho \vec{u} \cdot \nabla h_h = -\nabla \cdot \vec{q}_h + \dot{Q}_{eh}
\]

heavy particle energy

\[
\rho \frac{\partial h_e}{\partial t} + \rho \vec{u} \cdot \nabla h_e = -\nabla \cdot \vec{q}_e - \dot{Q}_{eh} + \vec{J}_q \cdot \vec{E} - \dot{Q}_r
\]

electron energy

- species conservation equations including diffusion fluxes
  - rate equations determine composition
  - need diffusion coefficients for fluxes $J_s$

\[
\frac{\partial n_s}{\partial t} + \nabla \cdot (\vec{u} n_s) = -\nabla \cdot \vec{J}_s + \dot{n}_s^c
\]

- properties for different ratios $T_e/T_h$, for different non-equilibrium compositions

- significantly increases computational effort

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Approach for property calculations in 2-temperature plasma

**PROPERTY CODE**

Function of: Te, Th, P, Non-equilibrium fluxes

A. THERMODYNAMIC

- N_M, N_A, N_i, N_D, N_e, T_e, T_h

B. TRANSPORT

- σ (Elec. Cond.)
- k_e (Th. Cond. e)
- k_h (Th. Cond. h)
- μ (Viscosity)
- v_c (Coll. freq.)
- Diffusion coef.

Effect of kinetic non-equilibrium

Number densities in Ar plasma

Thermal conductivity of oxygen plasma

Pfender and Heberlein, 2007

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Turbulence Modeling

Challenging because turbulence is characterized by large span of scales (i.e. flow features from $l_1 \ldots l_n$)

Three common approaches:

1. **Direct Numerical Simulation (DNS)**
   - Solves all the scales of the flow (very expensive!)
   - Unfeasible for industrial-type problems
   - Requires no “modeling” of turbulence (i.e. no extra equations, assumptions, etc.)

2. **Large Eddy Simulation (LES)**
   - Solves for the large scales of the flow and models the small scales
   - Turbulence model needed to approximate the small scales

3. **Reynolds-Averaged Navier-Stokes (RANS)**
   - Most common approach for industrial-type problems
   - Models all scales of the flow
   - Many models developed, usually a model is adequate for a specific problem
   - Common models: 0 eqns: mixing length; 1 eqn: Spalart-Allmaras; 2 eqns: k-ε, k-ε RNG, k-ω; 7 eqns: Reynolds Stresses

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The k-ε model

- As most models, relies on Boussinesq hypothesis: turbulence is mostly dissipative → model it as an “extra” diffusion mechanism (a.k.a. turbulent viscosity $\mu_t$)
- Models transport of *turbulent kinetic energy* $k$ and its *dissipation* $\varepsilon$: $\mu_t = \rho \frac{k^2}{\varepsilon}$
- Need to solve additional transport equations for $k$ and $\varepsilon$:

$$\frac{\partial (\rho k)}{\partial t} + \text{div}(\rho k \mathbf{U}) = \text{div} \left[ \frac{\mu}{\sigma_k} \text{grad} \ k \right] + 2\mu \varepsilon \text{E}_{y} \text{E}_{y} - \rho \varepsilon$$

  - Rate of increase
  - Convective transport
  - Diffusive transport
  - Rate of production
  - Rate of destruction

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \text{div}(\rho \varepsilon \mathbf{U}) = \text{div} \left[ \frac{\mu}{\sigma_{\varepsilon}} \text{grad} \ \varepsilon \right] + C_{\mu} \frac{\varepsilon}{k} 2\mu \varepsilon \text{E}_{y} \text{E}_{y} - C_{\omega} \rho \frac{\varepsilon^2}{k}$$

  - Rate of increase
  - Convective transport
  - Diffusive transport
  - Rate of production
  - Rate of destruction

> This are equations of the “standard” k-ε model: fully turbulent steady-state flow, no body forces, constant properties, etc.

