SAND2012-1369 C

Ablation Thermochemistry for TACOT

5th Ablation Workshop

February 28, 2012

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Motivation

Gas phase and gas/surface ablation thermochemistry

- **STANJAN and CEA chemical equilibrium codes**
- **ACE and MAT ablation thermochemistry codes**
- **Thermochemical ablation data has historically been interpolated from tabular data by an ablation code**
- **Computing on-the-fly has several advantages**
  - **Eliminate interpolation error**
  - **Eliminate multi-dimensional (4D and up) interpolation**
    - **Interpolate from P, T, B'_g, C_M, C_h, diff. coeff., etc.**
  - **Enable previously intractable computations**
  - **Ultimately eliminate the need for B'_c**

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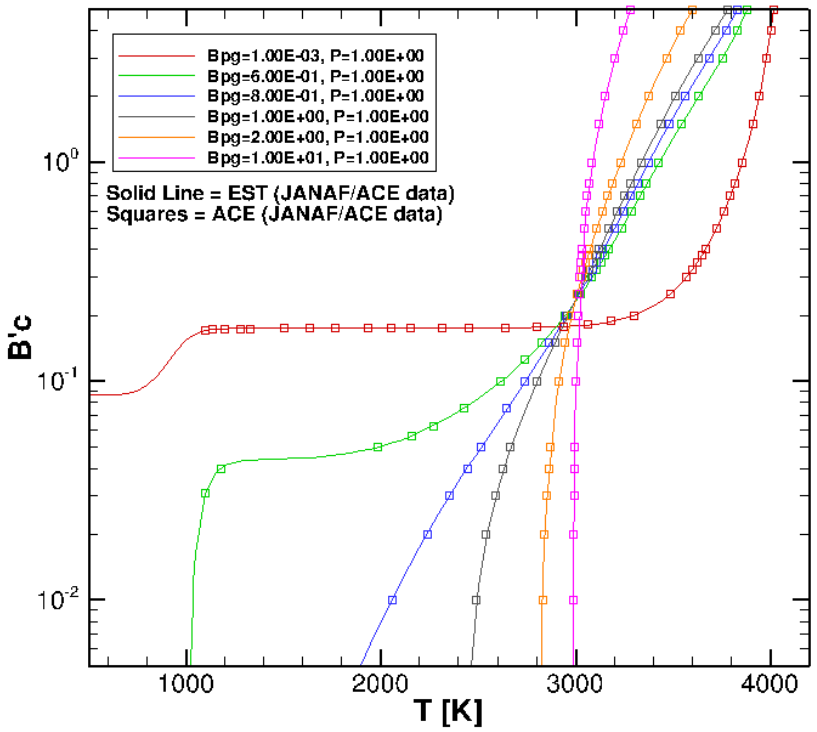
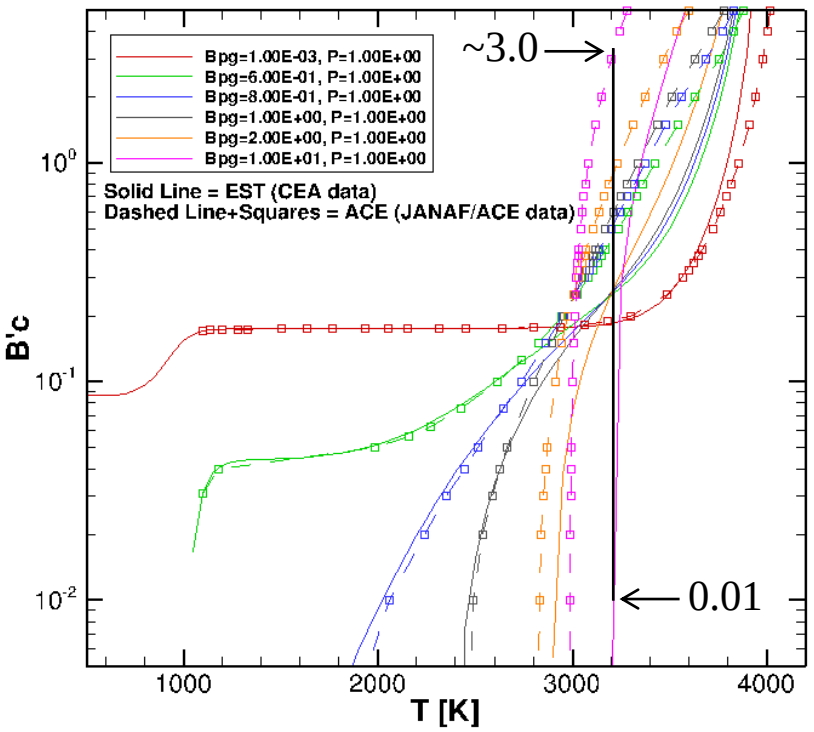
B'_c for TACOT in Air: Methods & Databases

