

The Influence of Chemical Mechanisms on PDF Calculations of Non-Premixed Piloted Jet Flames

Supplementary Material

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7/16/2005

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Description of supplementary material

The supplementary material presented here pertains to the joint PDF calculations of the Barlow & Frank [1] piloted jet flames described in the paper “*The influence of chemical mechanisms on PDF calculations of non-premixed piloted jet flames*,” R.R. Cao & S.B. Pope, *Combust. Flame* (2005). The numerical parameters are the same as those specified in the main paper, and the base configuration is used throughout, with two exceptions: in some calculations radiation is neglected; and in some calculations the pilot temperature T_p is changed (by 20K).

The Table on the following pages specifies the conditions of each calculation – the flame, the mechanism used, radiation model, pilot temperature – and a corresponding “case label” is defined. The radiation models used are “optically–thin” and “adiabatic”, and are indicated by “Y” and “N”, respectively, in the Table.

The results are reported in three parts: burning indices; conditional means and rms’s; and unconditional means and rms’s. The Table of contents provides a useful guide to the organization of the results. In the figures, the symbols have the same meanings as in the main paper, and the figure titles and legends provide a full description of the results reported. The experimental data shown are from [1] and [22].

[1] Barlow, R.S. and J.H. Frank, *Proc. Combust. Inst*, 27 (1998) 1087-1095

[22] Web site for the International Workshop on Measurement and Computation of Turbulent Non-premixed Flames (TNF), R. S. Barlow, Ed., Sandia National Laboratories, <http://www.ca.sandia.gov/tdf/Workshop>.

List of test cases

Test cases with EMST, $C\phi=1.5$, ISAT $\epsilon_{tol}=2\times 10^{-5}$

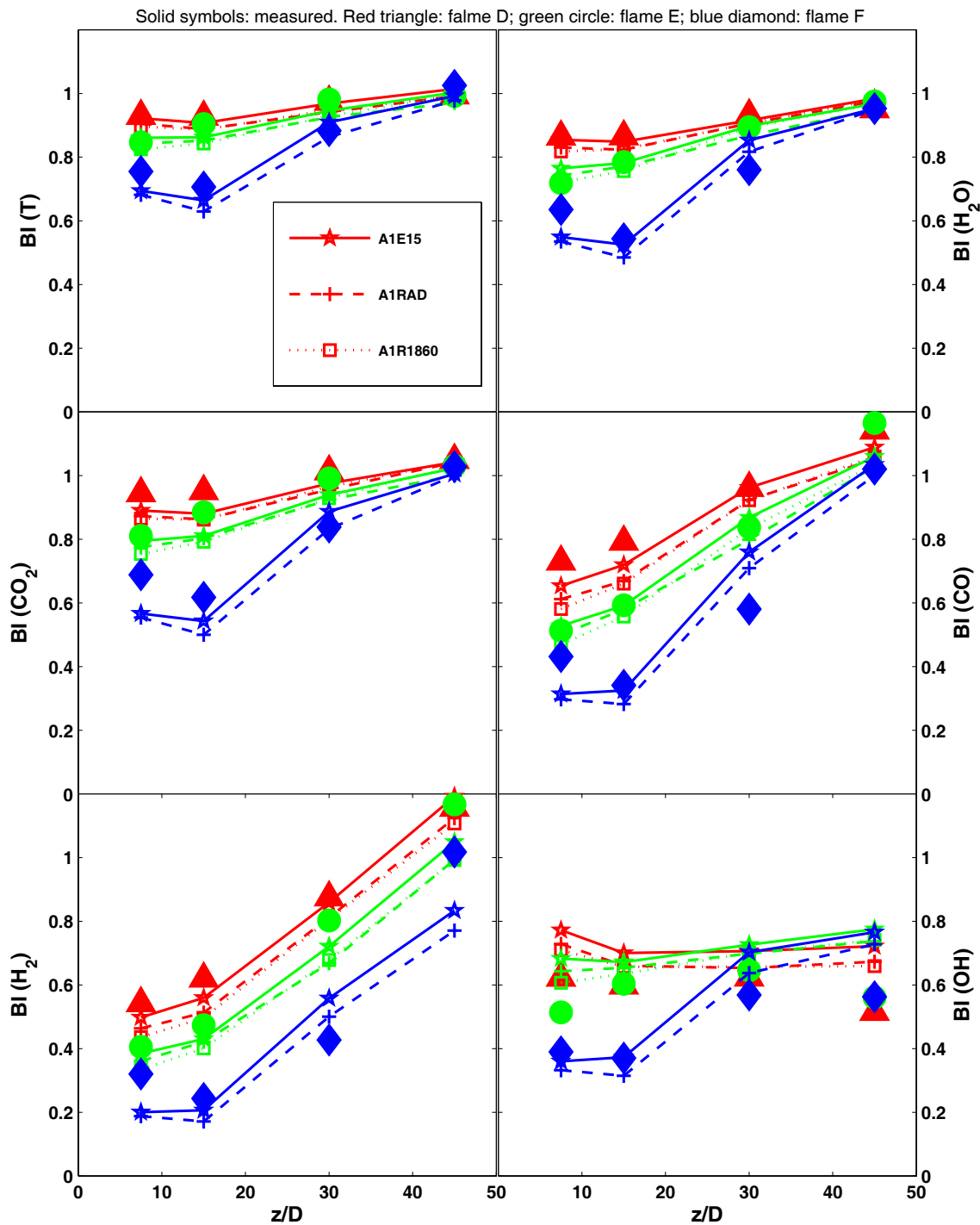
Mechanisms	Flame	Radiation	Pilot temperature (K)	Case Label	Note	
ARM1	D	N	1880	A1E15		
		Y	1880	A1RAD		
		Y	1860	A1R1860		
	E	N	1880	A1E15		
		Y	1880	A1RAD		
		Y	1860	A1R1860		
	F	N	1880	A1E15		
		Y	1880	A1RAD		
		Y	1860	A1R1860	Extinguished	
ARM2	D	N	1880	A2E15		
		Y	1880	A2RAD		
		Y	1860	A2R1860		
	E	N	1880	A2E15		
		Y	1880	A2RAD		
		Y	1860	A2R1860		
	F	N	1880	A2E15		
		Y	1880	A2RAD	Extinguished	
		Y	1860	A2R1860	Extinguished	
		N	1860	A21860		
	GRI2.11	D	N	1880	G2E15	
			Y	1880	G2RAD	
E		N	1880	G2E15		
		Y	1880	G2RAD		
F		N	1880	G2E15		
		Y	1880	G2RAD		

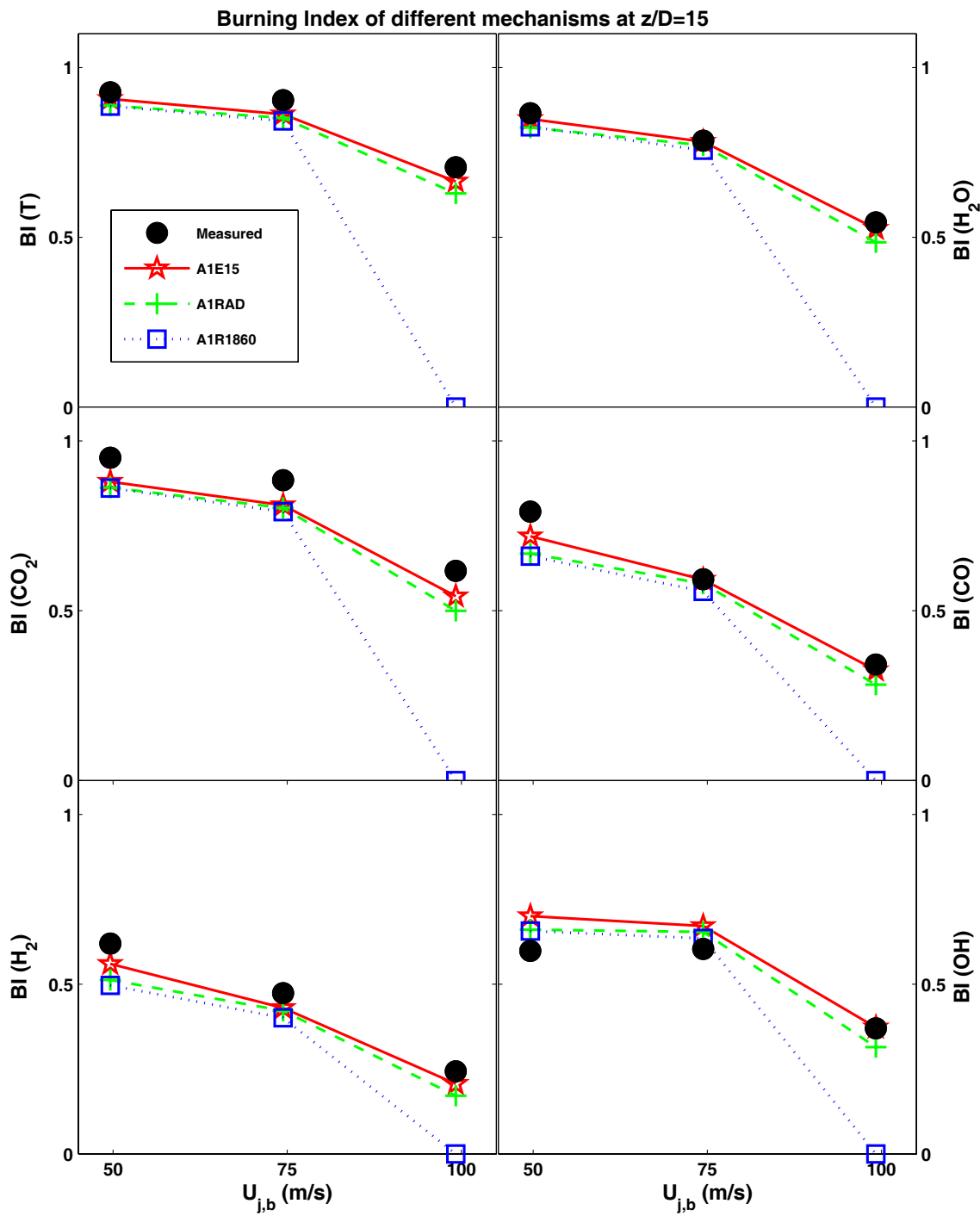
		Y	<i>1860</i>	G2R1860	
GRI3.0	E	N	1880	G3E15	
		Y	1880	G3RAD	
	F	N	1880	G3E15	
		Y	1880	G3RAD	
		Y	<i>1860</i>	G3R1860	
Skeletal	D	N	1880	SkE15	
		Y	1880	SkRAD	
	E	N	1880	SkE15	
		Y	1880	SkRAD	
	F	N	1880	SkE15	
		Y	1880	SkRAD	
		Y	<i>1860</i>	SkR1860	
Smooke	D	N	1880	SmE15	
		Y	1880	SmRAD	
	E	N	1880	SmE15	
		Y	1880	SmRAD	
	F	N	1880	SmE15	Extinguished
		Y	1880	SmRAD	Extinguished
S5G211	D	N	1880	S5E15	
		Y	1880	S5RAD	
	E	N	1880	S5E15	
		Y	1880	S5RAD	
	F	N	1880	S5E15	
		Y	1880	S5RAD	
		Y	<i>1860</i>	S5R1860	