> But yet, very often used for more complex flows, i.e. thermal plasmas

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Two fluid approach to simulate large scale turbulence

Plasma jet consists of hot and cold fluid parcels exchanging energy and momentum

(P.C. Huang et al., 1995)

Two-fluid turbulence simulation results

Comparison of time averaged results with experimental data
Two-fluid simulation results of temperature and velocity distributions and particle heating

Plasma and Particle Temperatures

Plasma and Particle Velocities

Particle Trajectories

• all particles injected with same velocity
• particles see widely varying plasma temperature and velocities
• strong effect on particle properties and trajectories

7. Examples of recent calculations

Two example calculations

(1) Highly constricted arc in plasma cutting torch
• two-dimensional geometry
• assuming non-equilibrium, \( T_e \neq T_h \), \( n_e \) affected by diffusion
• oxygen as plasma gas

(2) Time dependent three dimensional plasma spray torch
• describes anode attachment instability
• assuming kinetic non-equilibrium
• argon as plasma gas

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(1) Plasma cutting torch

Ghorui et al., 2007

[Image of a plasma cutting torch]

- Highly constricted arc
- Nozzle diameter ~2 mm
- 200 A, 150 V arc transferred to work piece
- Oxygen is plasma gas

Courtesy of Hypertherm Inc.

Modeling domain that of a plasma cutting torch

- Models including a downstream region have little influence on results

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**Boundary conditions**

<table>
<thead>
<tr>
<th>Boundary Condition</th>
<th>$p$</th>
<th>$v_z$</th>
<th>$v_r$</th>
<th>$v_\theta$</th>
<th>$T_a$ (K)</th>
<th>$T_b$ (K)</th>
<th>$\phi$ (V)</th>
<th>$\sigma$</th>
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<td>-</td>
<td>$\frac{\partial \phi}{\partial z} = 0$</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

**Boundary condition at cathode surface**

- assumed current density profile derived from experimental temperature measurements
**2T-Non-equilibrium Model**

1. Electrons have \( T_e \), all heavy particles have \( T_h \)

2. Two separate energy equations are solved: one for electrons and the other for ions, in addition to momentum, mass, species and charge conservation

3. Electrons receive energy through Ohmic heating

4. Heavy particles receive energy from electrons through collisions

5. Viscous dissipation term appears only in heavy particle equation

6. Radiation loss appears only in electron energy equation

---

**Chemical non-equilibrium modeling approach**

Number density \( n_k \) of species ‘k’ inside a plasma control volume under chemical non-equilibrium is computed using the convective diffusive equation:

\[
\frac{\partial n_k}{\partial t} + \nabla \cdot (n_k \vec{u}) + \nabla \cdot \vec{g}_k = \dot{n}_k
\]

\( n_k \vec{u} \) is the convective flux, \( \vec{g}_k \) is the diffusive flux:

\[
g_k = \frac{n^2}{\rho} \sum_{j=1}^{\nu} m_j D_{kj} \left[ \nabla x_j + \frac{\rho_j}{\rho} \nabla \ln \rho \right] - \frac{n}{\rho} \sum_{j=1}^{\nu} \left( \frac{n_j Z_j e D_{kj}}{k_B T_k} \right) E^x - \frac{D_{kj}}{m_k} \nabla \ln T_k
\]

\( E^x \) is the external electric field, \( \rho \) is the total mass density, \( k_B \) is the Boltzmann constant, \( x_j \) and \( \rho_j \) are respectively the mole fraction and the mass density of species \( j \), \( D_{kj}^q \), \( D_{kj}^{\theta \theta} \) are general ambipolar and thermal diffusion coefficients.
Chemical non-equilibrium

- Net rate of accumulation or depletion of species inside a plasma volume will influence 2-T chem. Equil. rate equations:

\[
\begin{align*}
\dot{R}_A &= \frac{n_A}{n_M} \Delta R_A \\
\dot{R}_I &= \frac{n_A n_I}{n_A} \Delta R_I \\
\dot{R}_P &= \frac{n_A n_P}{n_I} \Delta R_P \\
Q_k &= \frac{R_k}{S_k}
\end{align*}
\]

- Inside plasma, it is assumed for any species k: \(0.5 < Q_k < 2\)

- Properties are tabulated as a function of \(T_e\) for every: \(p, (T_e/T_h), Z_A, Z_I, Z_D\) in discrete steps.

