In the present paper, synchrotron VUV photoionization mass spectrometry is used to study the detailed chemistry of co-flow methane diffusion flames with different dilution ratios. The experimental results constitute a comprehensive characterization of species important for PAH and soot formation under conditions that resemble those of practical flames. In addition to the main C1/C2 species, unsaturated C3 (C3H2, C3H3, aC3H4, pC3H4), C4 (C4H2, C4H4, C4H6), and C6 (C6H2) species as well as first aromatics (C5H6, C6H6, C7H8, C10H8, C12H8) are detected. The laminar, co-flow flames were simulated using an original CFD code based on the operator-splitting technique, specifically conceived to handle large kinetic mechanisms. The detailed kinetic modeling was effectively used to describe and analyze the fuel consumption and the formation of PAH. Experimental measurements and numerical predictions were found to be in satisfactory agreement and showed the relative importance of the C2 and C3 mechanisms in the formation of the first aromatics.

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