Part A: Summary of Burning Index

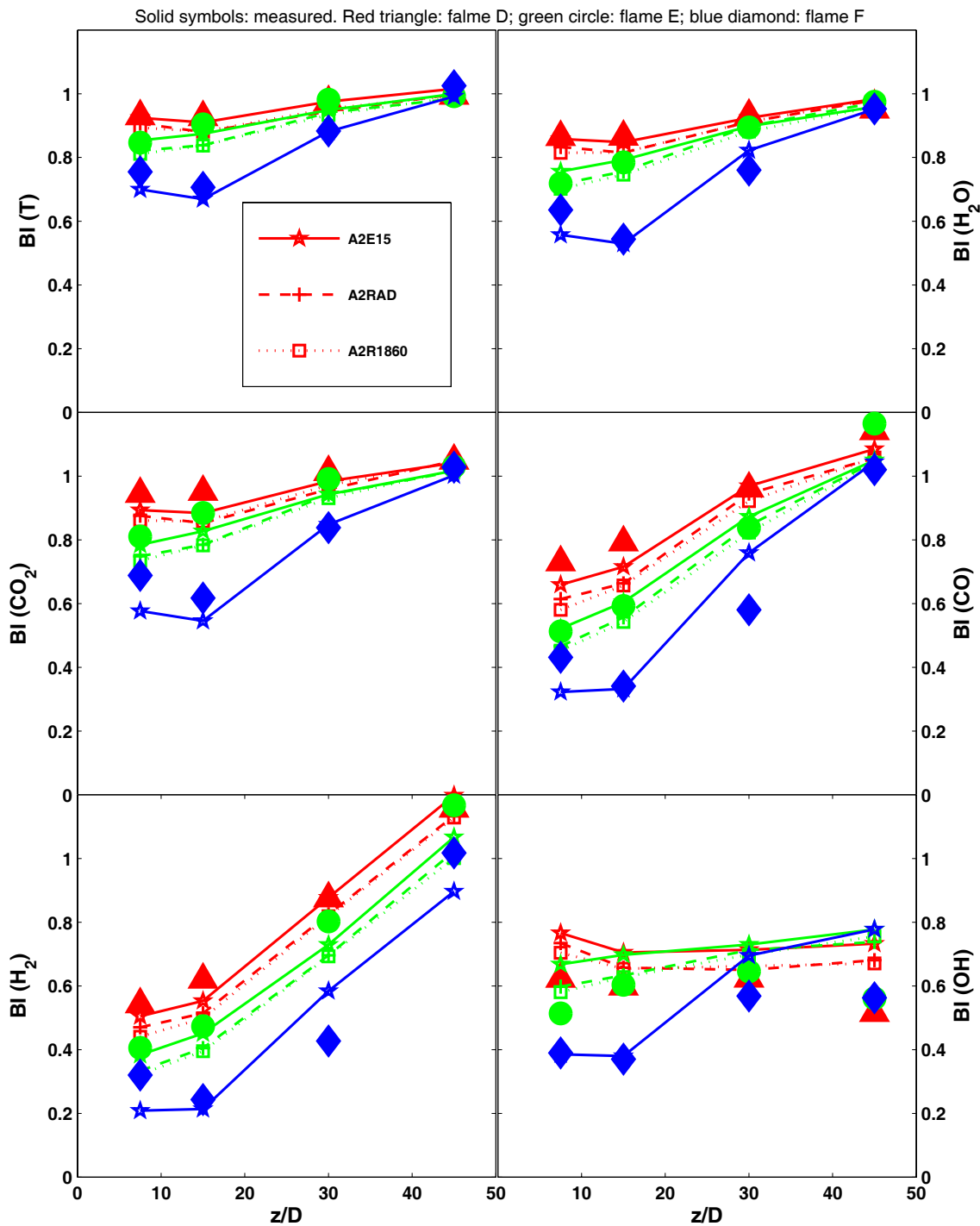
A-1 performance of single mechanisms

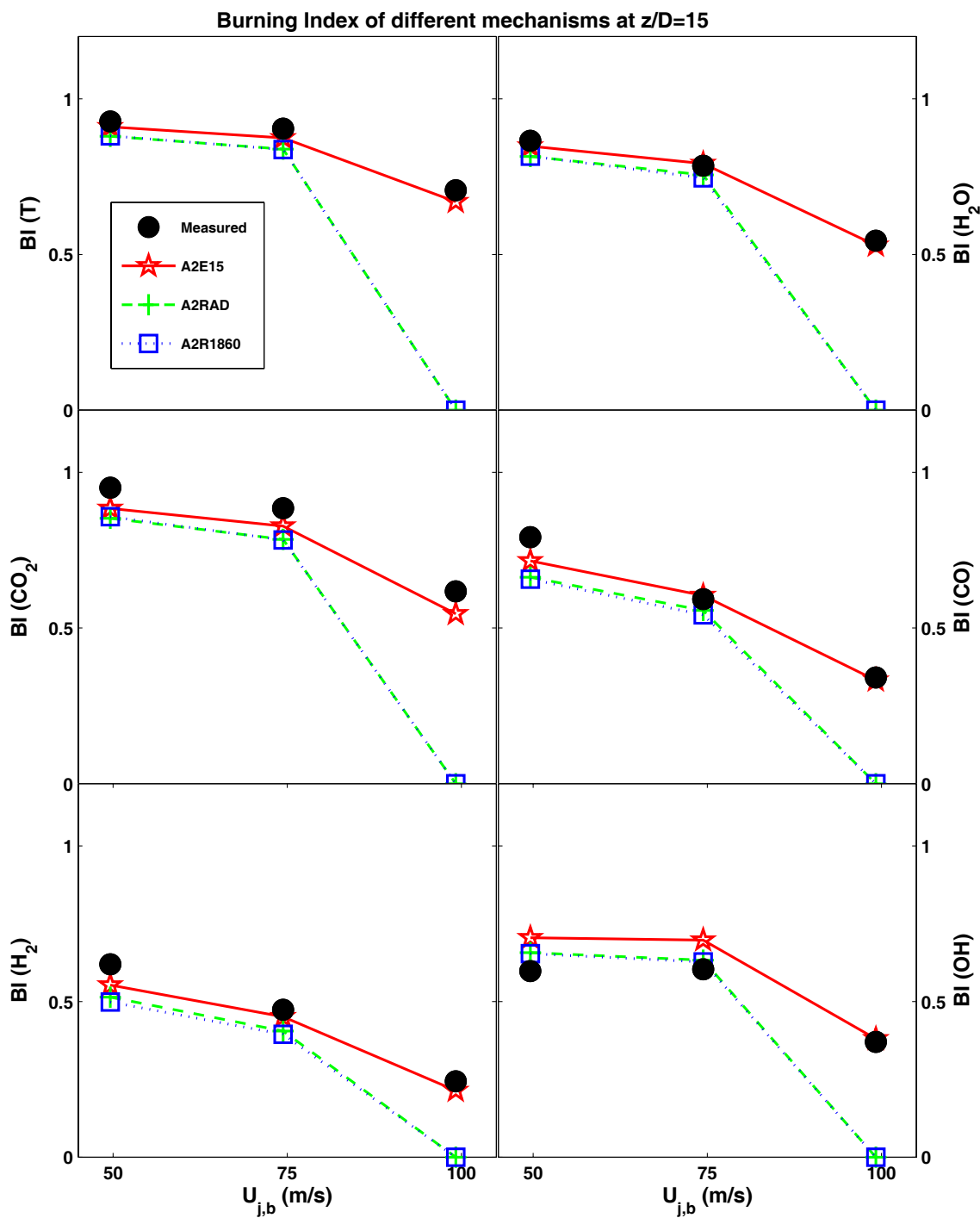
(1) ARM1 mechanism



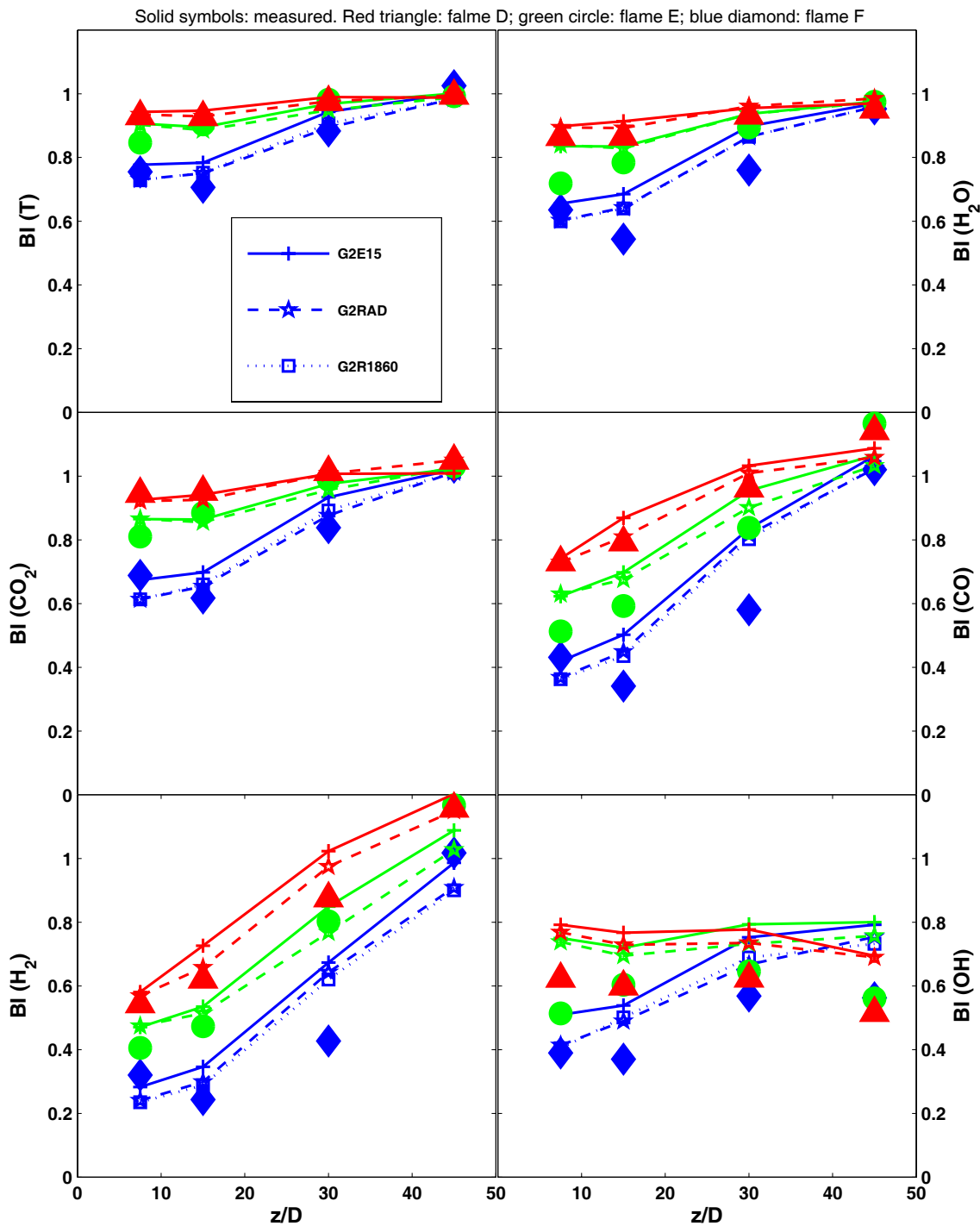


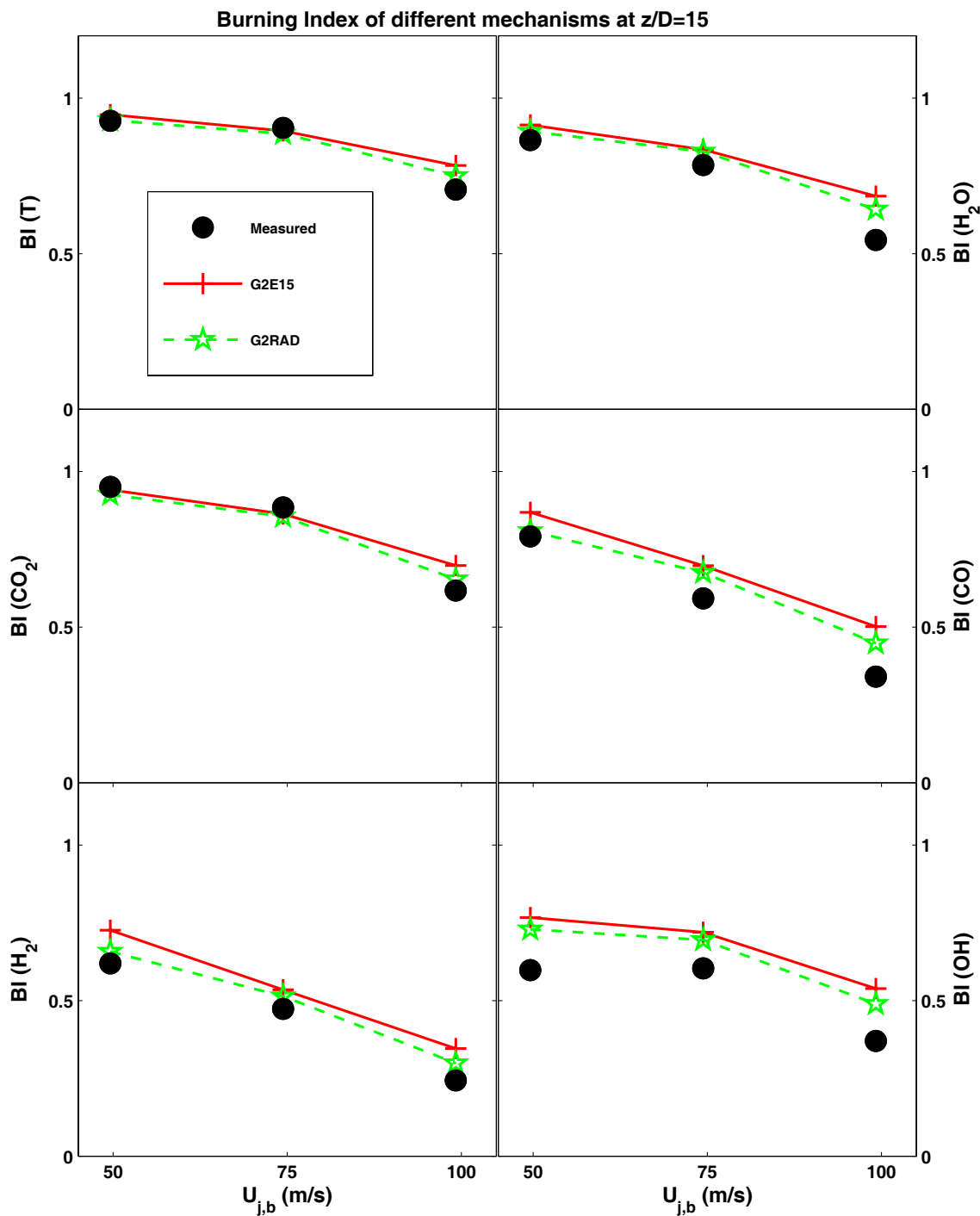
(2) ARM2 mechanism



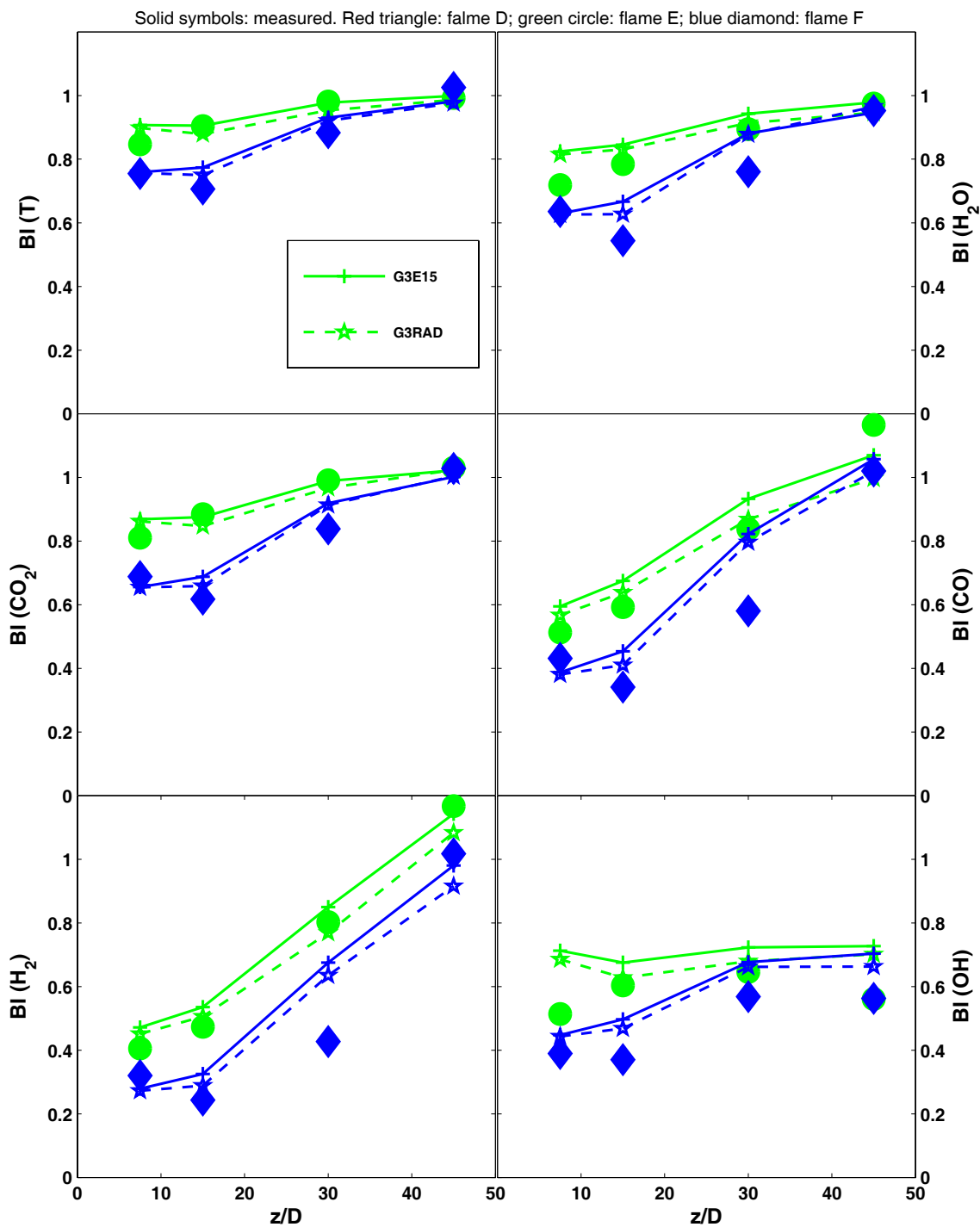


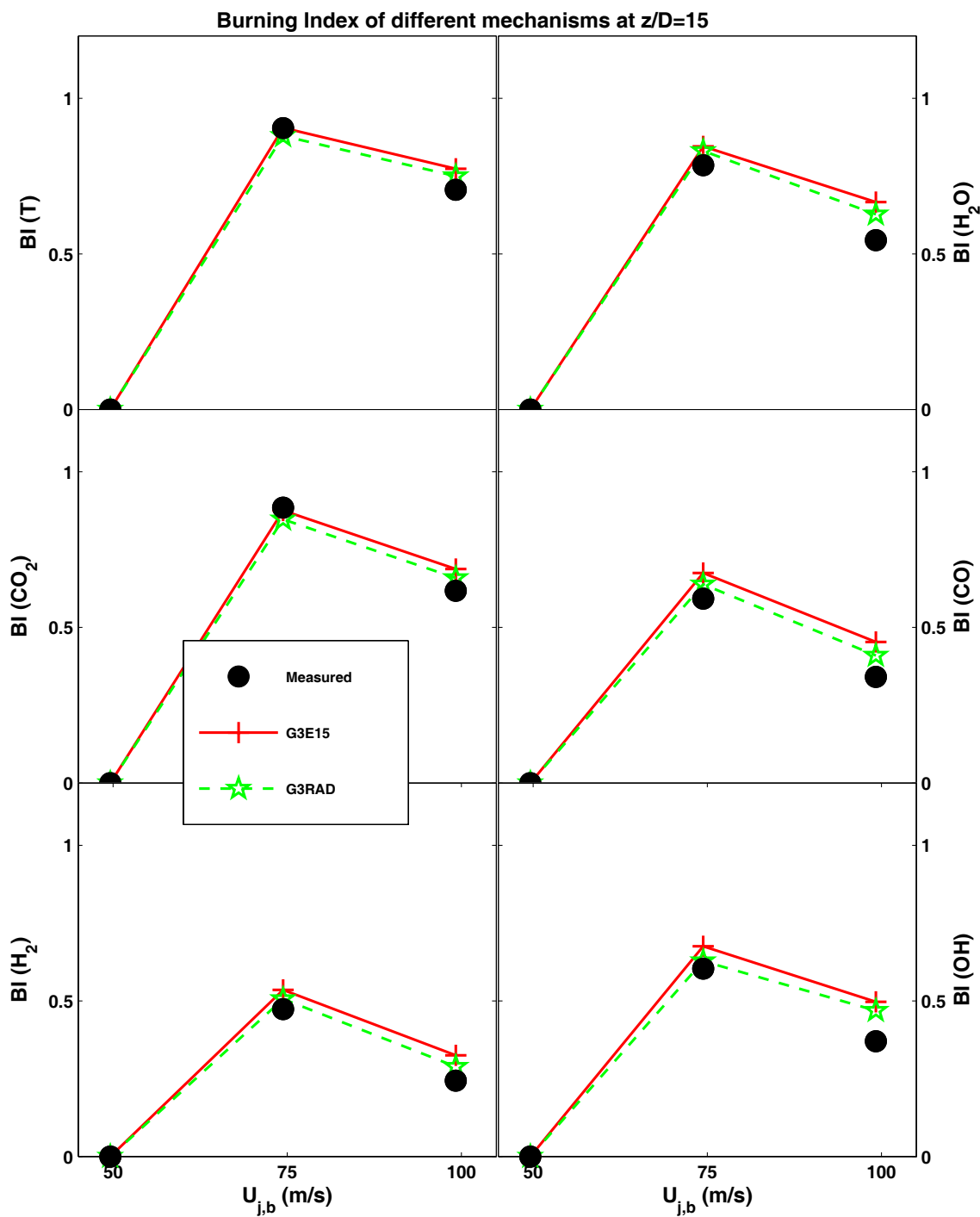
(3) GRI2.11



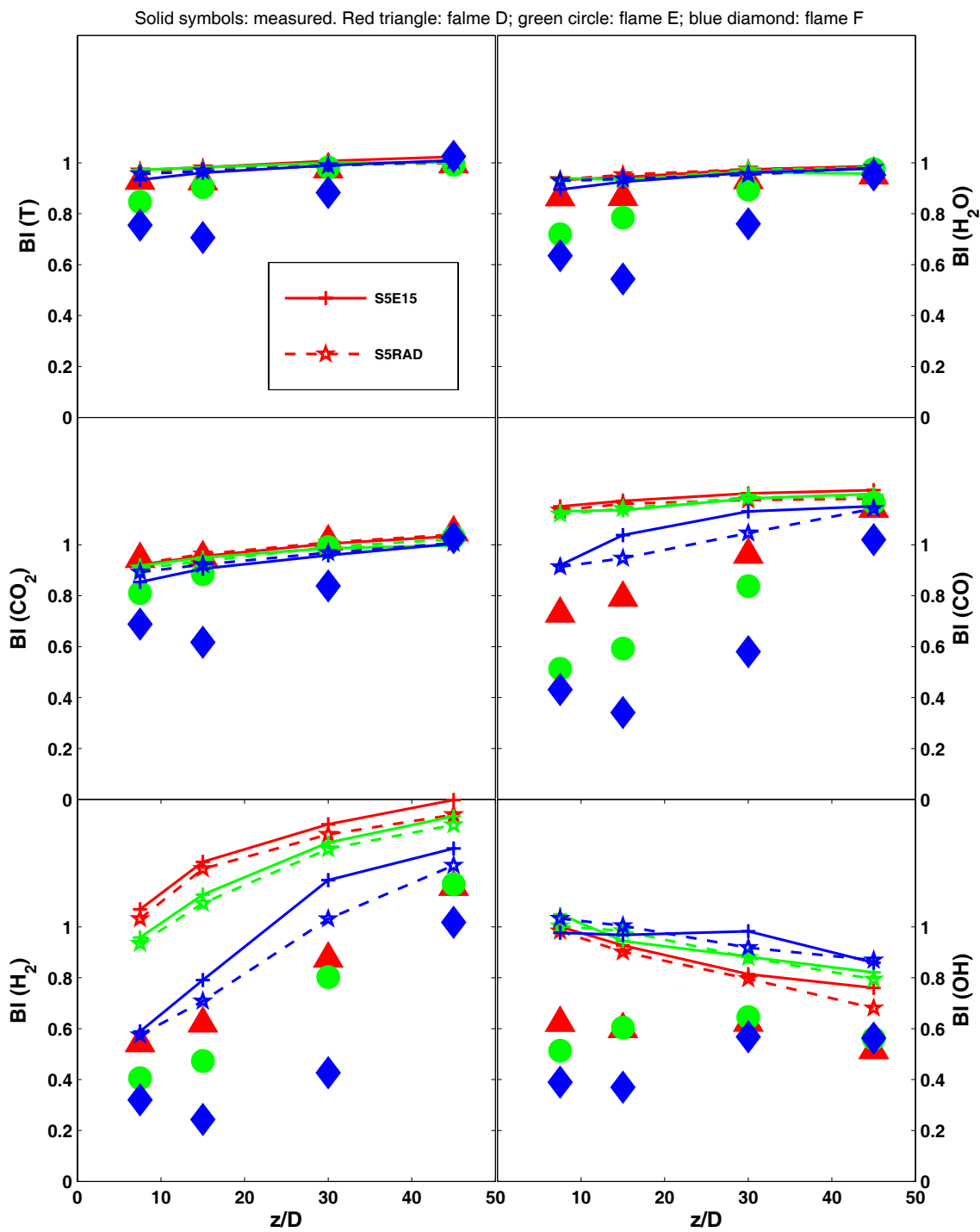


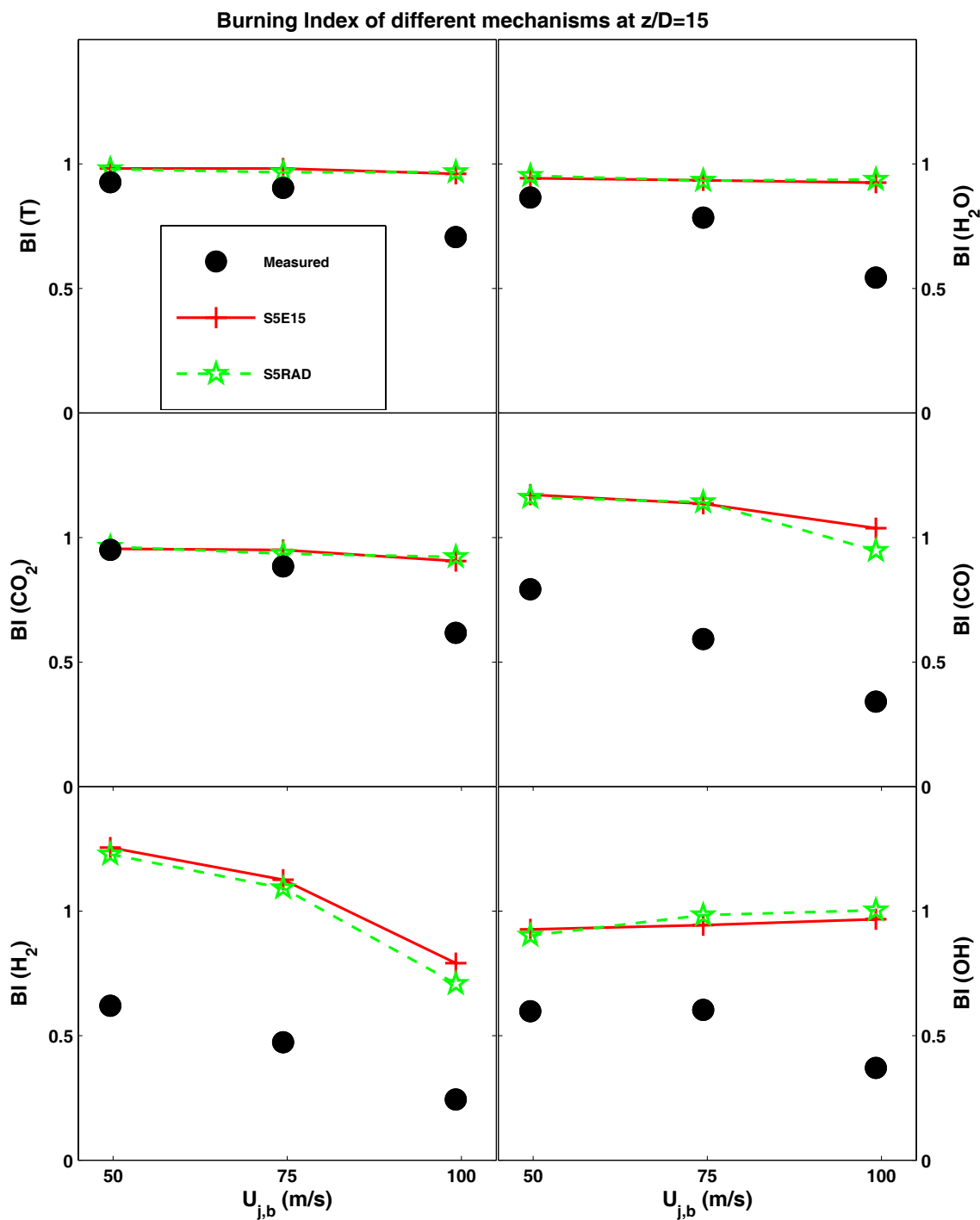
(4) GRI3.0



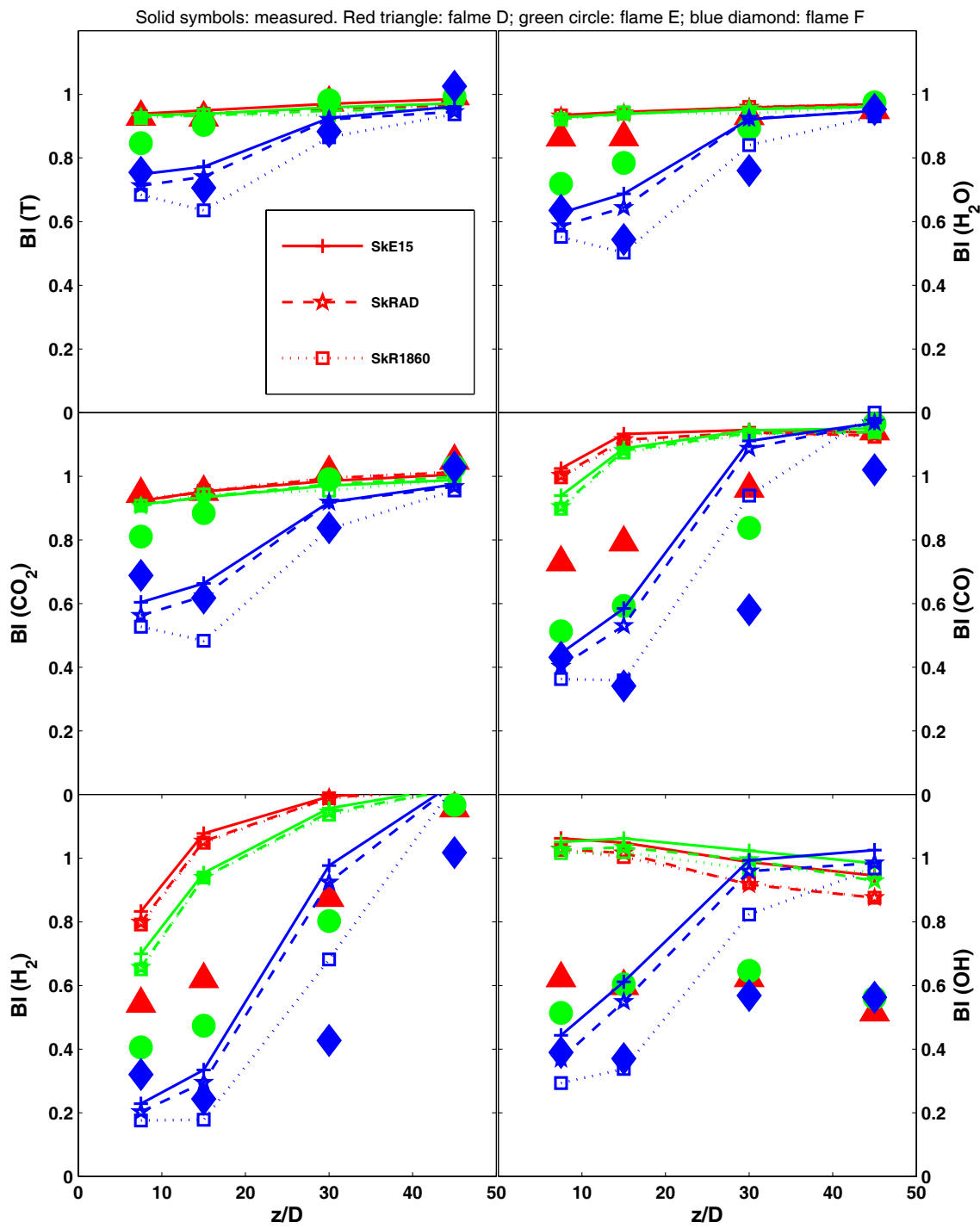


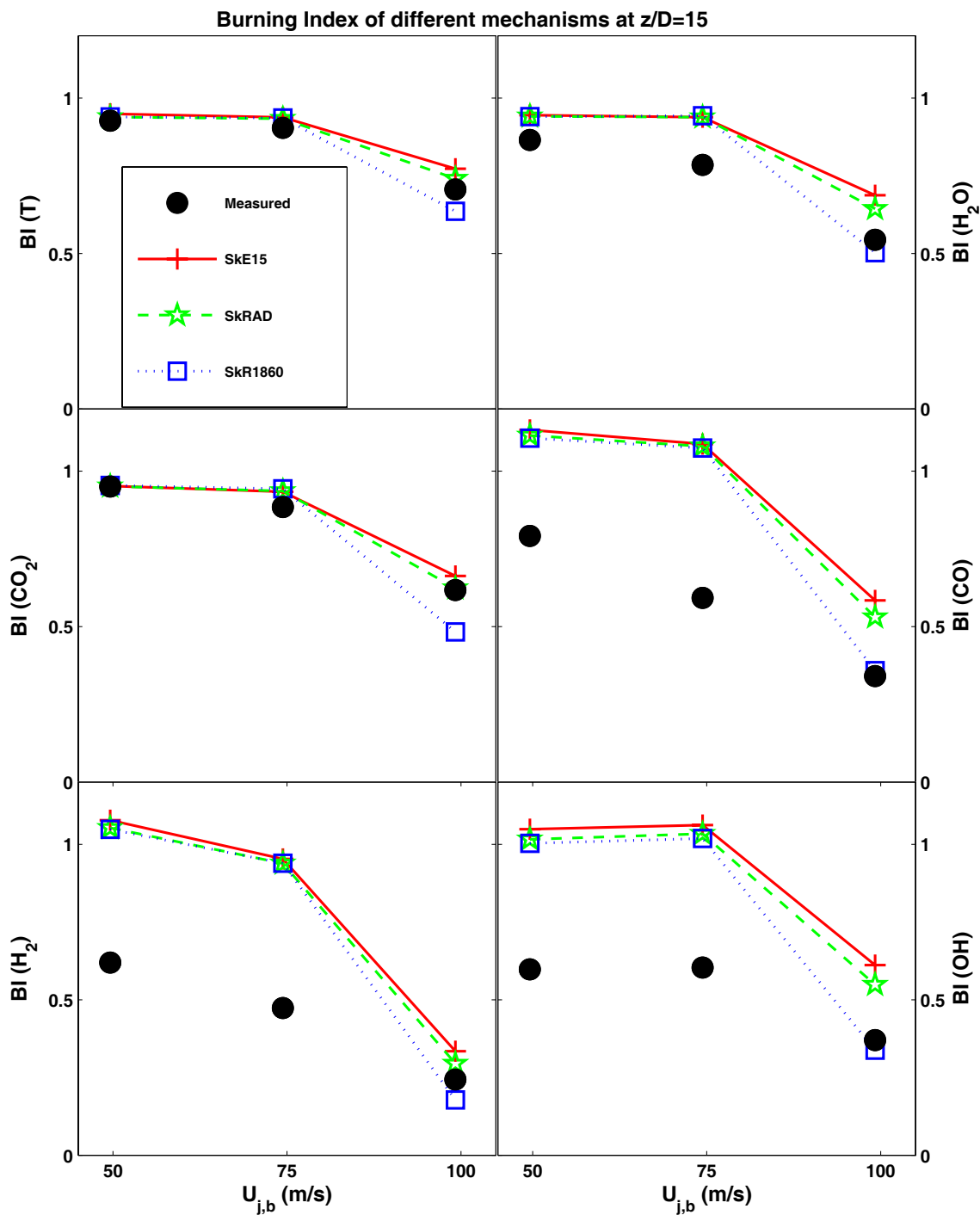