---

LTE model results

Arc Temperature Distribution

---

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Non-equilibrium model results

temperature distributions: $T_e$ upper half, $T_h$ lower half

- distinct difference between $T_e$ and $T_h$ in entrance region and close to wall

Non-equilibrium model results

- comparison with experiment shows acceptable agreement
  - modeling results at nozzle exit, experimental 2 mm downstream

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Collisional coupling between $T_e$ and $T_h$

- collision frequencies for different $T_e/T_h$ ratios and different non-equilibrium factors

- maximum in collision frequency coincides with temperature region where $T_e$ and $T_h$ are closest

Axial temperature distributions

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Non-equilibrium model results

Radial $n_e$ distribution

Comparison with experiment shows acceptable agreement

Radial $n_e$ distributions with and without composition non-equilibrium

Noticeable effect at intermediate radii

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Non-equilibrium model results

Axial velocity

- strongest acceleration near nozzle exit

Non-equilibrium model results

Axial current density distribution

- strong variations in nozzle entrance region

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(2) Time dependent model of plasma spray torch
Trelles and Heberlein, 2006

**Numerical Approach: Stabilized FEM**

- **System of transient – advective – diffusive – reactive equations:**

\[
\frac{\partial Y}{\partial t} + (A \cdot \nabla)Y - \nabla \cdot (K \nabla Y) - (S_1 Y + S_0) = R(Y) = 0
\]

- **Stabilized and Multi-scale Methods:** \( Y = \bar{Y} + Y' \)

\[
\int_{\Omega} \mathbf{W} \cdot R(\bar{Y}) d\Omega + \int_{\Omega'} \mathbf{P}(\bar{Y}) \delta \cdot R(\bar{Y}) d\Omega' = 0
\]

- **Solution:** \(\alpha\)-method, Globalized Inexact-Newton, Pre-Cond. GMRES

**Computational Domain \(\Omega\)**

- capture arc + jet
- hexahedral elements
  (8 nodes / element)
- unknowns per node:
  - 9 for LTE model
  - 10 for NLTE model

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Boundary Conditions

| Side 1: inlet | \( p = p_0 \) | \( \omega = \omega_{0,\text{in}} \) | \( T = T_{\text{in}} \) | \( \phi_{\text{in}} = 0 \) | \( A_{\text{in}} = 0 \) |
| Side 2: cathode | \( p_{\text{in}} = 0 \) | \( u_{\text{in}} = 0 \) | \( T = T_{\text{c}} \) | \( \phi_{\text{c}} = 0 \) | \( A_{\text{c}} = 0 \) |
| Side 3: cathode tip | \( p_{\text{in}} = 0 \) | \( u_{\text{in}} = 0 \) | \( T = T_{\text{c}} \) | \( -\alpha \nabla_{\text{c}} \cdot \vec{f} \) | \( A_{\text{c}} = 0 \) |
| Side 4: outlet | \( p_{\text{out}} = 0 \) | \( u_{\text{out}} = 0 \) | \( T_{\text{out}} = 0 \) | \( \phi_{\text{out}} = 0 \) | \( A_{\text{out}} = 0 \) |
| Side 5: anode | \( p_{\text{an}} = 0 \) | \( u_{\text{an}} = 0 \) | \( -\kappa T_{\text{an}} = h_{\text{an}}(T - T_{\text{an}}) \) | \( \phi = 0 \) | \( A_{\text{an}} = 0 \) |

Cases Studied

<table>
<thead>
<tr>
<th>Gas</th>
<th>Current [A]</th>
<th>Flow Rate [slpm]</th>
<th>Injection</th>
</tr>
</thead>
<tbody>
<tr>
<td>Torch 1</td>
<td>Ar-H₂</td>
<td>600</td>
<td>60</td>
</tr>
<tr>
<td>Torch 2</td>
<td>Ar-H₂</td>
<td>600</td>
<td>60</td>
</tr>
<tr>
<td>Torch 3a</td>
<td>Ar-H₂</td>
<td>600</td>
<td>60</td>
</tr>
<tr>
<td>Torch 3b</td>
<td>Ar-H₂</td>
<td>600</td>
<td>60</td>
</tr>
</tbody>
</table>

Arc and Jet Dynamics

undulating and fluctuating nature of jet captured by simulation

movement of arc → jet forcing

Schlieren image plasma jet turbulence

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Arc Dynamics: Approach 1 (LTE)

Old attachment

New attachment forms

New attachment remains

Too large voltage drop !!!