Considering all available gas species (JANAF/ACE=90 species, CEA=156 species)

Different Methods/Same Database



Same Method/Different Databases



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h for TACOT in Air: Methods & Databases

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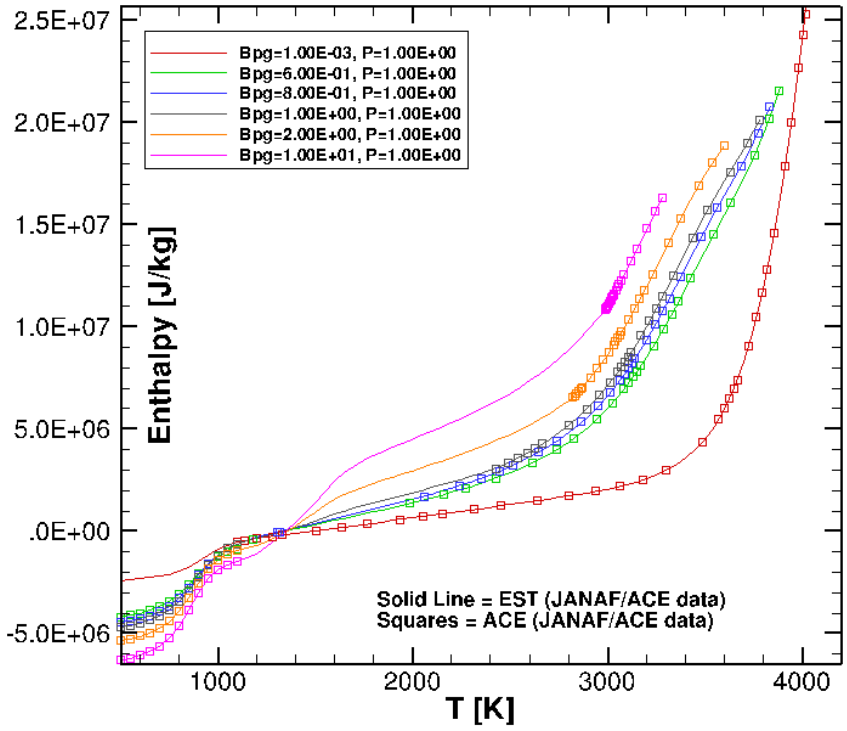