(5) S5G211 mechanism



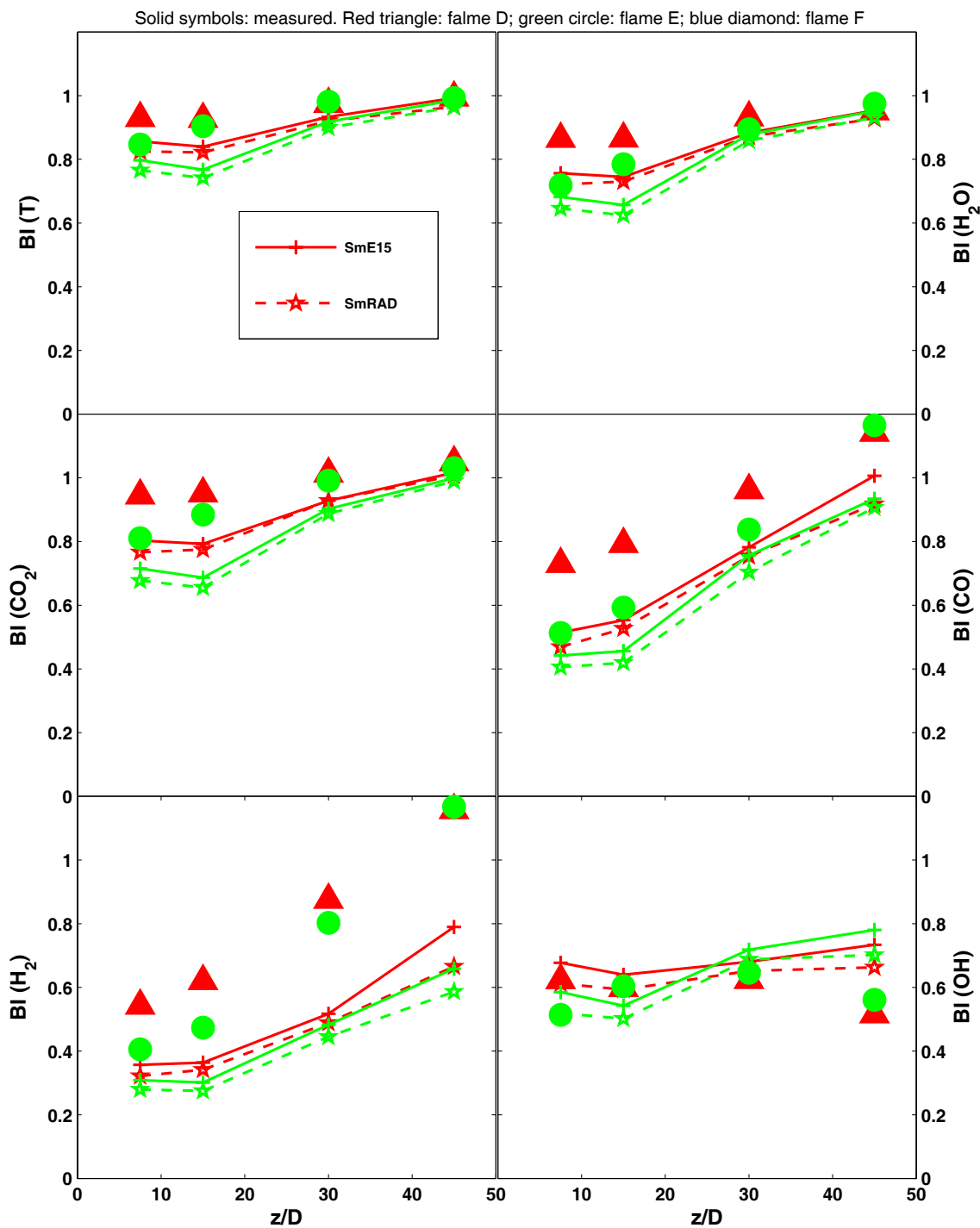


(6) Skeletal mechanism



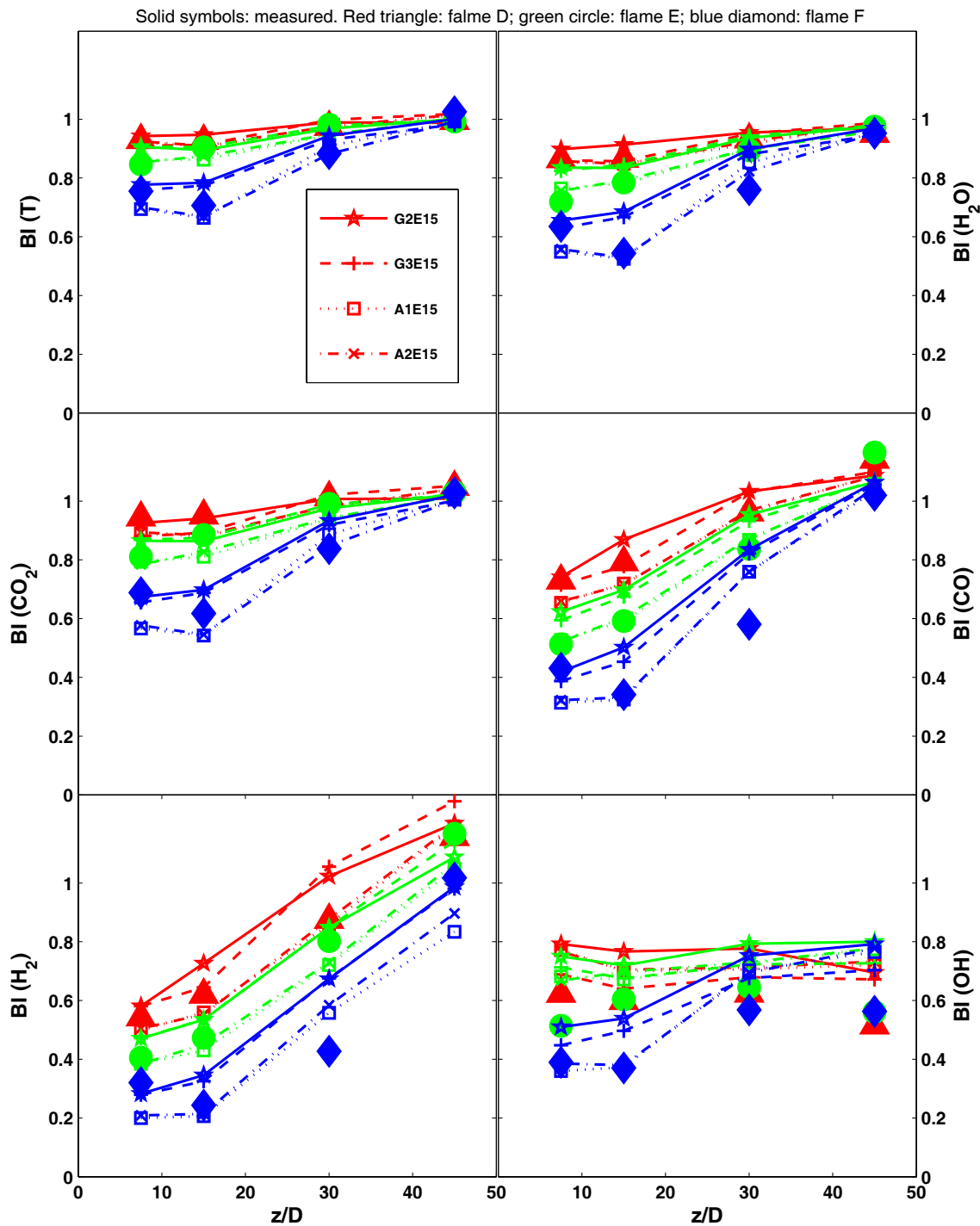


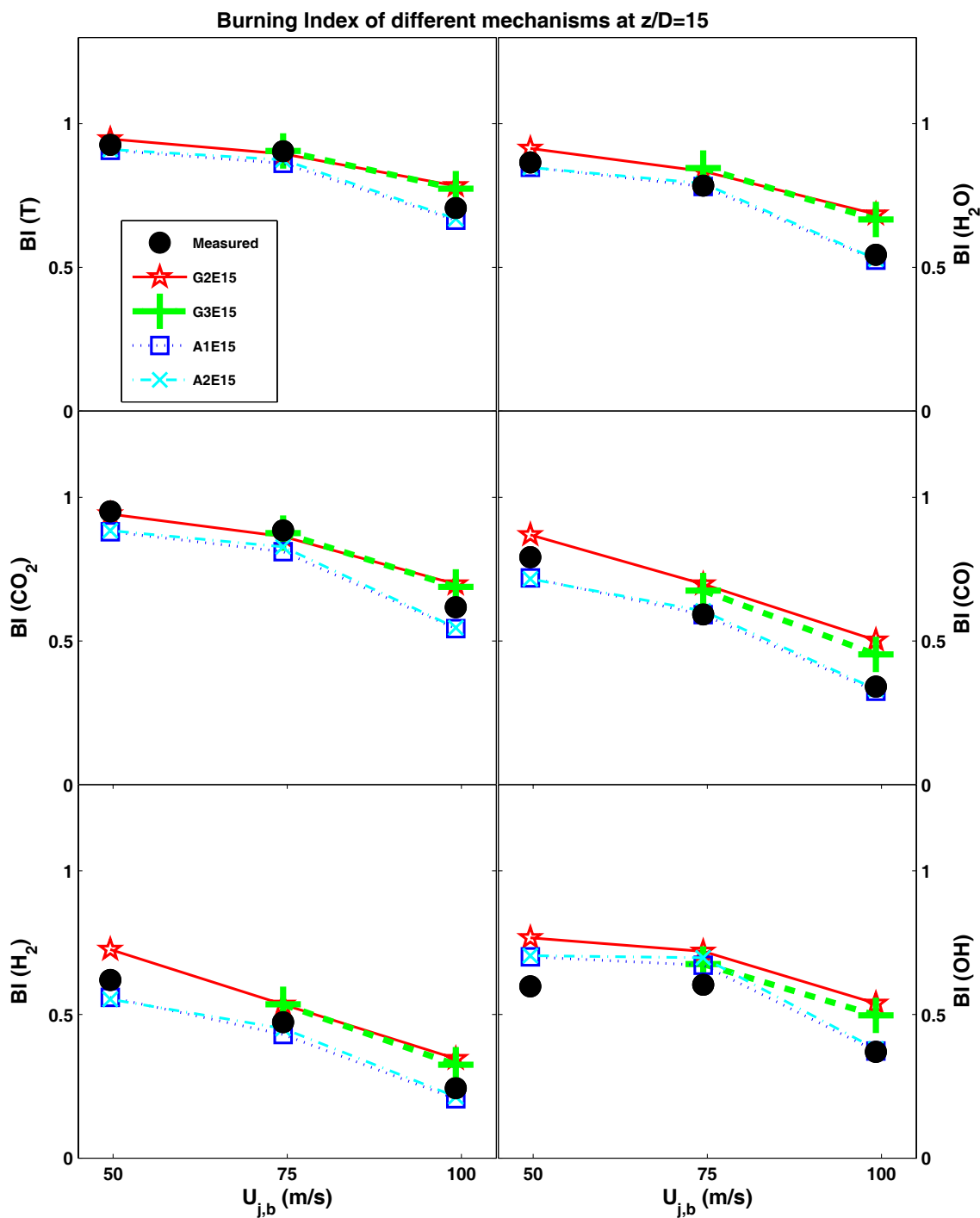
(7) Smooke mechanism



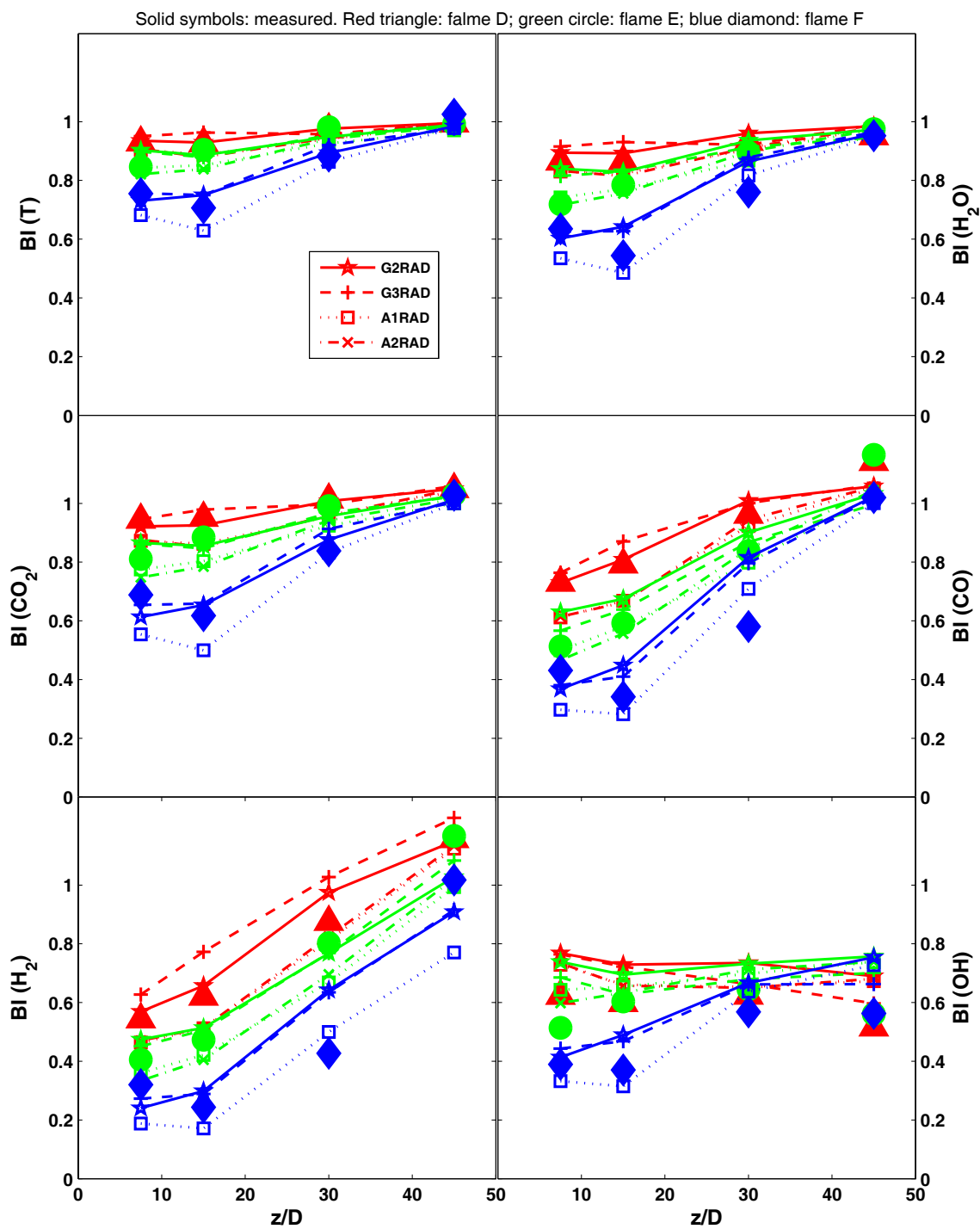
A-2 Comparison of different mechanisms

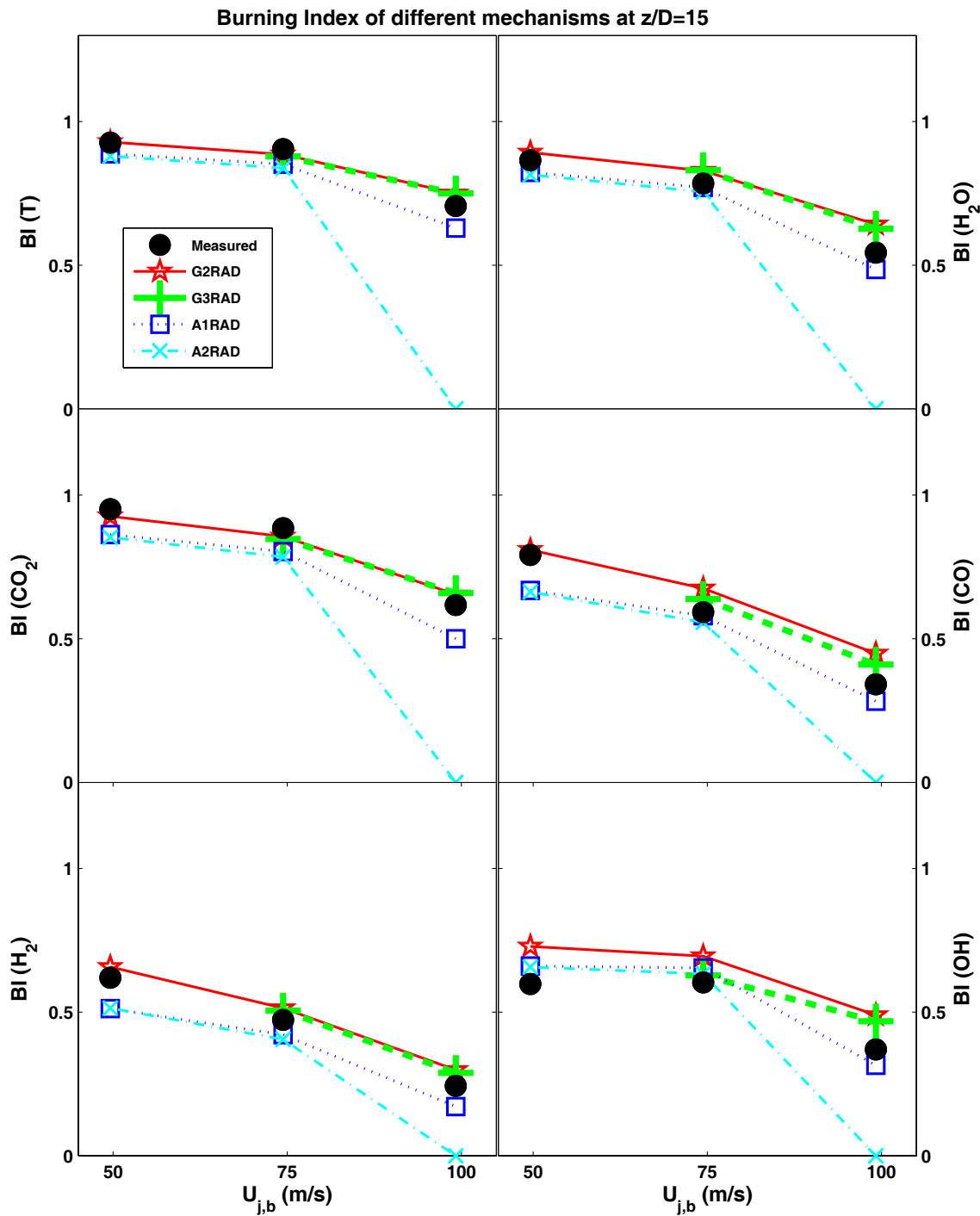
(1) Comparison of A1, A2, G2, G3 mechanisms without radiation



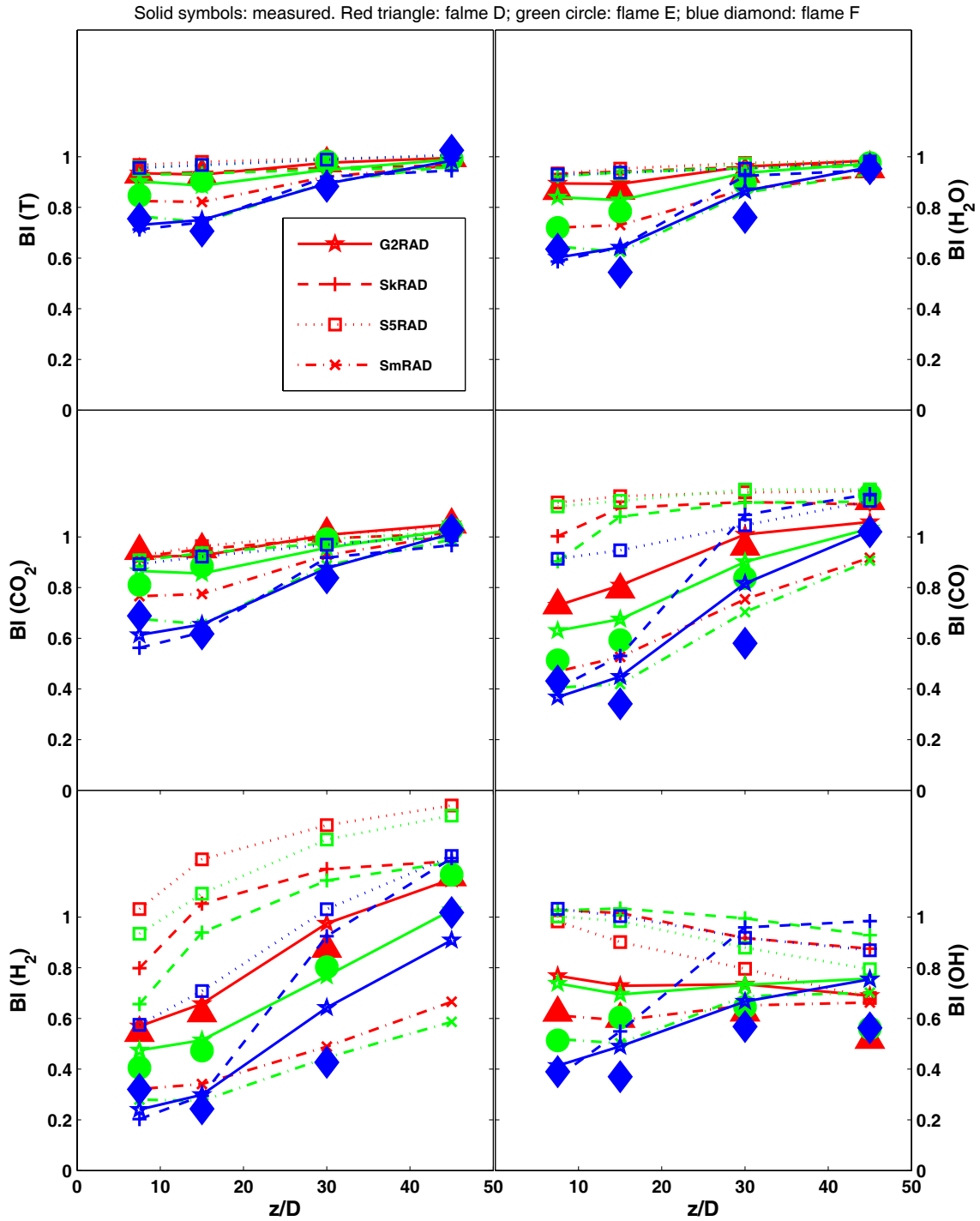


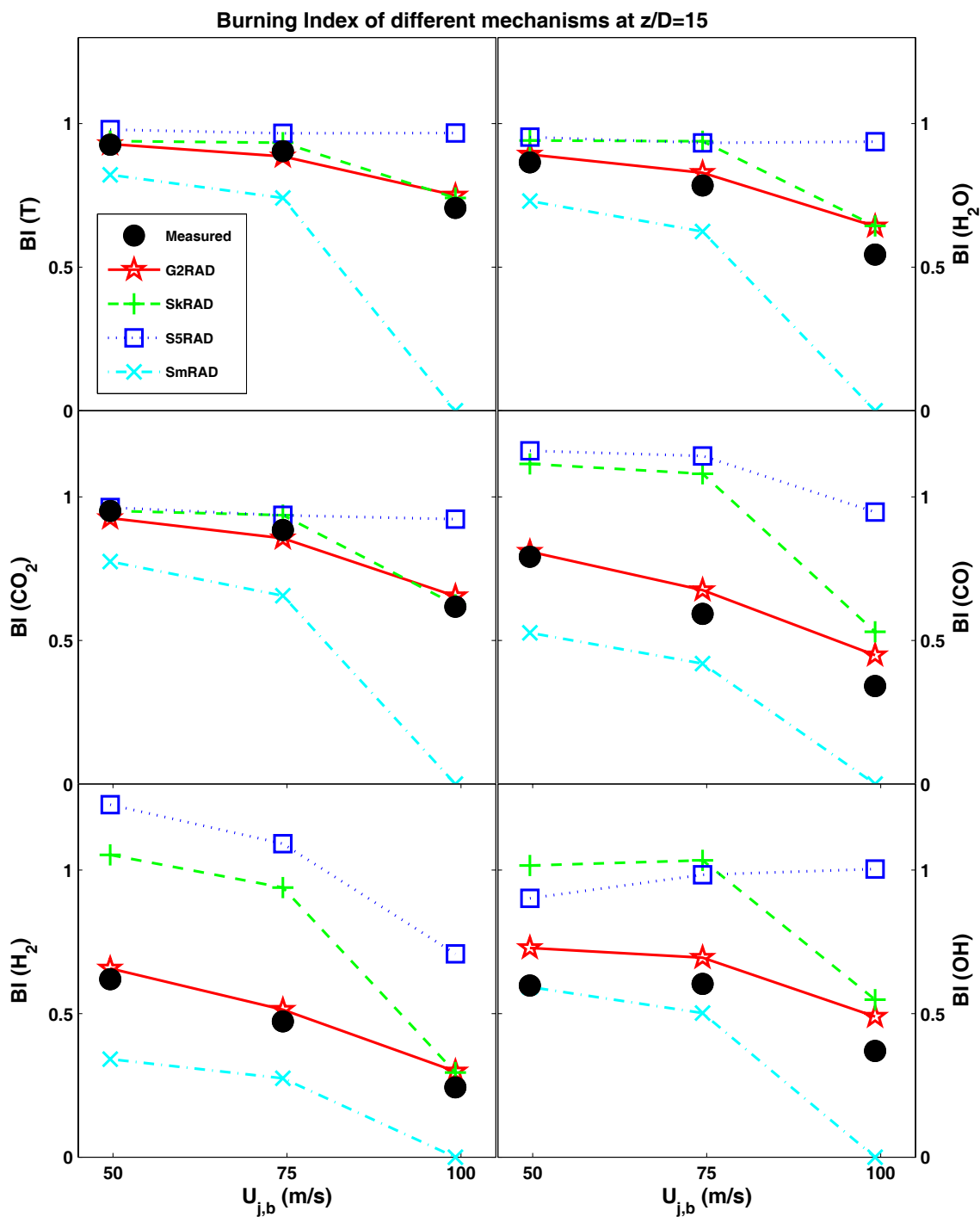
(2) Comparison of A1, A2, G2, G3 mechanisms with radiation