Improved Approach: Non-Equilibrium Model

• Thermal non-equilibrium ($T_e \neq T_h$) (NLTE):

\[
\begin{array}{cccccc}
  i & Y_i & \text{transient} & \text{advective} & \text{diffusive} & \text{reactive} \\
  1 & p & \rho \frac{\partial \rho}{\partial t} & \bar{u} \cdot \nabla \rho + \rho \nabla \cdot \bar{u} & 0 & 0 \\
  2 & \bar{u} & \rho \frac{\partial \bar{u}}{\partial t} & \rho \bar{u} \cdot \nabla \bar{u} - \nabla p & - \nabla \cdot \bar{\tau} & \bar{J}_q \times \bar{B} \\
  3 & T_h & \rho \frac{\partial h_h}{\partial t} & \rho \bar{u} \cdot \nabla h_h & - \nabla \cdot \bar{q}_h & \frac{Dp_h}{Dt} + \dot{Q}_{eh} \\
  4 & T_e & \rho \frac{\partial h_e}{\partial t} & \rho \bar{u} \cdot \nabla h_e & - \nabla \cdot \bar{q}_e & \frac{Dp_e}{Dt} + \dot{Q}_J - \dot{Q}_r - \dot{Q}_{eh} \\
  5 & \phi_p & 0 & 0 & - \nabla \cdot \bar{J}_q & 0 \\
  6 & \bar{A} & \frac{\partial \bar{A}}{\partial t} & \nabla \phi_p - \bar{u} \times \nabla \times \bar{A} & \eta \nabla^2 \bar{A} & 0 \\
\end{array}
\]

If $T_e = T_h \Rightarrow$ LTE model

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Arc Dynamics: Approach 3 (NLTE)

Comparison with Experiments

- Voltage frequencies **NLTE & LTE** can match
- BUT … more realistic voltage drops with **NLTE** model
- Wide spectra in exp. data due to pure Ar & new anode

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Electric Potentials and Fields

- Non-LTE model produces more realistic voltage drops

Pressure and Velocity

- Formation of cathode jet
- Cold flow avoids entering hot plasma
- Inflection point in velocity profiles → K-H instability (?)
8. Electrode Regions

Anode region

- drop of temperature and electrical conductivity near surface poses problem for describing current transfer
- modeling must consider all diffusion effects, charge flux influences on electric fields
- column fluid flow (mass and energy transport) affect anode region
- column models usually assume region with artificially high electrical conductivity between column and surface

Cathode region

- cathode electron emission model required
- always strong space charges, strong cathode fall
- numerous detailed models exist dividing cathode region into space charge sheath, ionization and thermalization zone
- column models usually assume current density distribution at cathode boundary

Relations Describing Arc Characteristics in Anode Region

Conservation equations including separate electron energy equations

Maxwell’s equations

Generalized Ohm’s law (without B-field, thermodiffusion)

\[ j = \sigma \left( E + \frac{1}{en_e} \frac{dp_e}{dx} \right) \]

\[ I = 2\pi \int_{r_o}^{r_k} j dr = 2\pi \int_{r_o}^{r_k} \sigma \left( E + \frac{1}{en_e} \frac{dp_e}{dx} \right) dr = \text{const.} \]

Heat loss from arc to anode requires heat into anode region
- Increased dissipation: \( \sigma(T) \uparrow , \ E \uparrow , \ R \downarrow \Rightarrow \text{constriction} \)
- Energy transport into anode region by convection \( R \uparrow \) or \( |\text{grad } n_o| \uparrow , \ E \downarrow \Rightarrow \text{diffuse attachment} \)

Decrease of \( E \) in anode region can mean negative anode fall
- Predicted theoretically, confirmed by some experiments

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Contributions to the total current density in an argon arc (I = 200 A) (Jenista et al., 1997)

- electron density gradient becomes principal current driver
- electric field reverses to reduce electron flux