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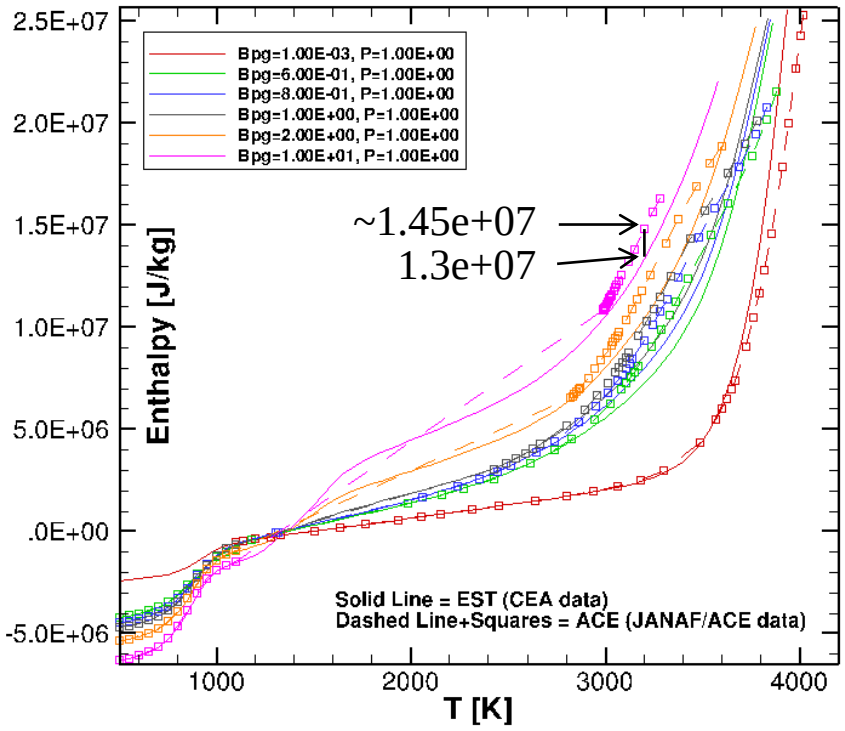

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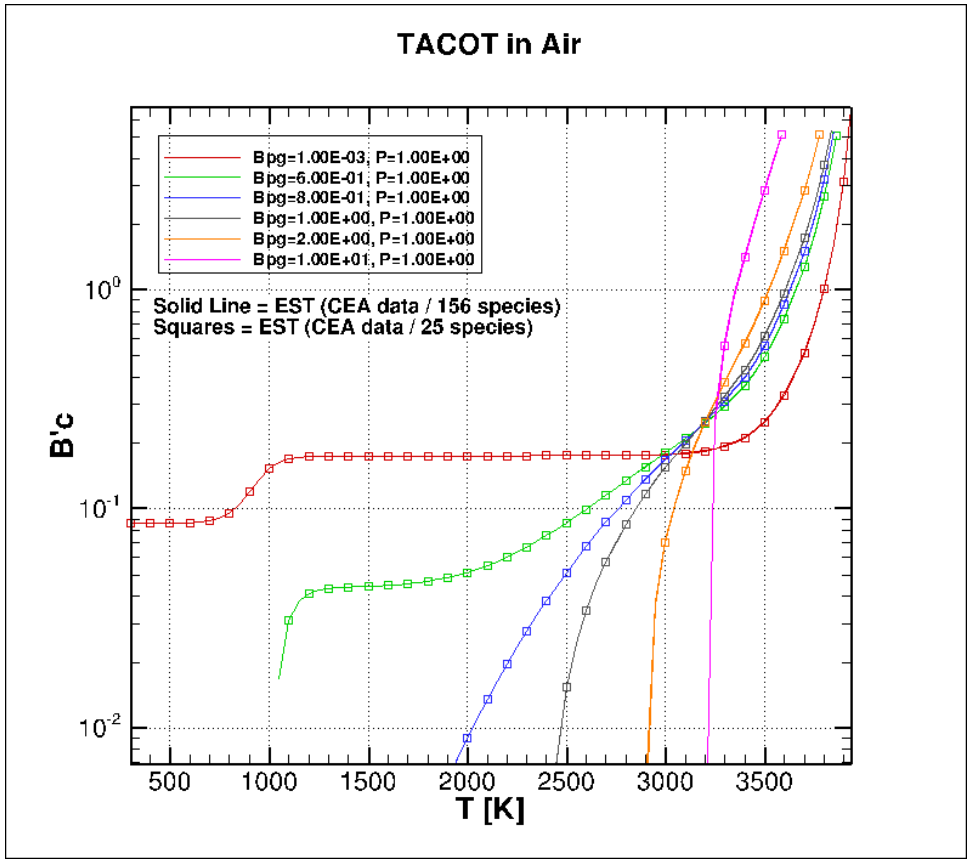
B'_c for TACOT in Air: Specie Selection