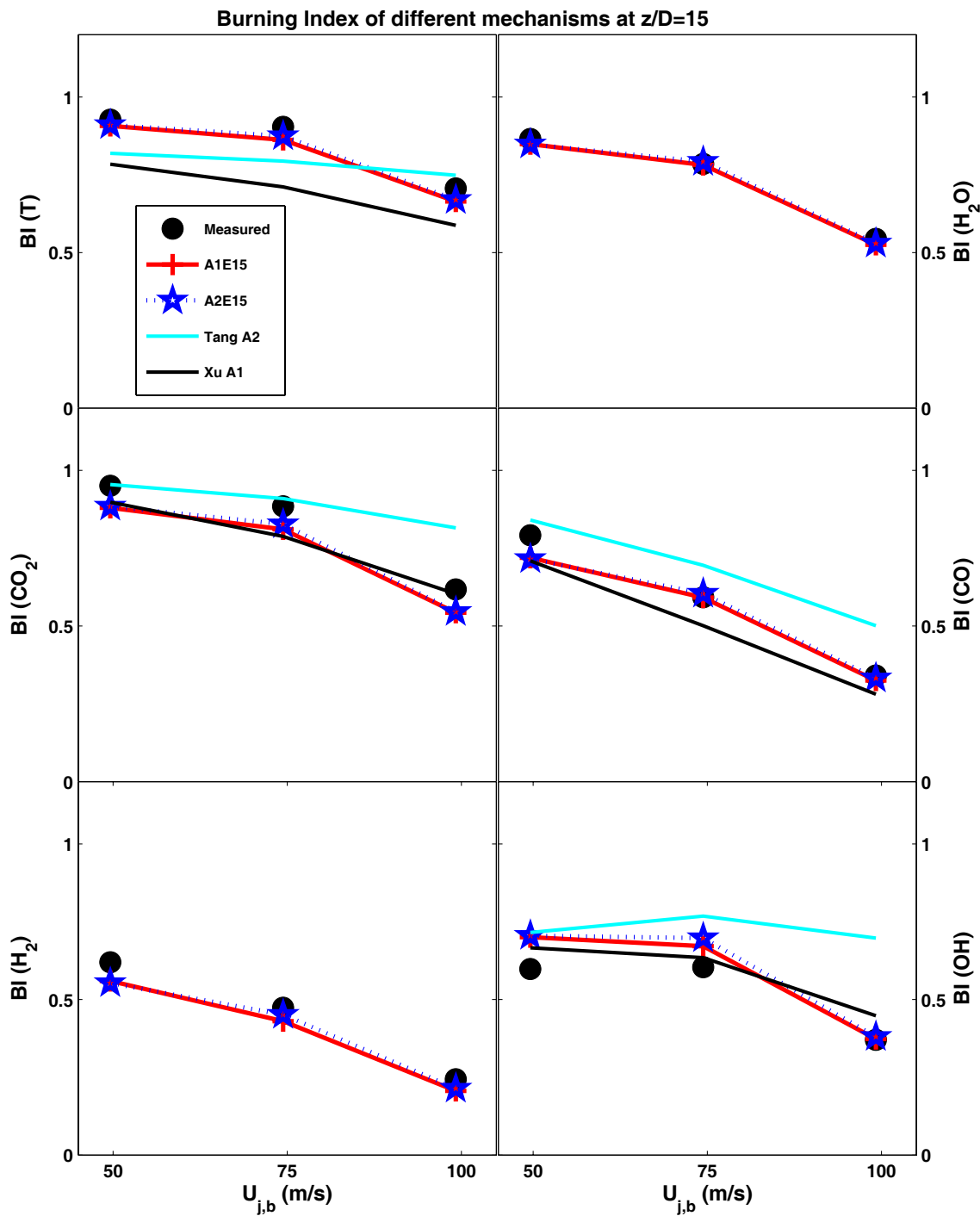


(3) Comparison of Skeletal, Smooke, S5G211 and G2 mechanisms





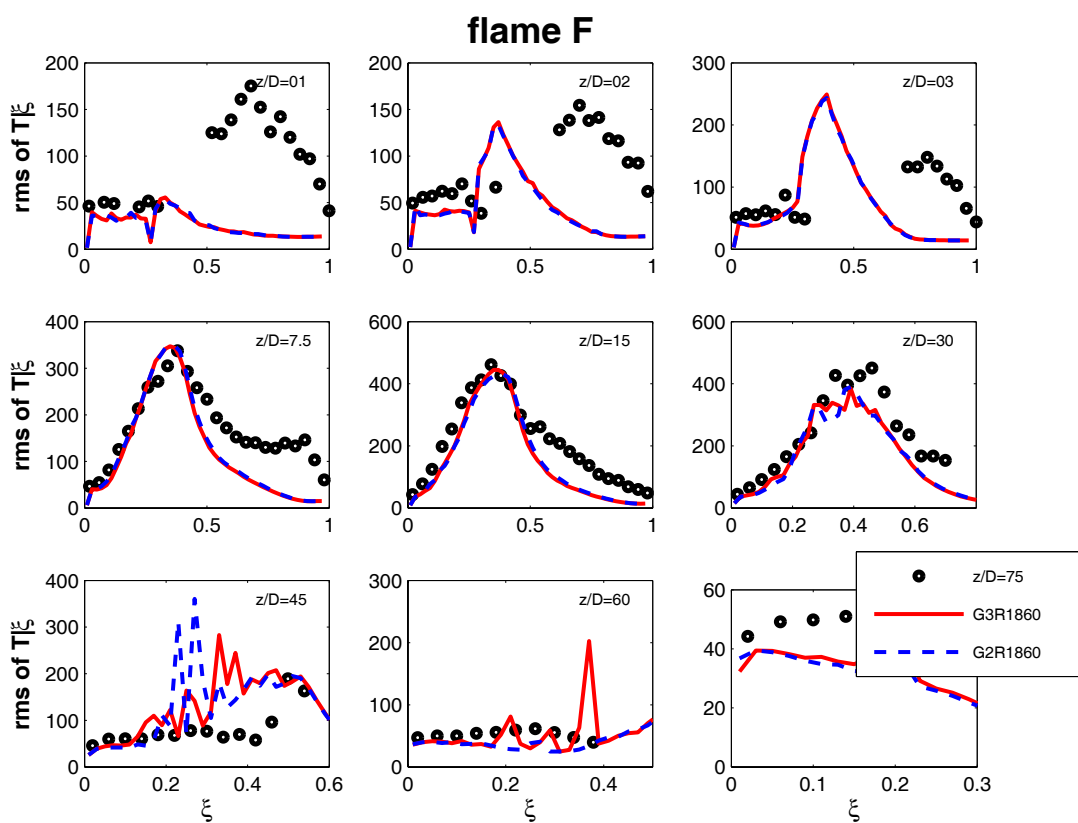
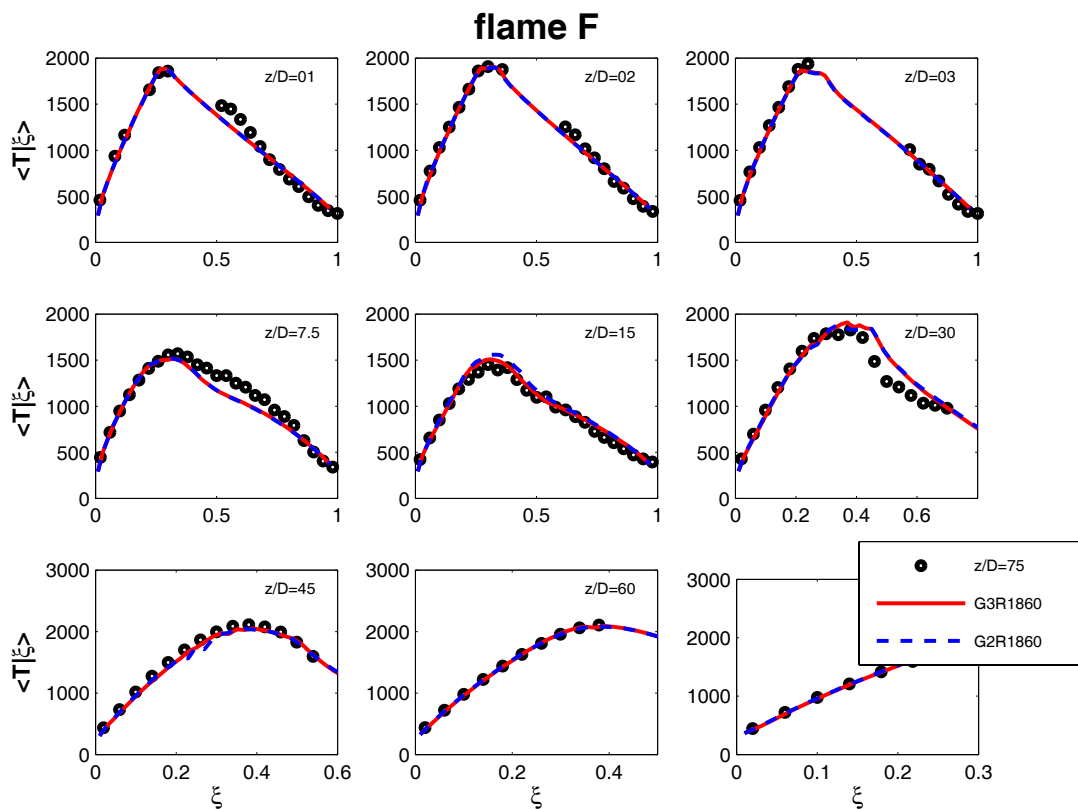
A-3 Comparison with previous calculations

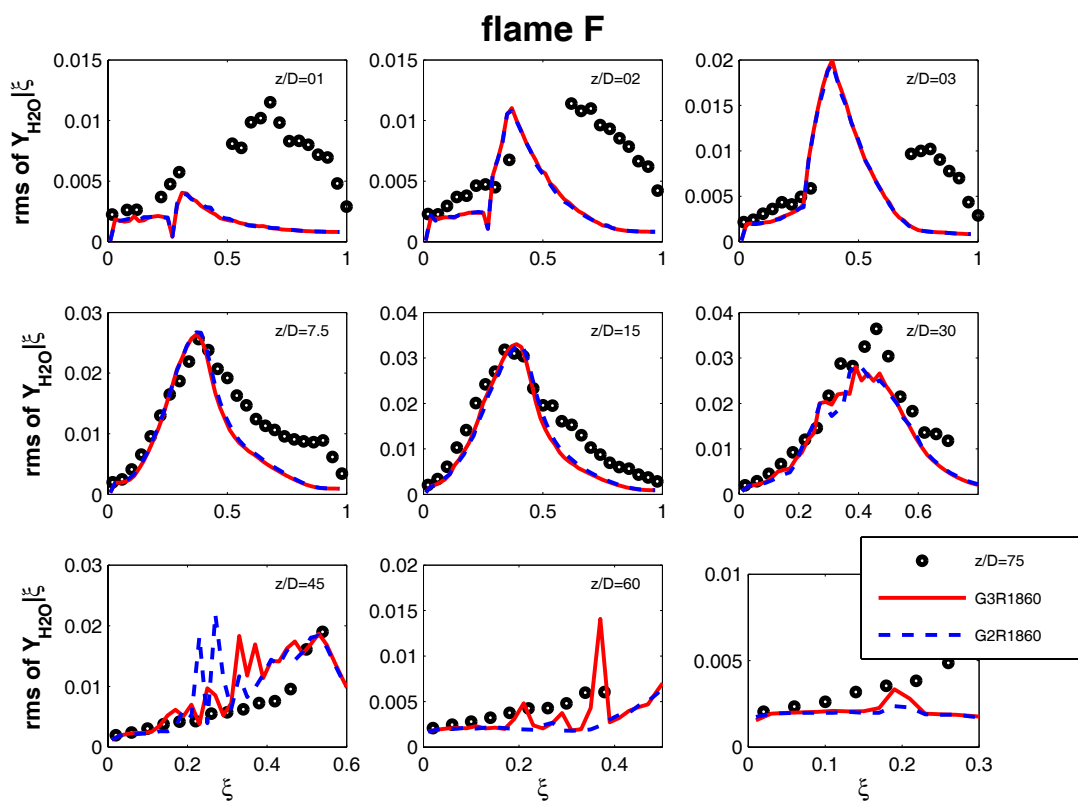
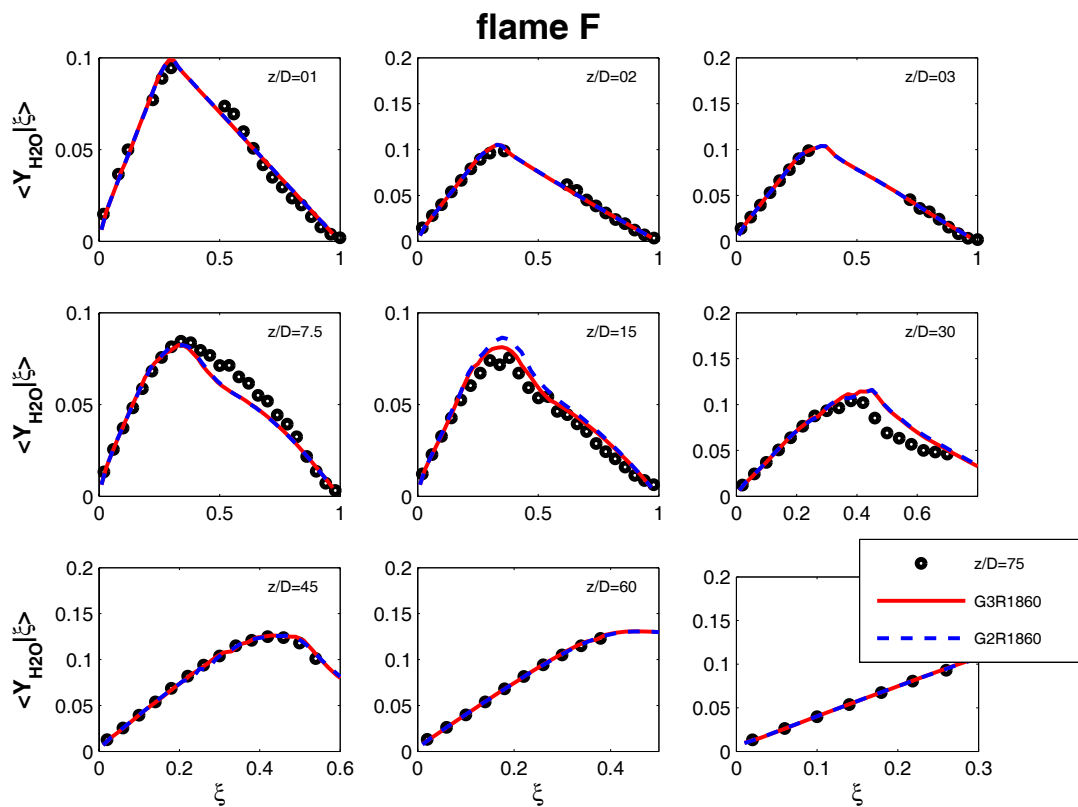


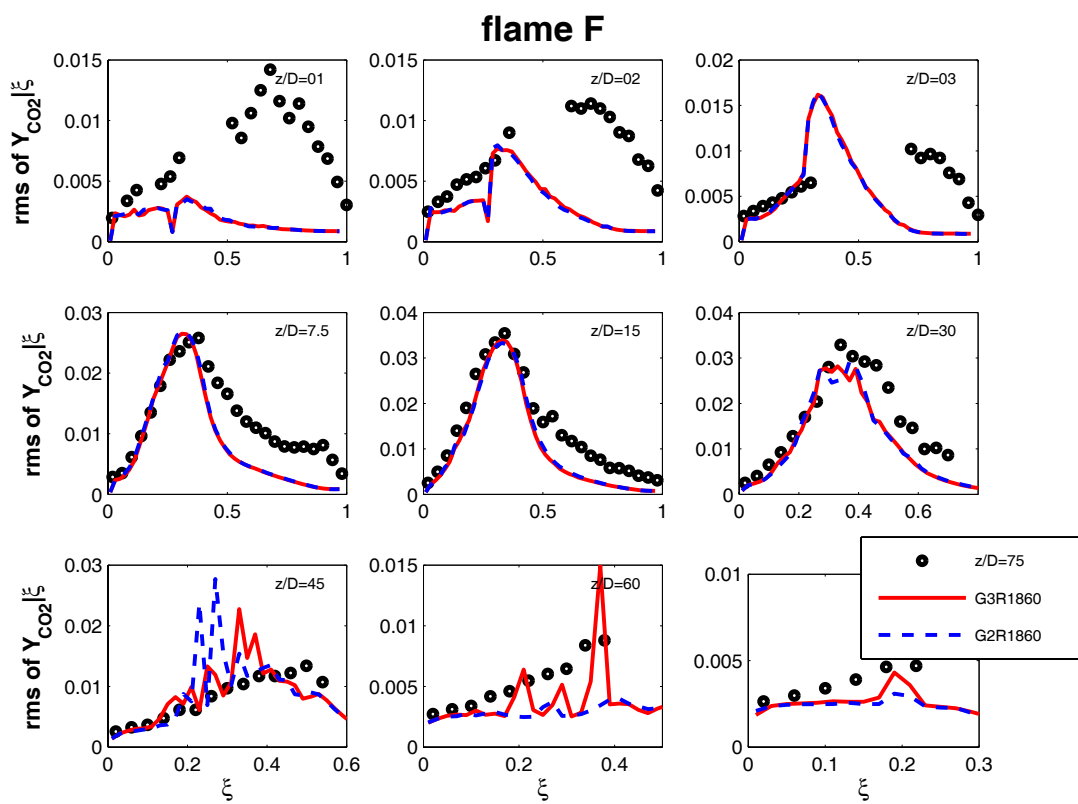
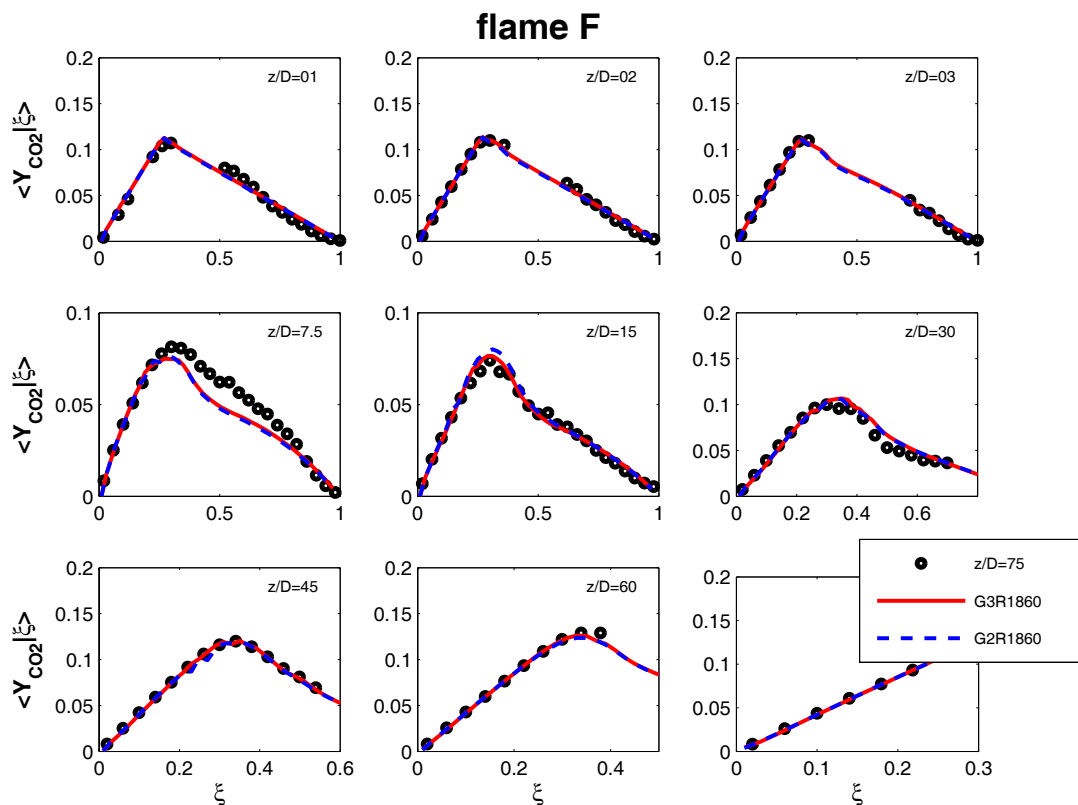
Part B: Conditional means and rms's

