

Abstract Submitted
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The influence of chemical mechanisms on PDF calculations of non-premixed turbulent flames¹ STEPHEN B. POPE, RENFENG RICHARD CAO, Cornell University — A series of calculations is reported of the Barlow & Frank non-premixed piloted jet flames D, E and F, with the aim of determining the level of description of the chemistry necessary to account accurately for the turbulence-chemistry interactions observed in these flames. The calculations are based on the modeled transport equation for the joint probability density function of velocity, turbulence frequency and composition (enthalpy and species mass fractions). Seven chemical mechanisms for methane are investigated, ranging from a five-step reduced mechanism to the 53-species GRI 3.0 mechanism. The results show that, for C-H-O species, accurate results are obtained with the GRI 2.11 and GRI 3.0 mechanisms, as well as with 12 and 15-step reduced mechanisms based on GRI 2.11. But significantly inaccurate calculations result from use of the 5-step reduced mechanism (based on GRI 2.11), and from two different 16-species skeletal mechanisms. As has previously been observed, GRI 3.0 over-predicts NO by up to a factor of two; whereas NO is calculated reasonably accurately by GRI 2.11 and the 15-step reduced mechanism.

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