Temperature profiles in anode boundary layer

Predicted $T_e$ and $T_h$ profiles (left) and measured $T_e$ profile (right)

- $T_e$ remains high

Jenista et al., 1997, Yang et al., 2006.
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Different Contributions to Anode Heat Flux

\[
q = j\phi_w + \left( \frac{5 k}{2 e} + \frac{\phi}{\sigma} \right) jT_e - k_a \frac{dT}{dx} - k_e \frac{dT_e}{dx} + j_i (\varepsilon_i - \phi_w)
\]

Comparison of calculated and experimental anode heat flux distributions

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Arc Anode Attachment: Constricted vs. Diffuse Mode

**Constricted Mode:**
- anode jet and cathode flow form stagnation layer away from anode

**Diffuse mode:**
- anode surface serves as stagnation plane

Streamlines in Anode Boundary Layer for Two Anode Attachment Modes

*Argon, 1 atm, 200 A*

- arc constriction for increased gas heating
- anode jet forces cold gas entrainment (thermal pinch)

- high flow compresses thermal boundary layer
- increases arc diameter in stagnation region
Temperature Distributions of Ions and Neutrals for Two Anode Attachment Modes
Argon, 1 atm, 200 A

• increased energy dissipation can lead to maximum for $T_h$, $T_e$, $n_e$
• monotonic drop in $T_h$, $T_e$, $n_e$

Electric potential distributions for a constricted and a diffuse attachment of an argon arc ($I = 200$ A)

• potential difference between column and anode positive for constricted mode, about zero for diffuse mode
• potential gradient shows increase for constricted mode, monotonic drop for diffuse mode
• both modes show negative gradients immediately in front of anode

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Anode heat flux distributions in an argon arc (I = 200 A)

- Constricted mode brings 4 fold increase in peak heat flux for approximately the same total heat transfer

![Graph showing heat flux distributions in an argon arc](image)

**Thermionic Cathode Emission Mechanism**

- Electrons from stationary hot spot (> 3500K)
- Spot is heated through ion bombardment
- High melting point materials e.g. W, C, Mo, Zr
- Typical current densities $\sim 10^4$ A/cm$^2$

**Current density given by Richardson-Dushman**

$$j = AT^2 \exp\left(-\frac{e \phi_{eff}}{kT}\right) \quad \phi_{eff} = \phi_W - \left(\frac{eE}{4 \pi \varepsilon_0}\right)^{1/2}$$

- $A \approx 60$ A/cm$^2$k$^2$ for most metals
- $\phi_W =$ work function = energy requirement for release of one electron
  - 4-5 V for electronegative metals (Cu, Ag, W)
  - 1.5 - 4 V for electropositive metals (Th, Ca, Ba)

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Thermionic current density as function of temperature

- at $10^4$ A/cm$^2$, a reduction of $\Phi$ by 2 V results in a cathode temperature reduction of about 1700 K

Arc cathode model
(Zhou and Heberlein, 1994)
Cathode temperature distribution
Comparison of modeling and experimental results

• Fast evaporation of thoria from the cathode spot may increase the work function of 2% ThO$_2$-W cathodes. (6.4 mm, truncated, 200 A, Ar)

Effect of Cathode Diameter on Temperature and Heat Transfer

• Cathode tip temperature is primarily a function of work function and of arc parameters
• Cathode tip cooling at 100 A is primarily through electron emission
Cathode tip temperatures

9. Conclusions

- Thermal plasma models rely on simplifications for obtaining results
  - some very good predictions have been obtained
- major issues are non-equilibrium regions, instabilities
  - 2-temperature properties, diffusion fluxes
  - time dependent calculations
- limited availability of transport properties of gas mixtures
  - very cumbersome to calculate
- present state of computer technology limits advances
  - run times of more than a month for realistic 3-D, non-equilibrium model
- electrode models usually describe effects in limited parameter range
- solution for contradictions with some experimental results will require novel modeling approaches
  - non-continuum formulation
- models for high currents/high current densities still needed
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X. Zhou

Selected Bibliography

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2. Properties

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3. Radiation


4. Modeling Results


5. Electrode Models


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