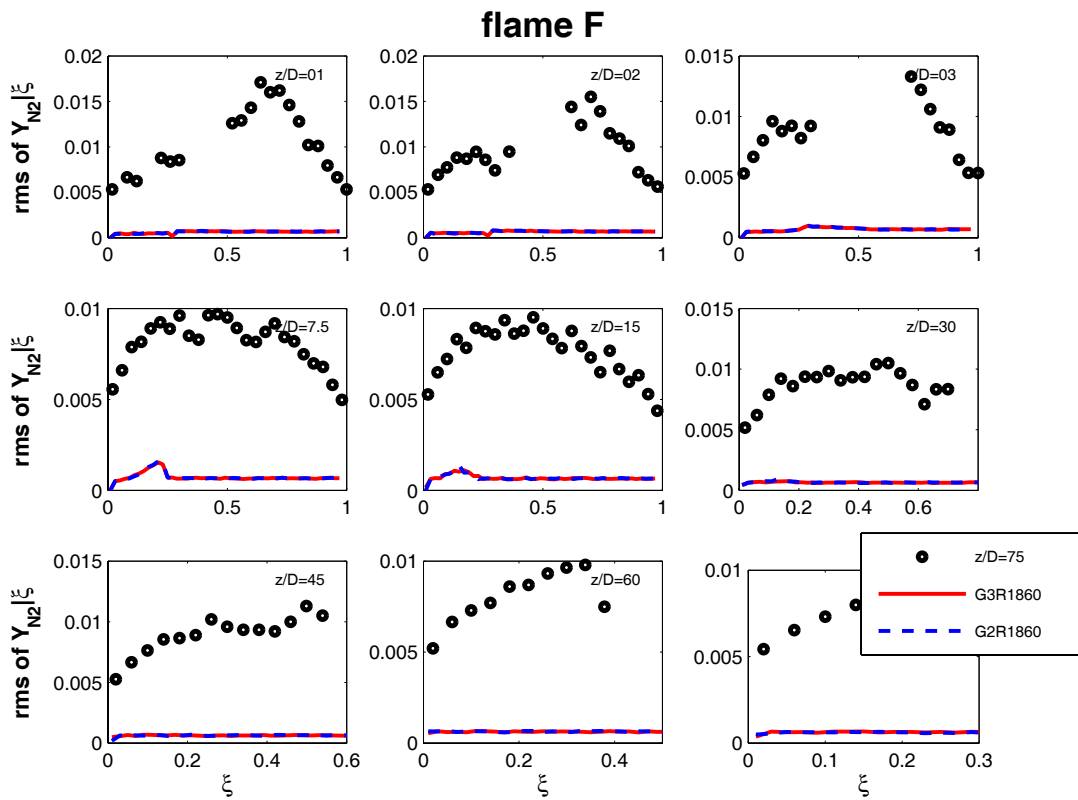
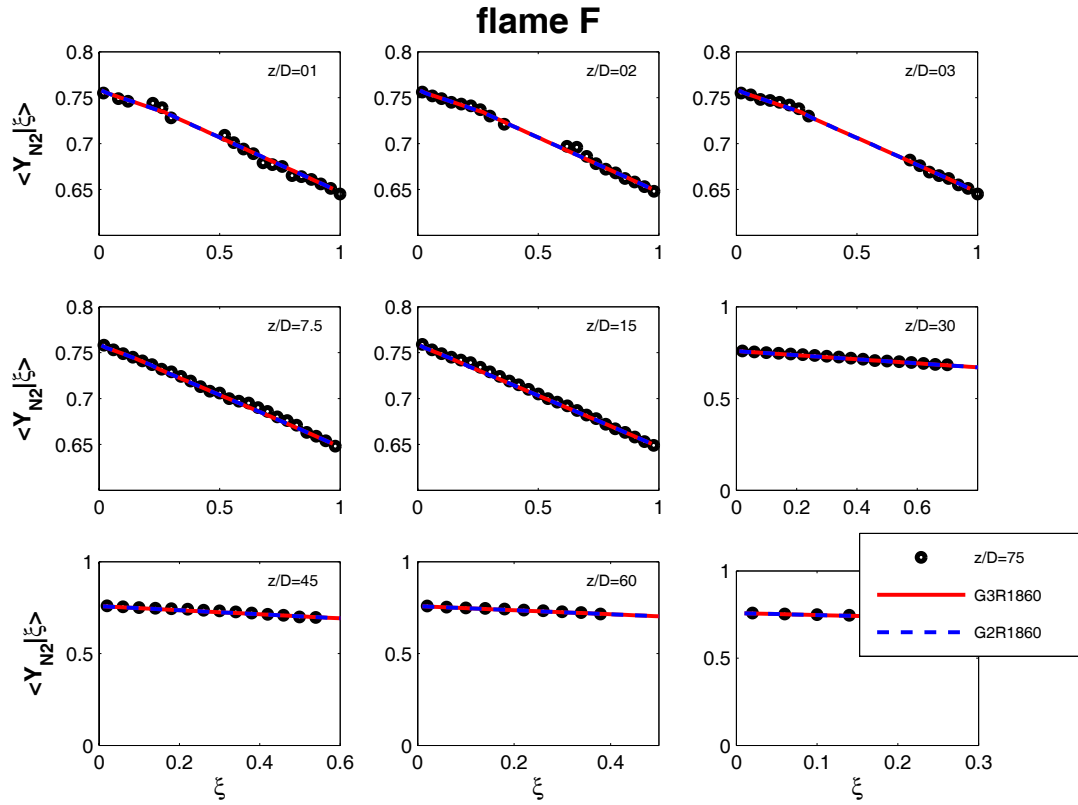
B-1 Calculations using GRI3.0 and GRI2.11 with base case configuration

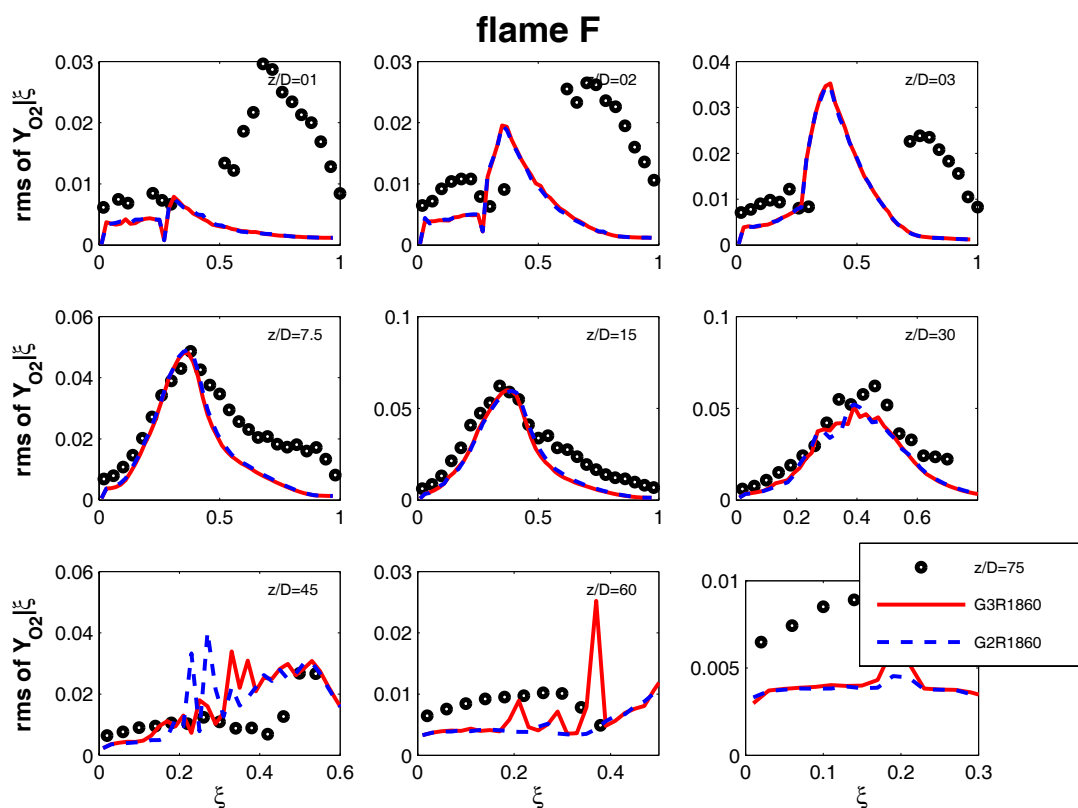
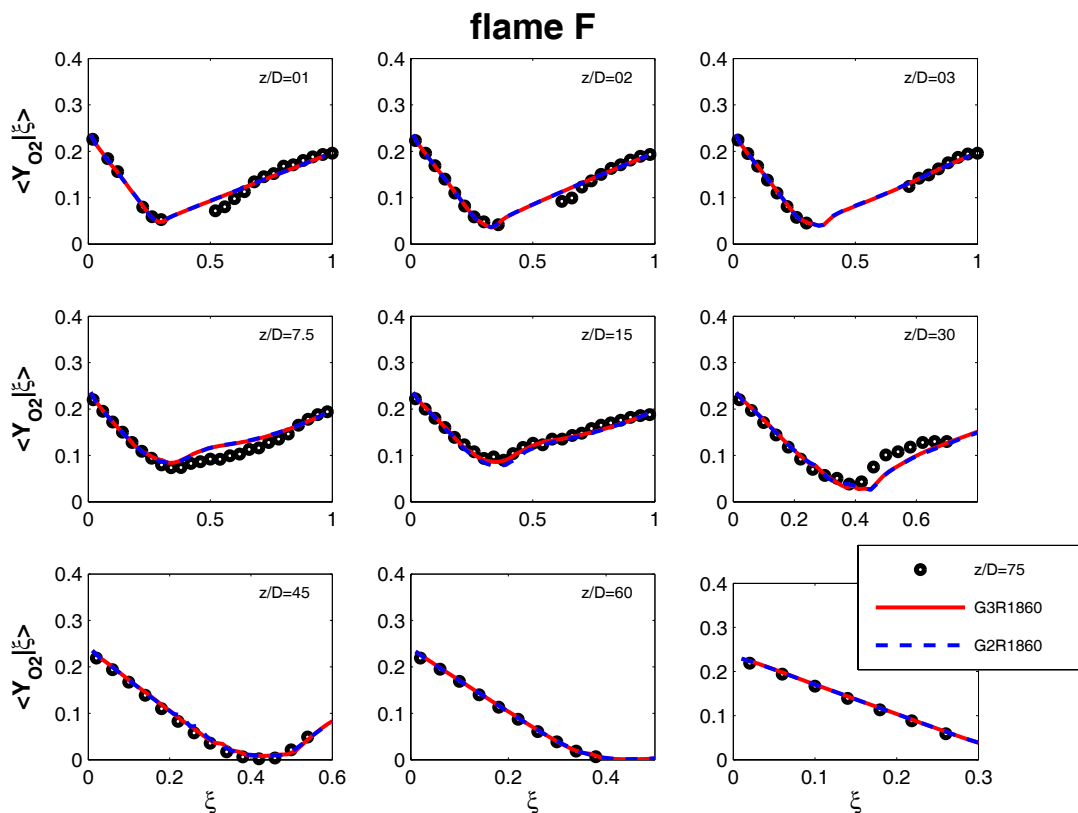
(1) Flame F

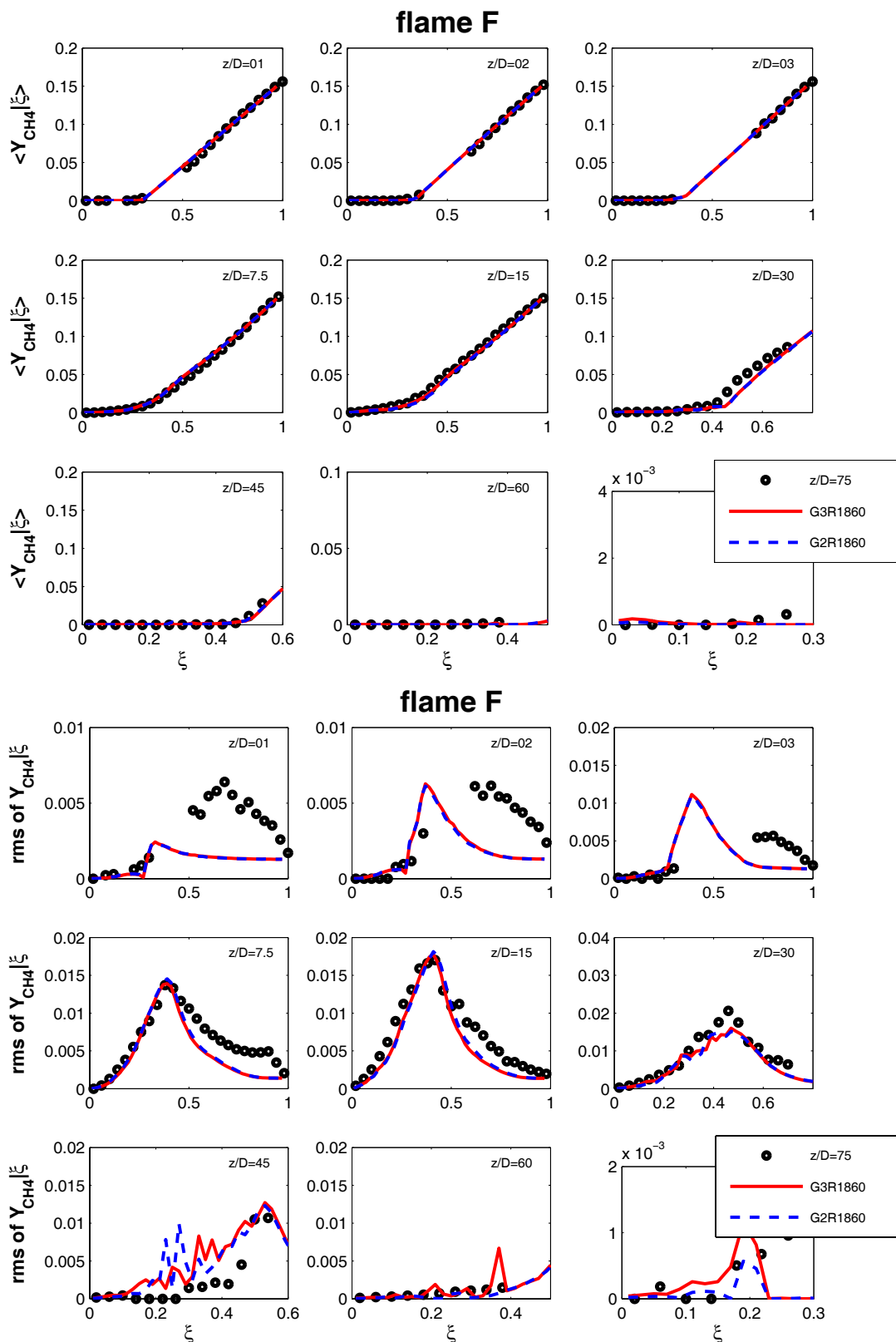


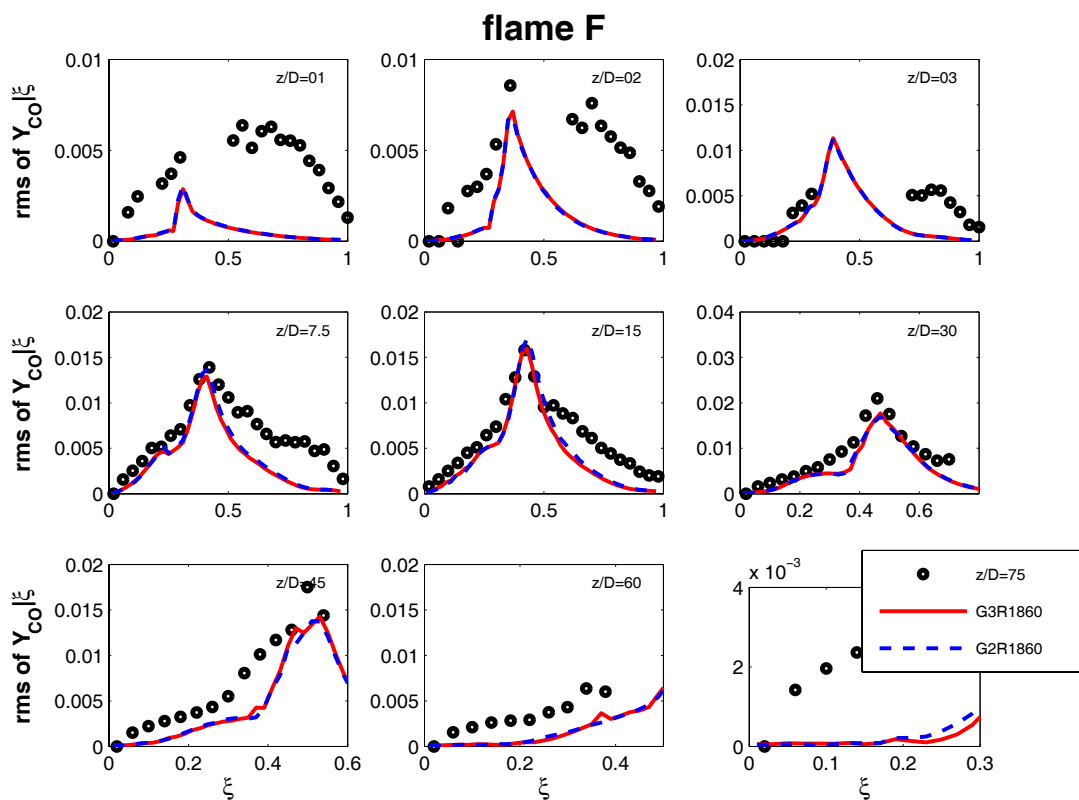
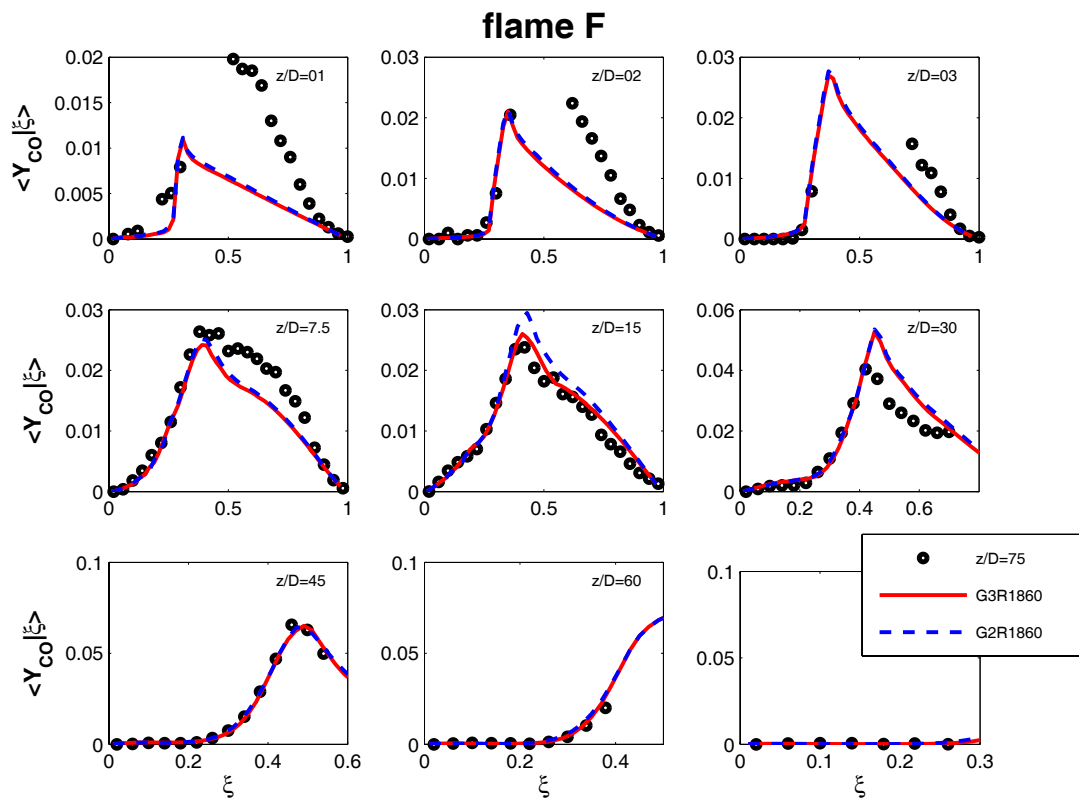