Considering all available gas species and a reduced set (156 species vs. 25 species)

25 species = C; H; O; N; CH4; CN; CO; CO2; C2; C2H; C2H2,acetylene; C3; C4; C4H2,butadiyne; C5; HCN; H2; H2O; N2; CH2OH; CNN; CNC; CNCOCN; C6H6; HNC



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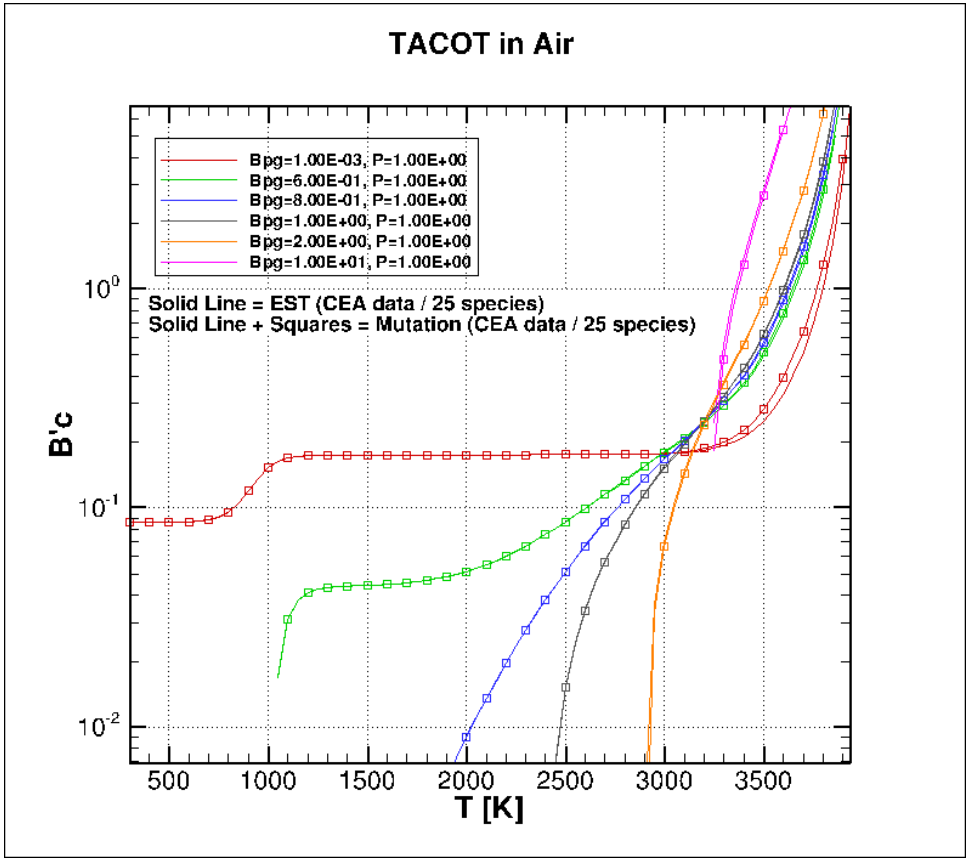
B'_c for TACOT in Air: Mutation Results

Considering 25 specie reduced set



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Conclusions

- Implementation of the element potential method for ablation thermochemistry problems
- Efficient nonlinear convergence via ‘smart’ initialization of the system
- B'_c and enthalpy comparisons with ACE favorable for a carbon-phenolic like material
- Integrated ablation tests with EST show negligible differences compared to using tabular B'_c data
- Differences resulting from different thermodynamic databases is concerning

Questions?

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