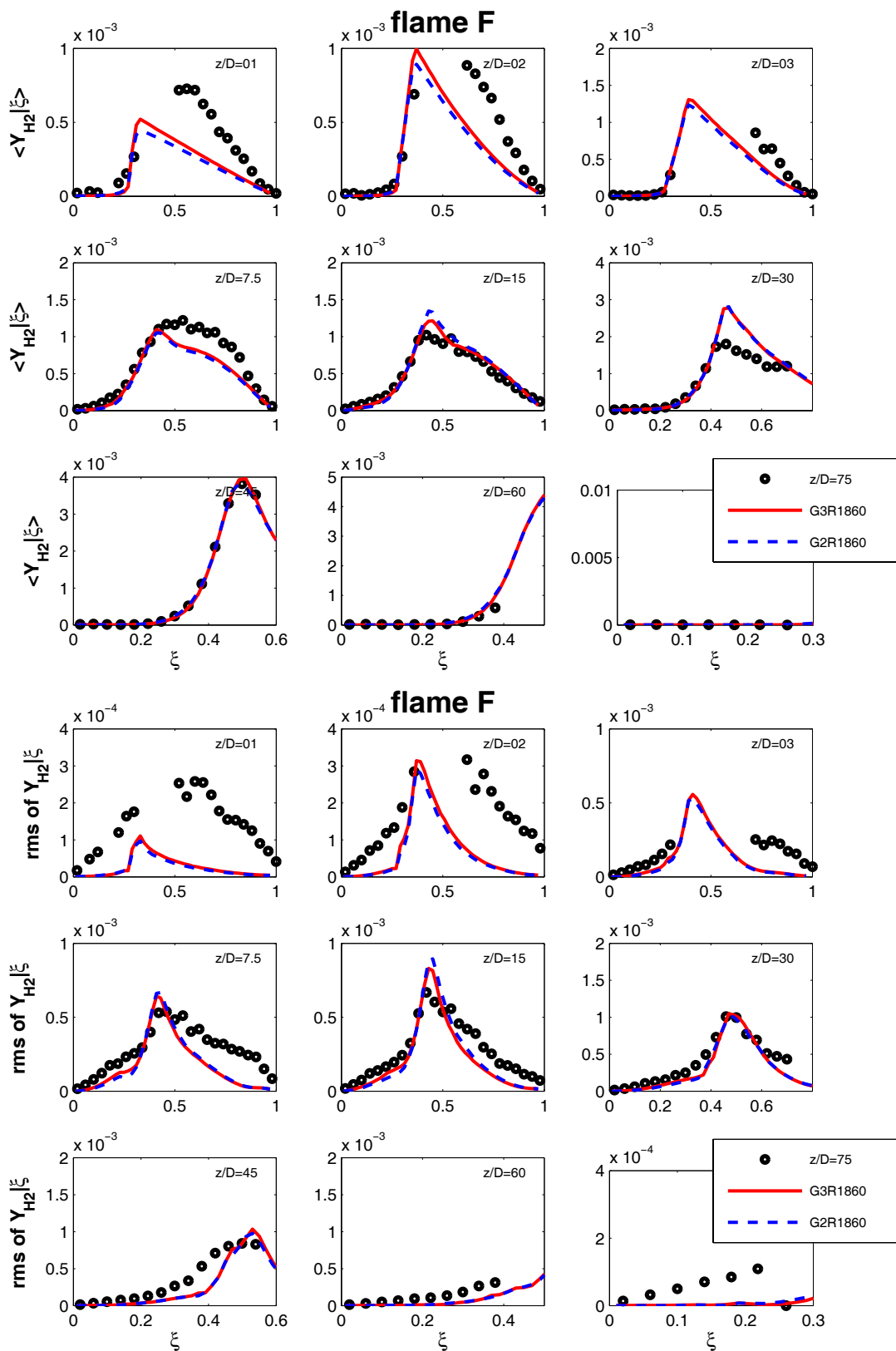


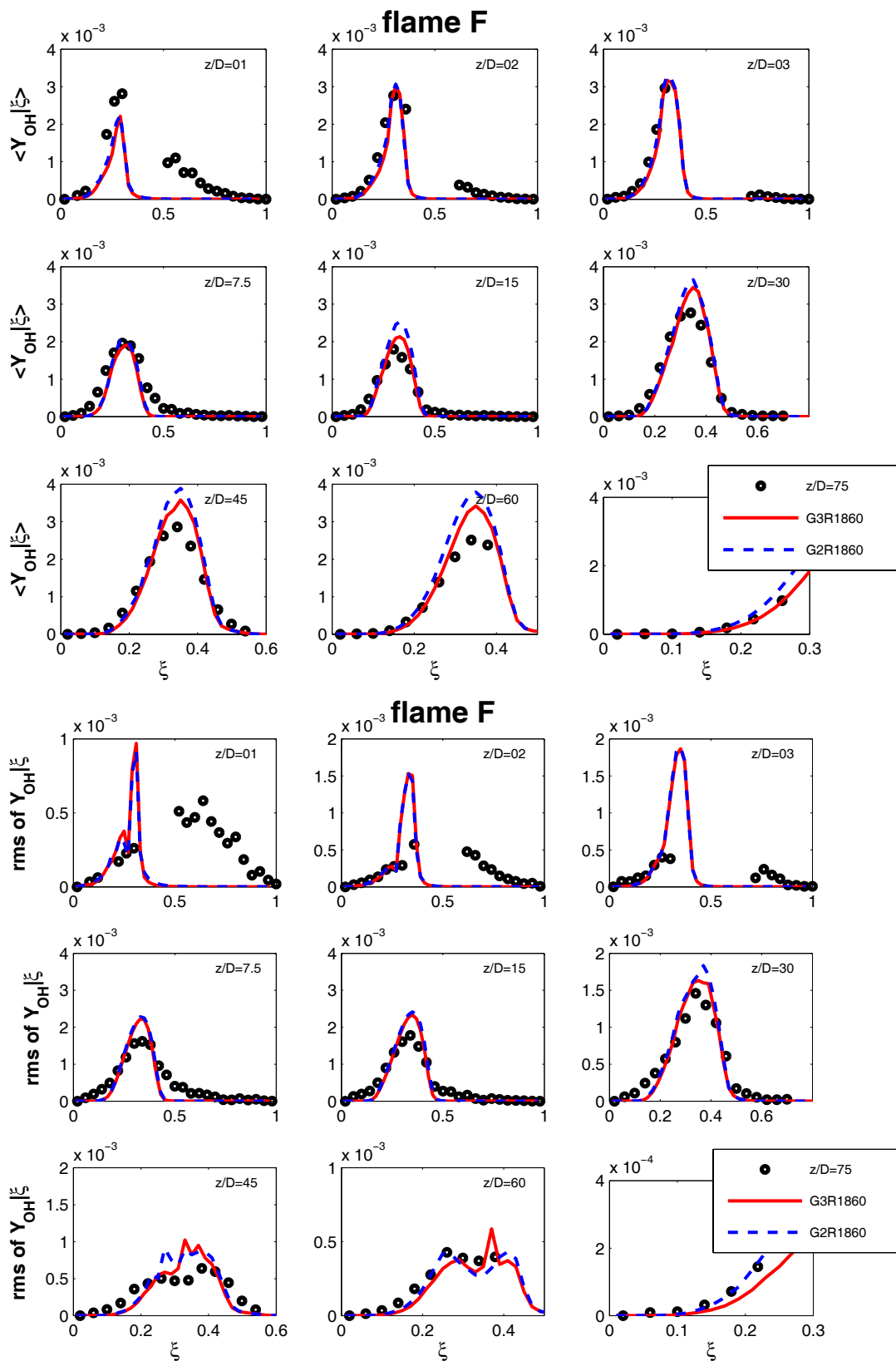


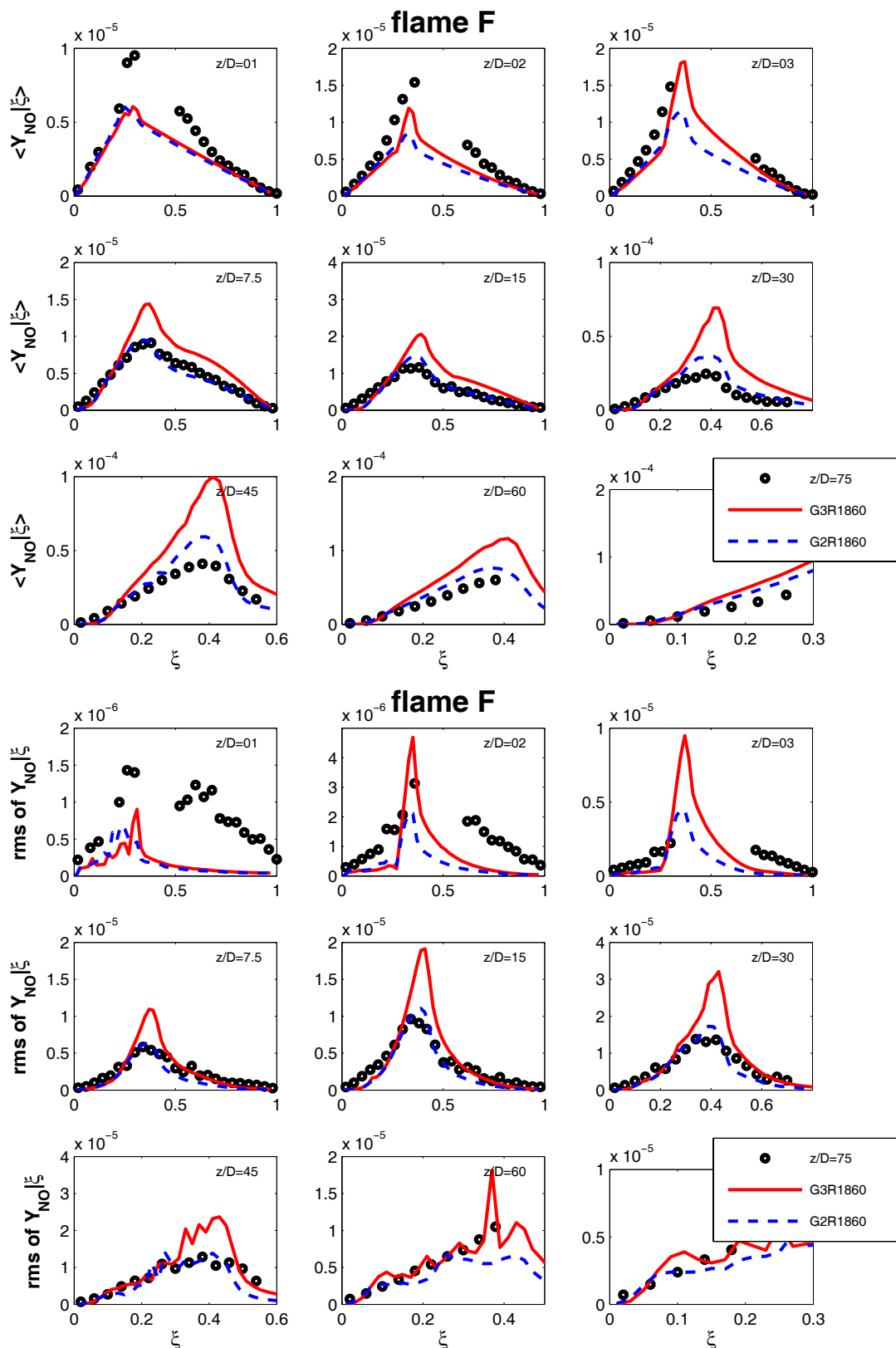




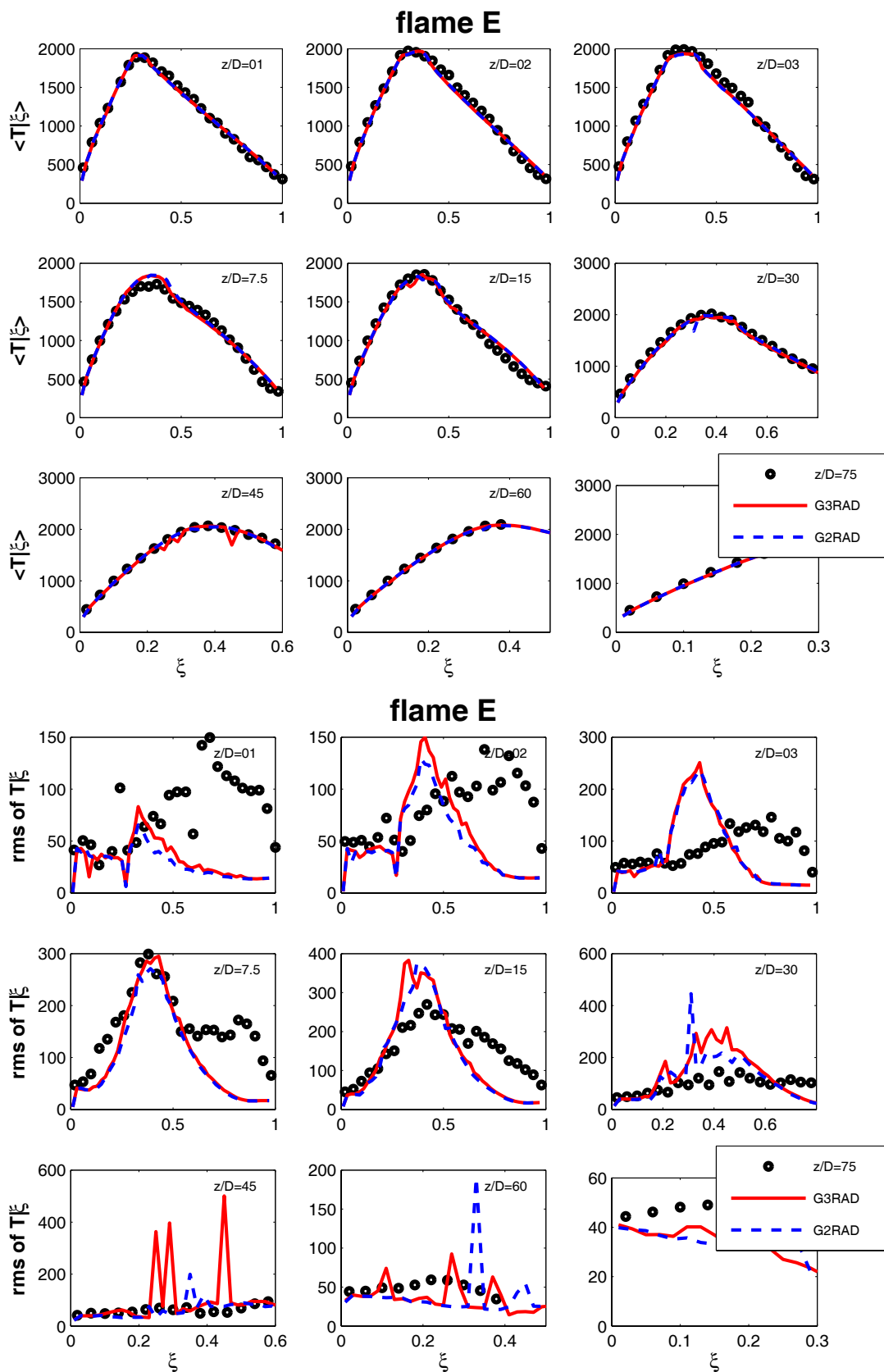


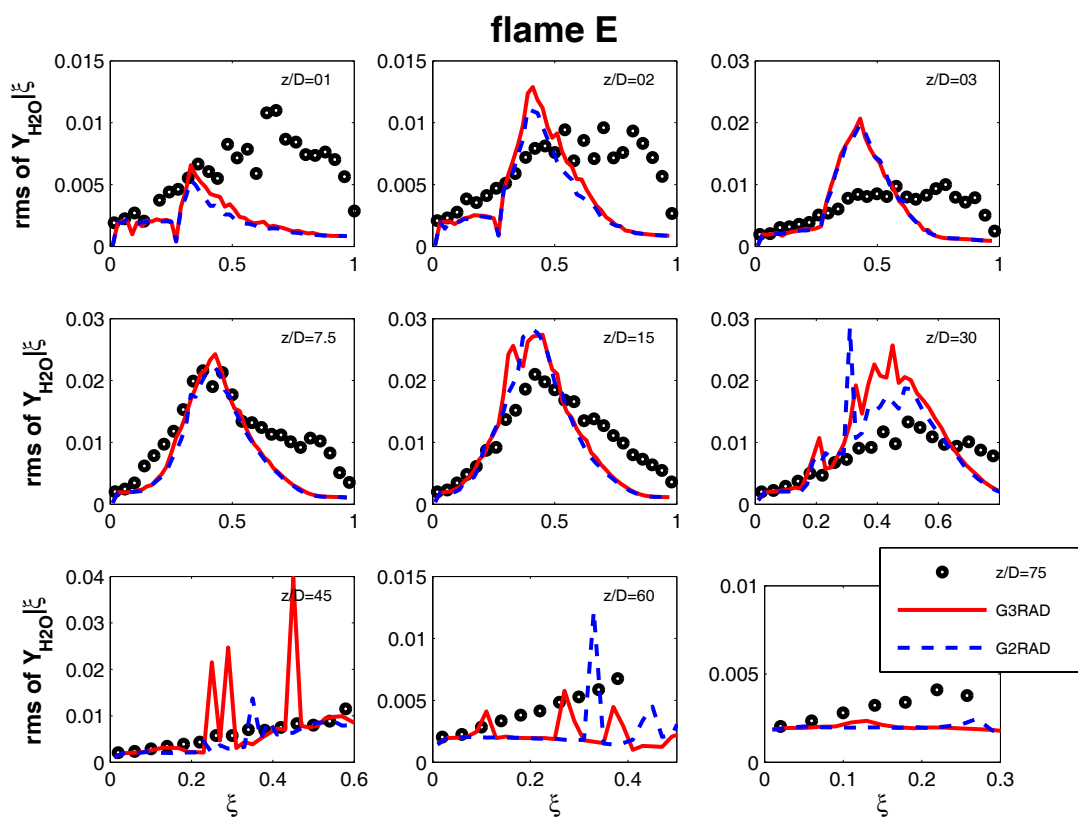
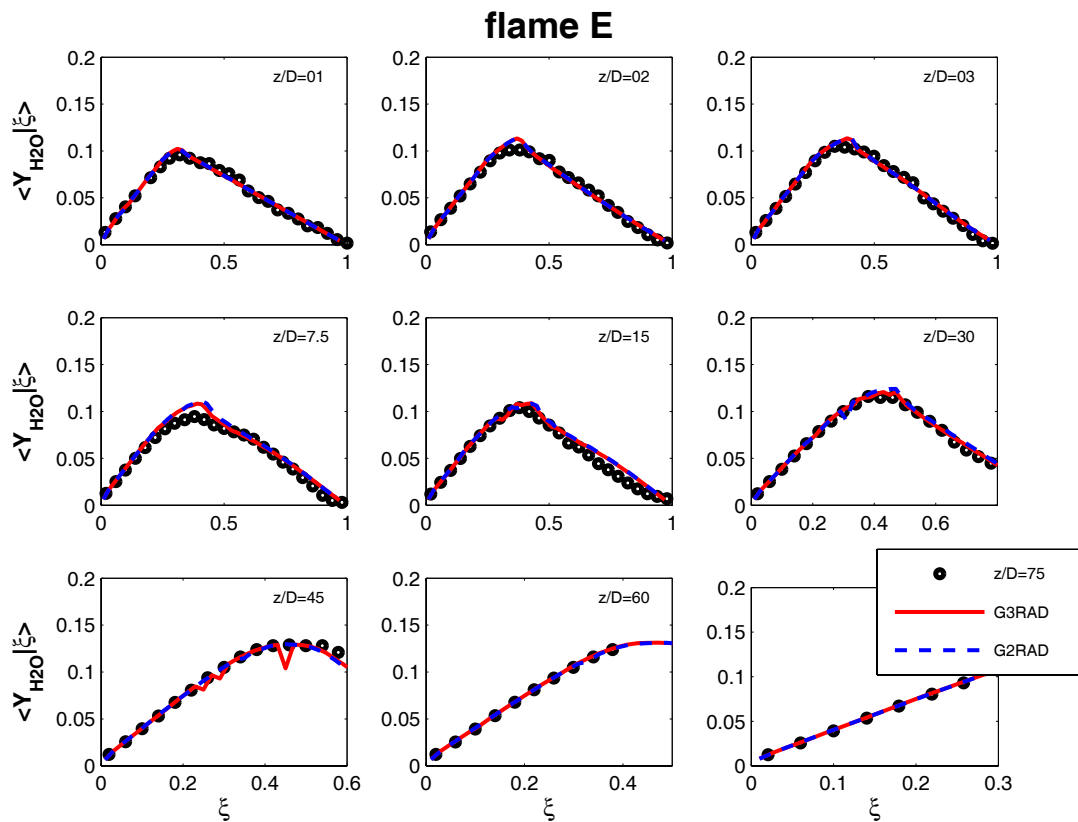


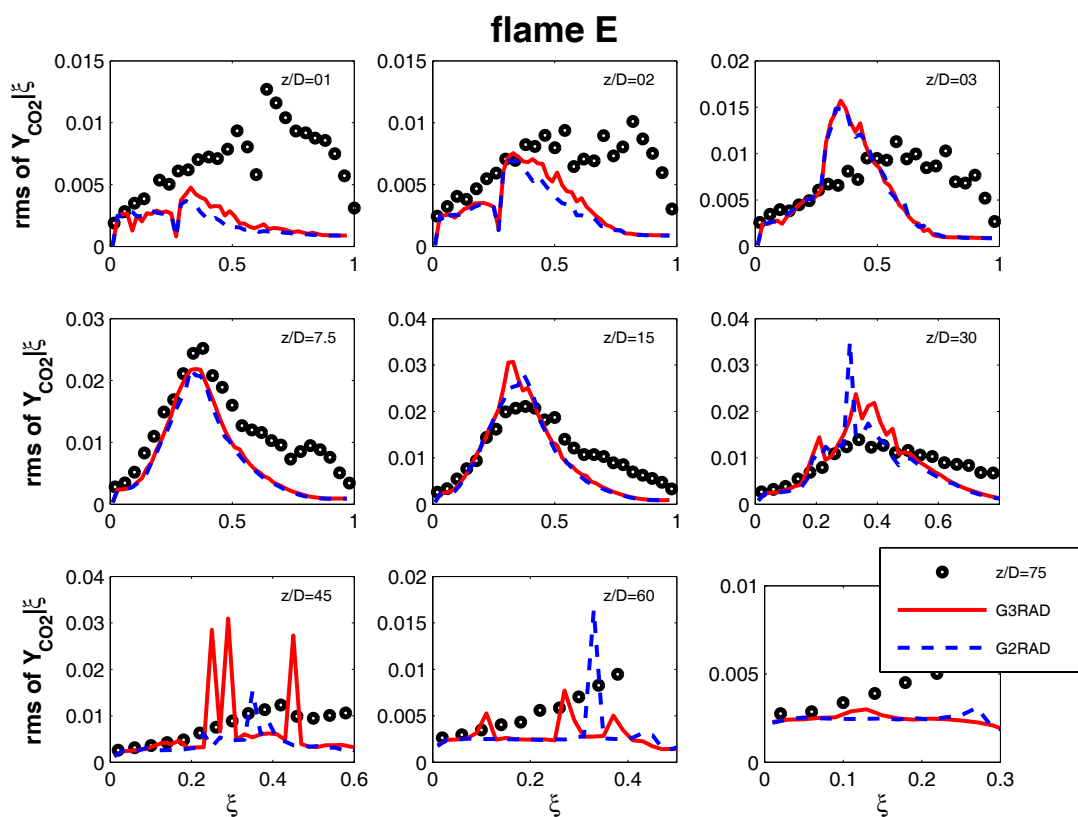
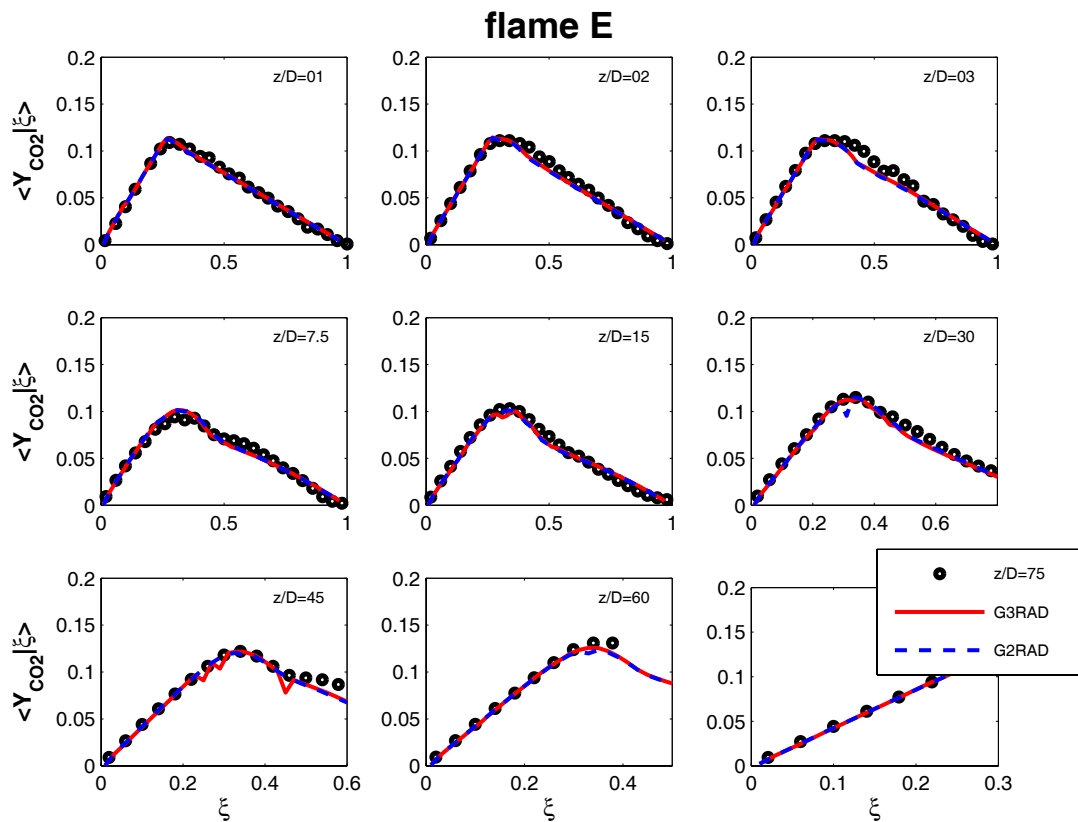


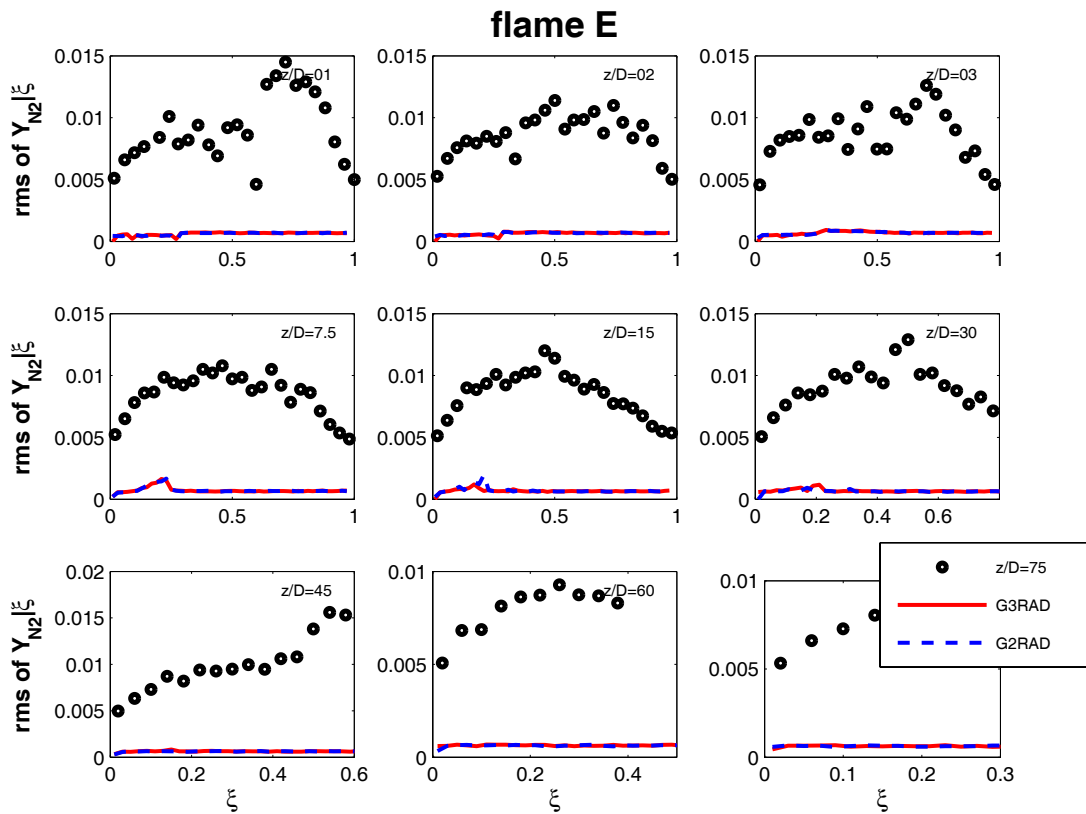
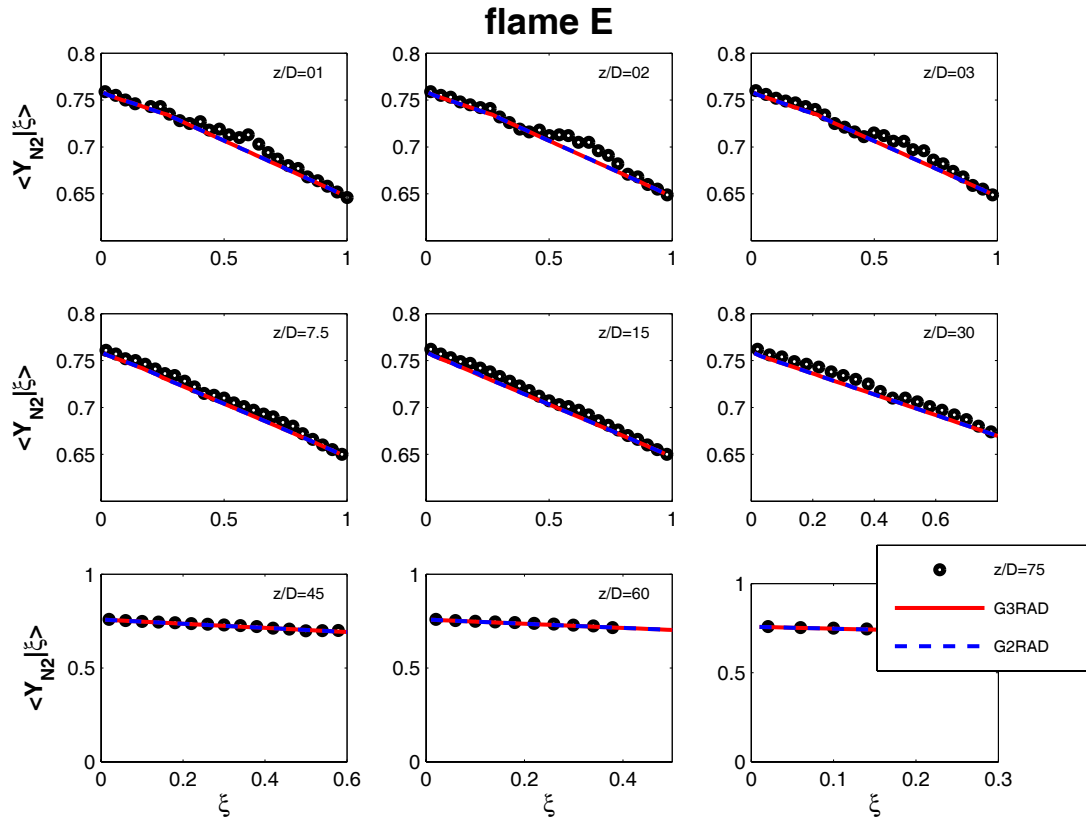


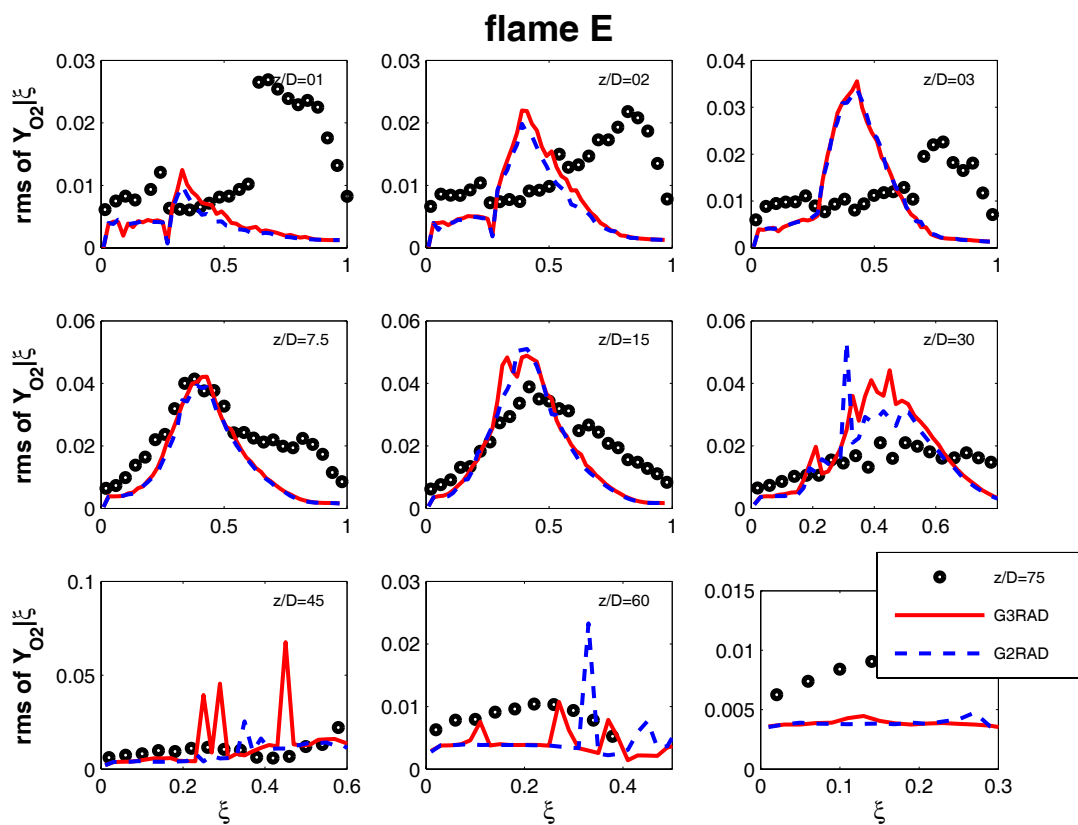
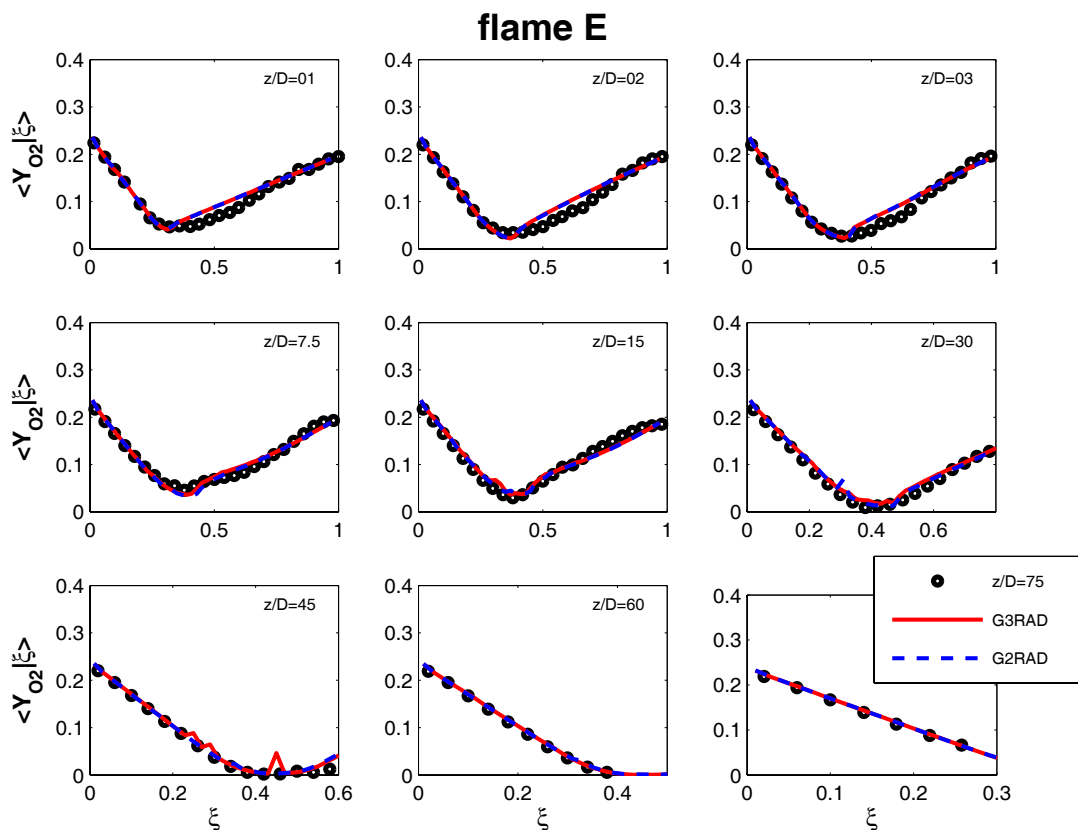
(2) Flame E

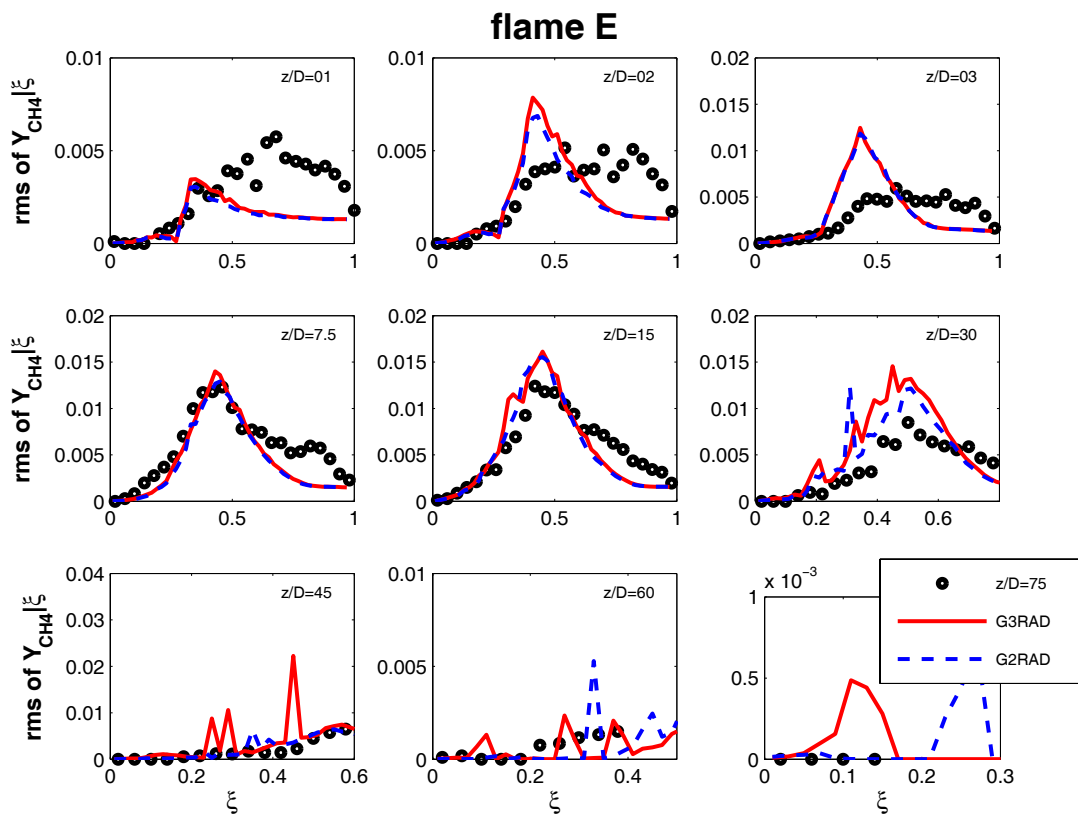
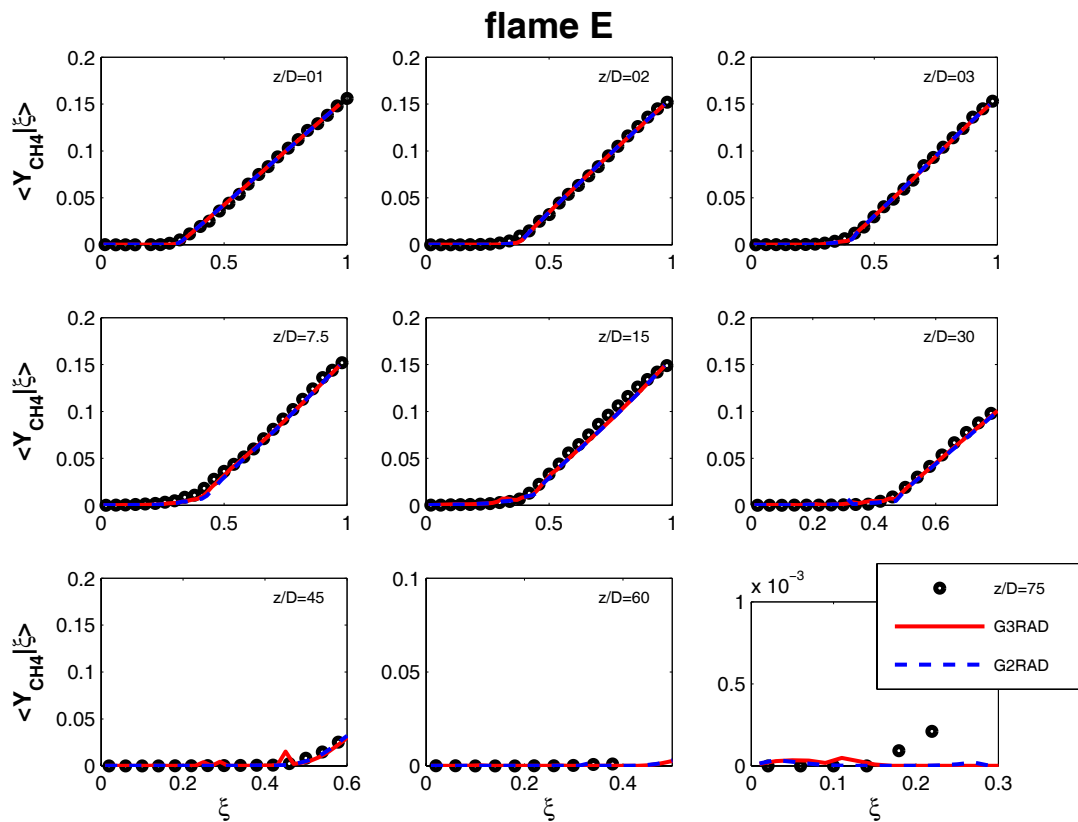


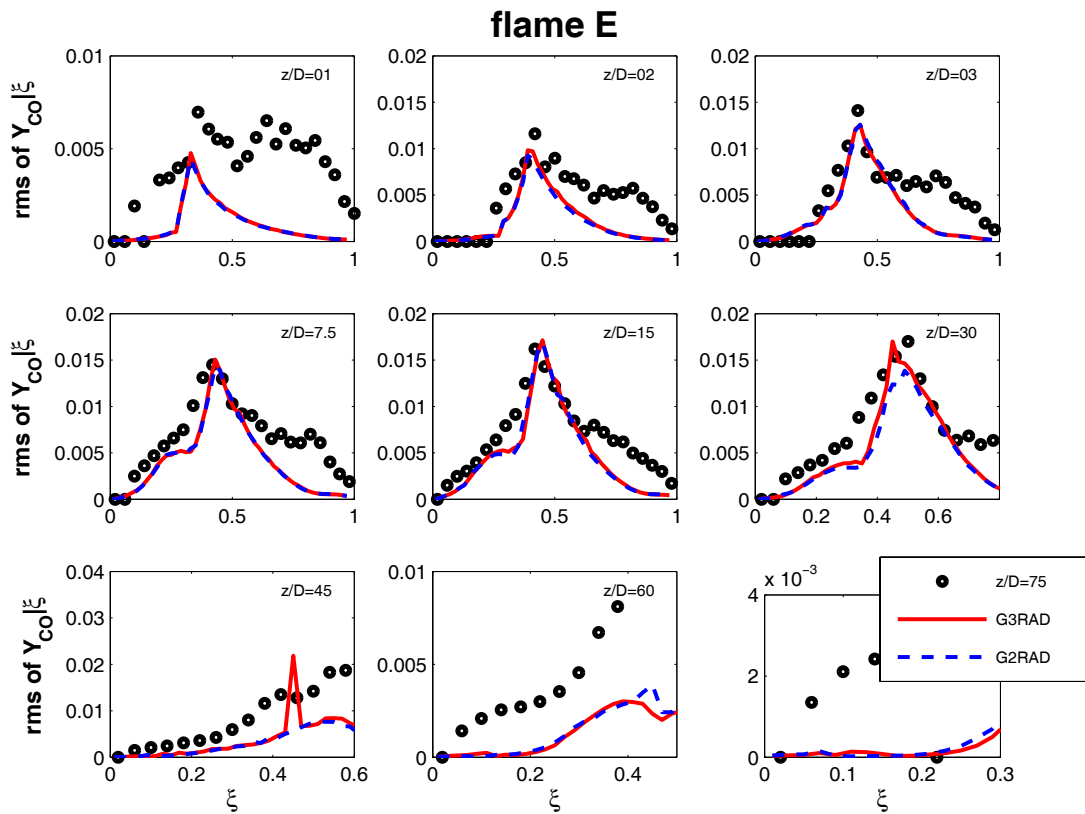
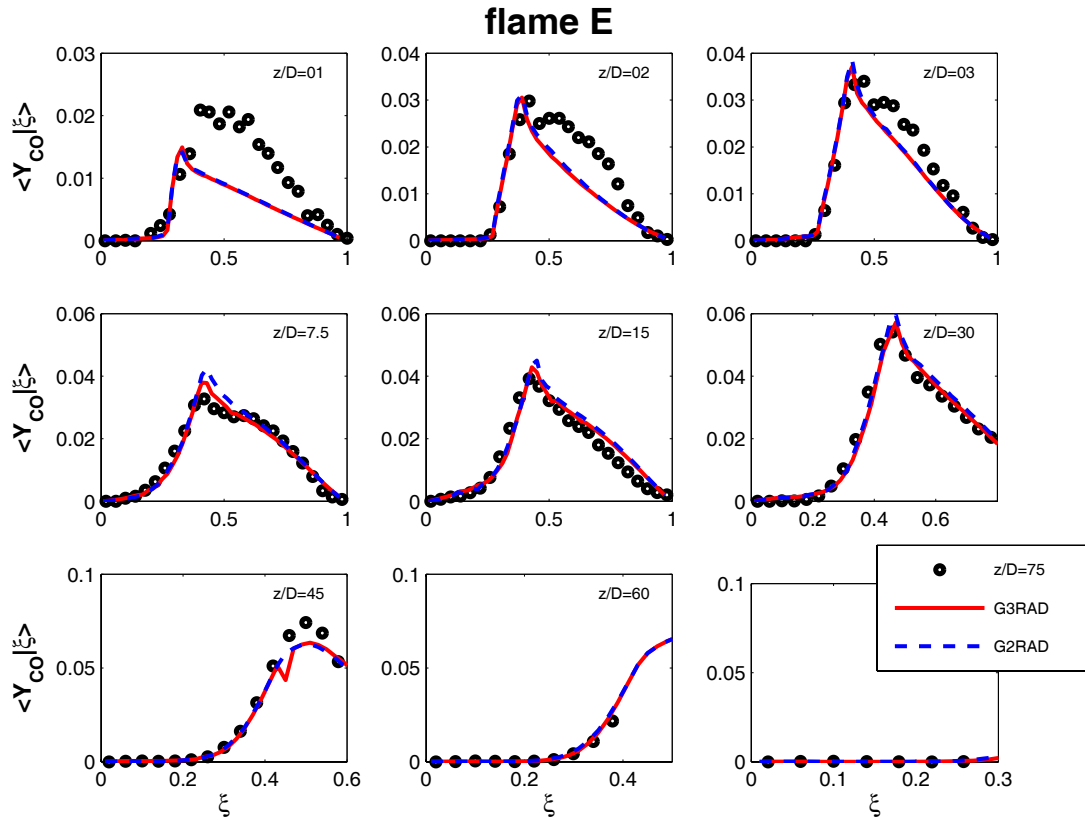


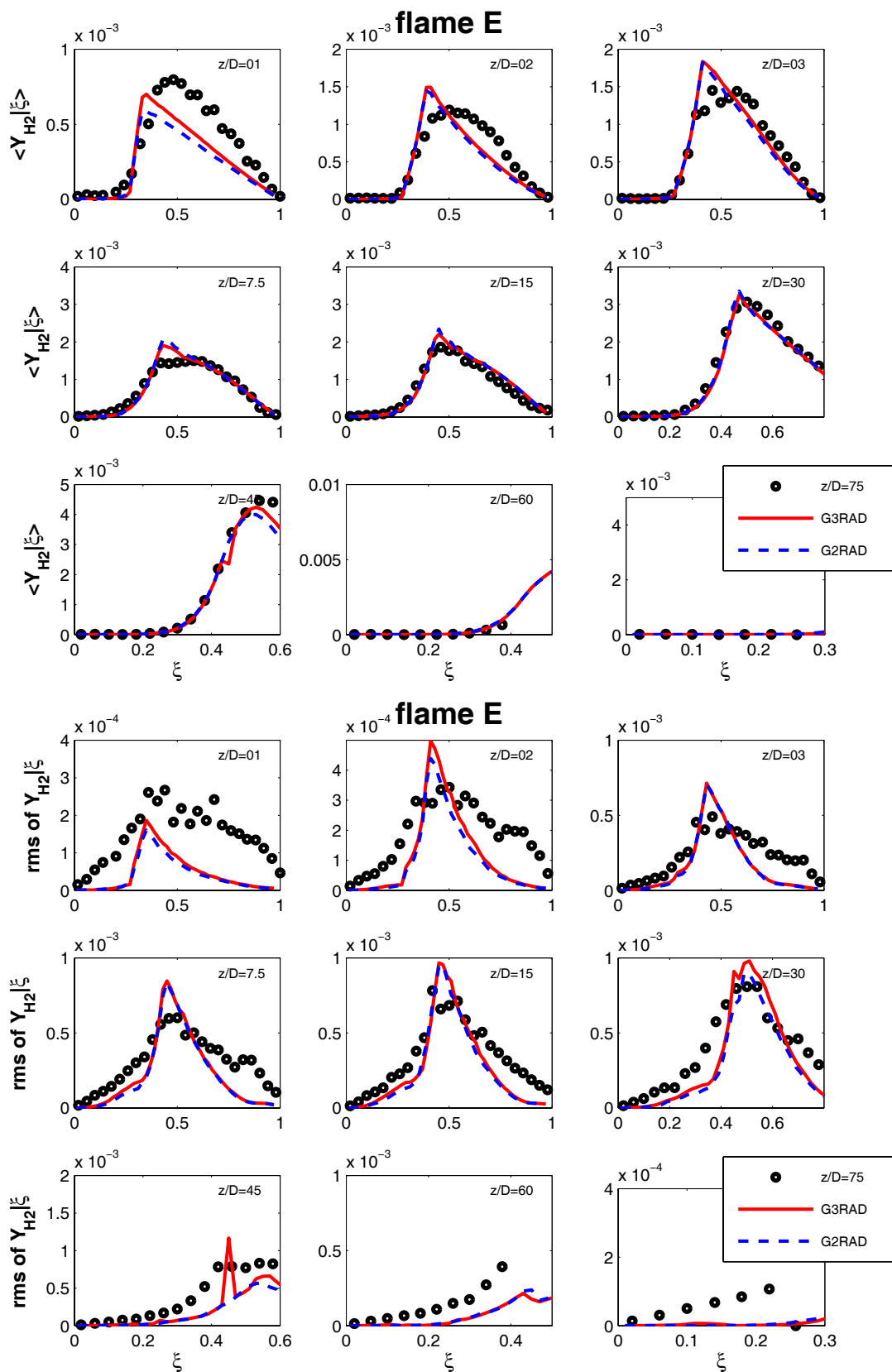


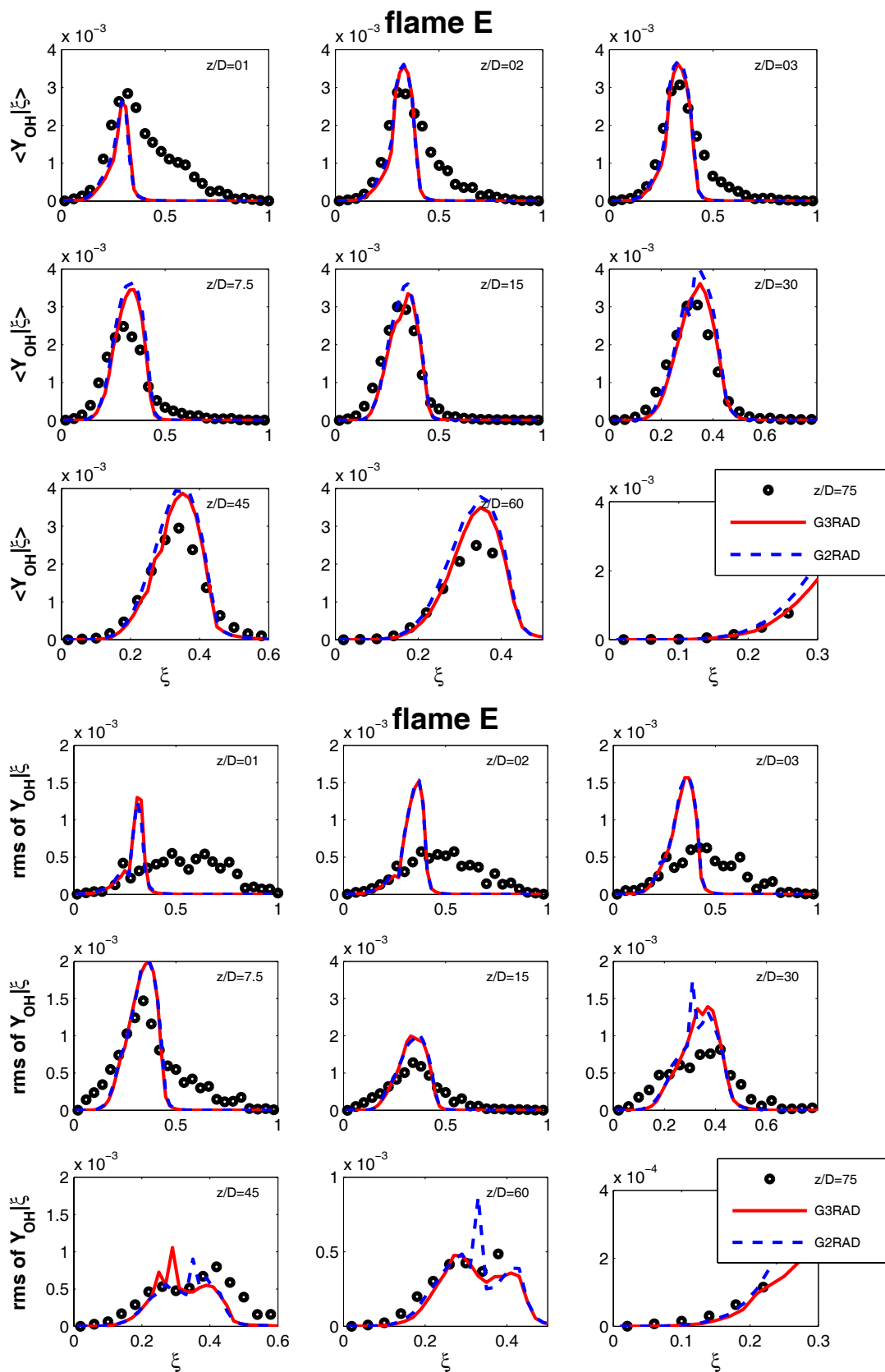


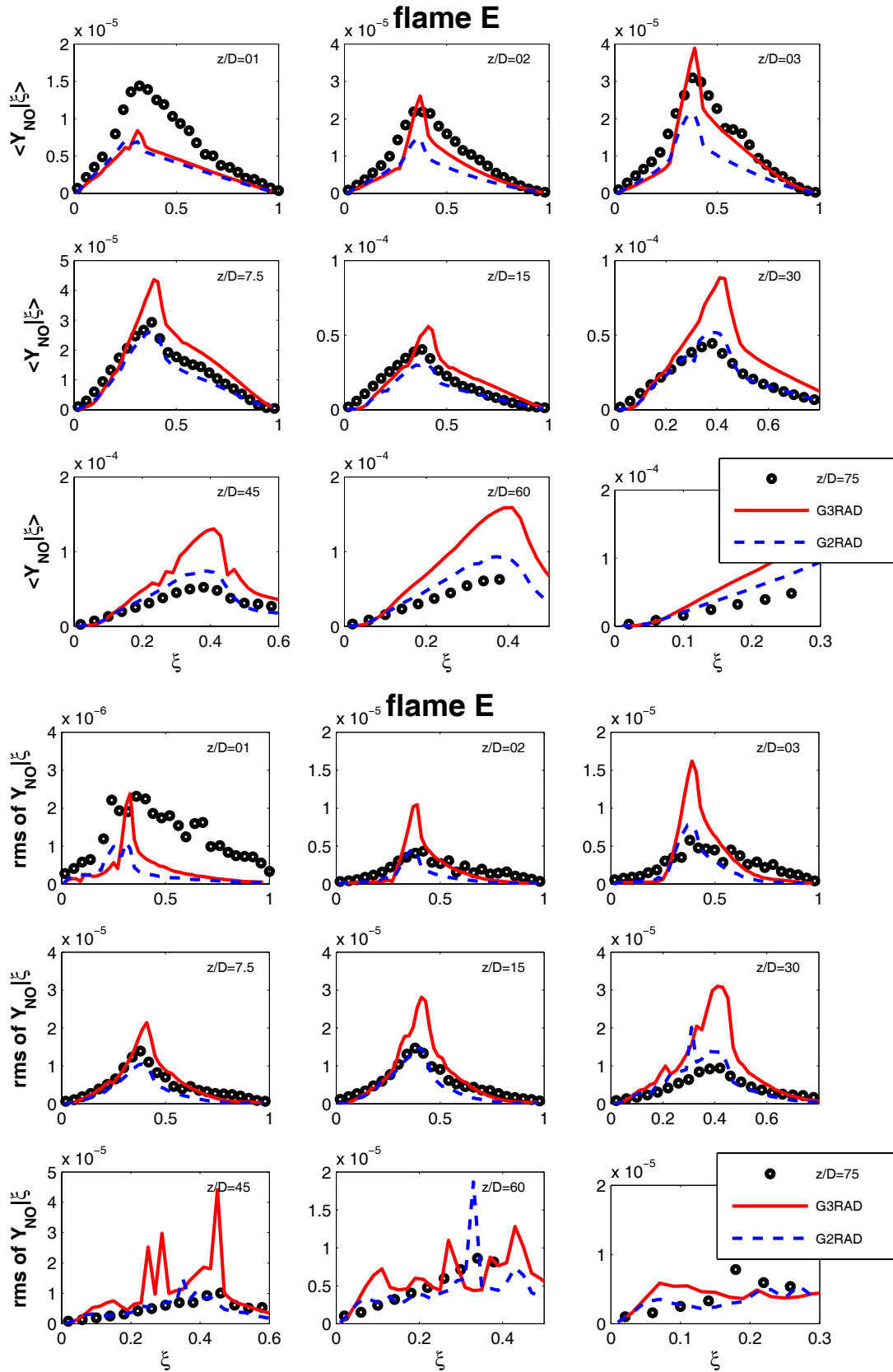




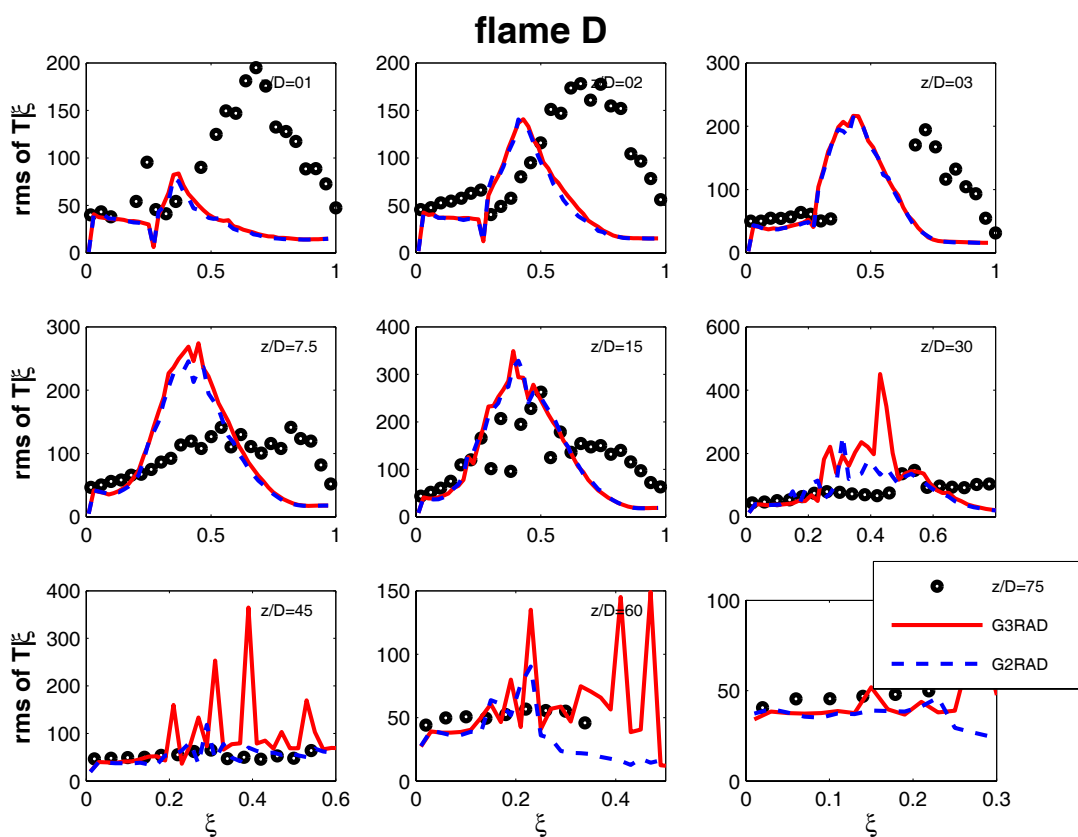
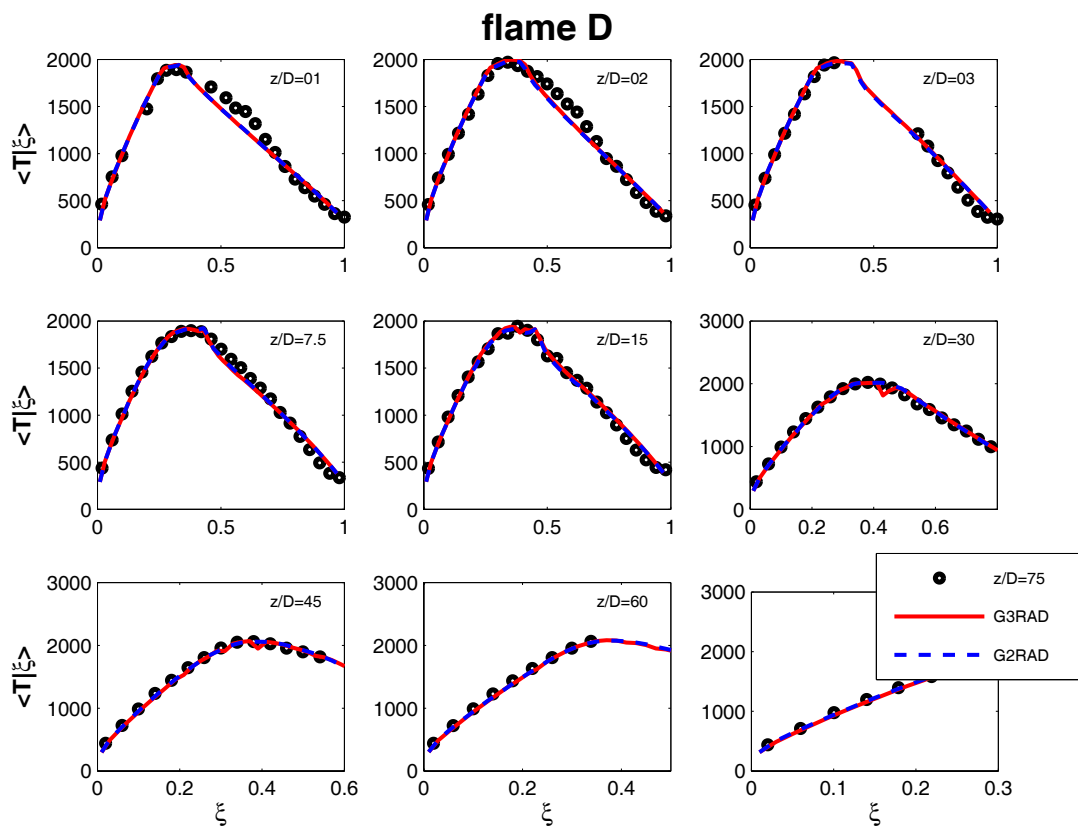


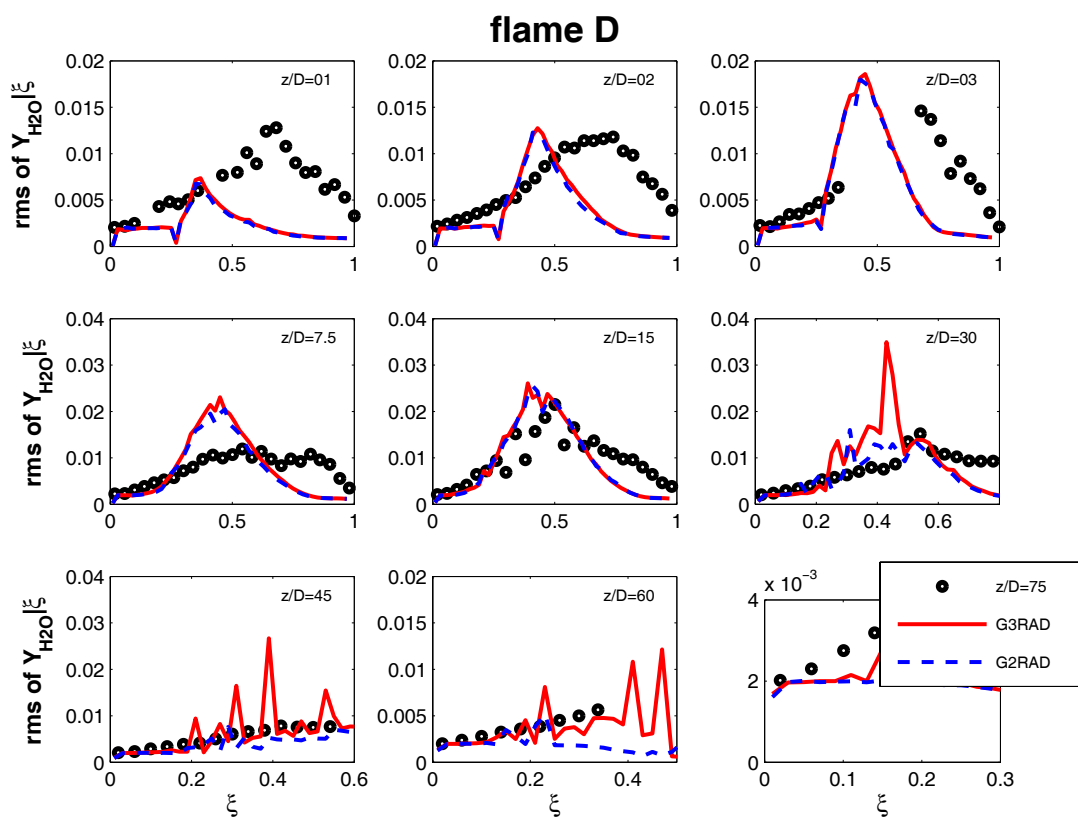
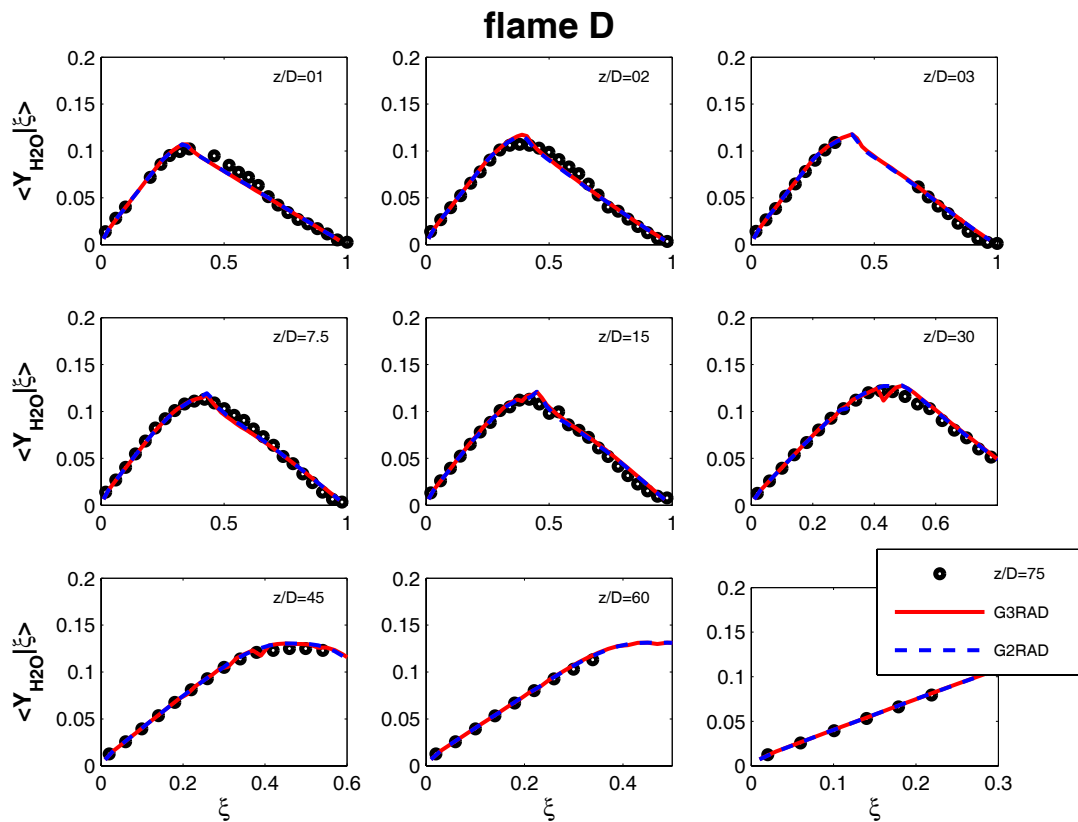


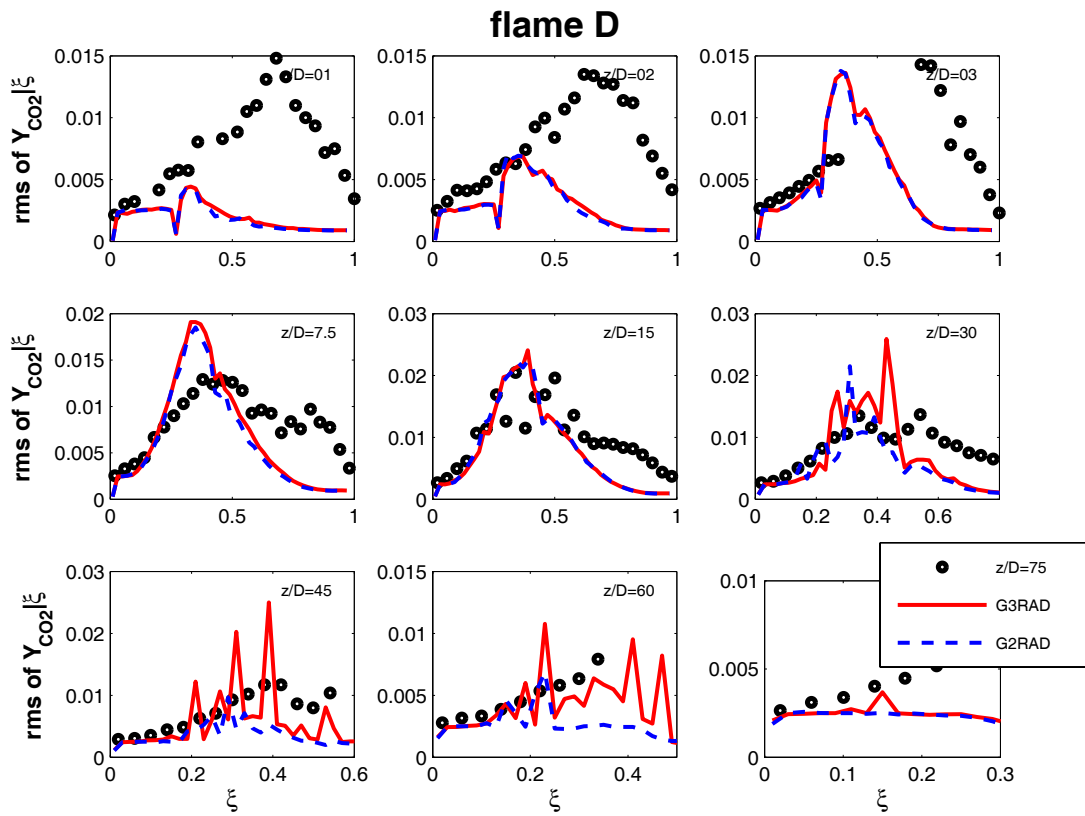
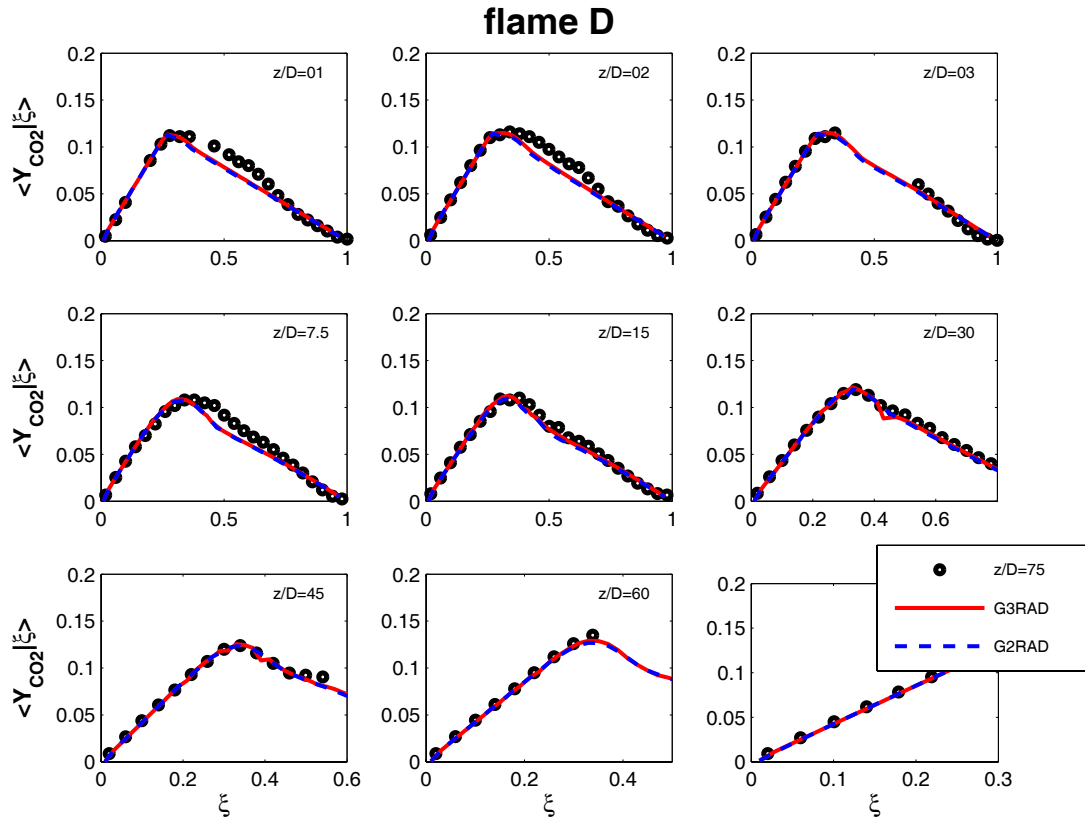


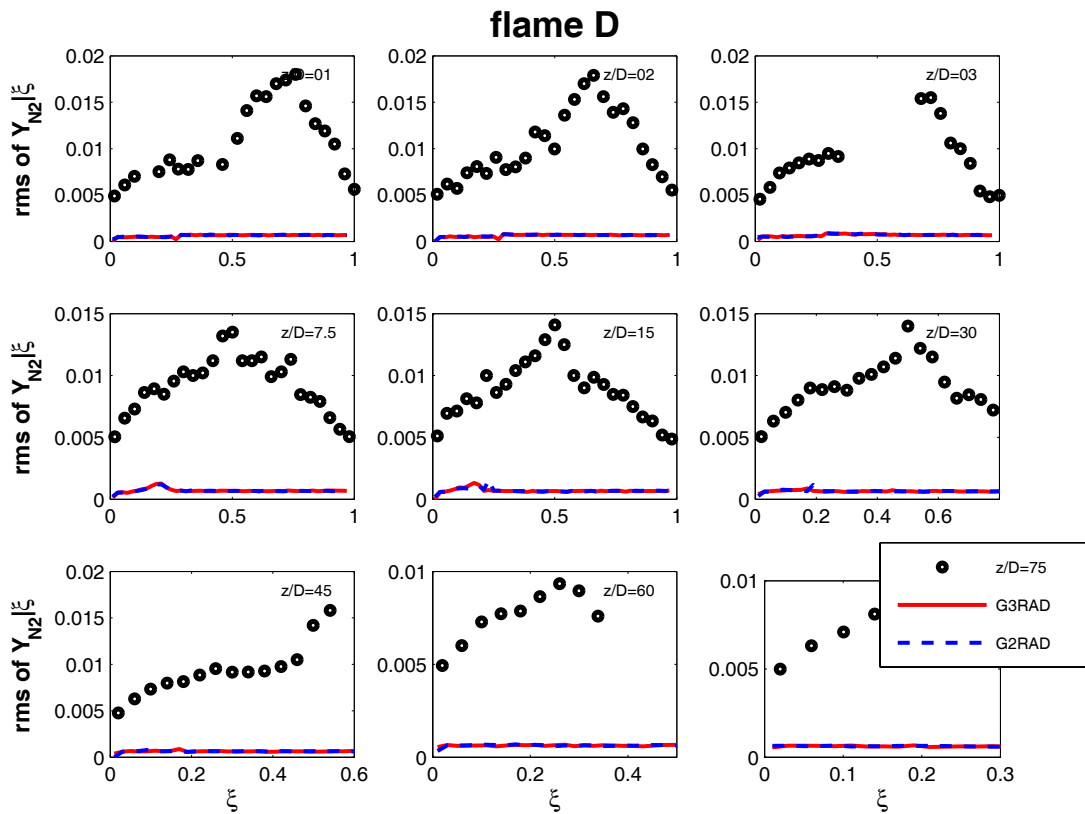
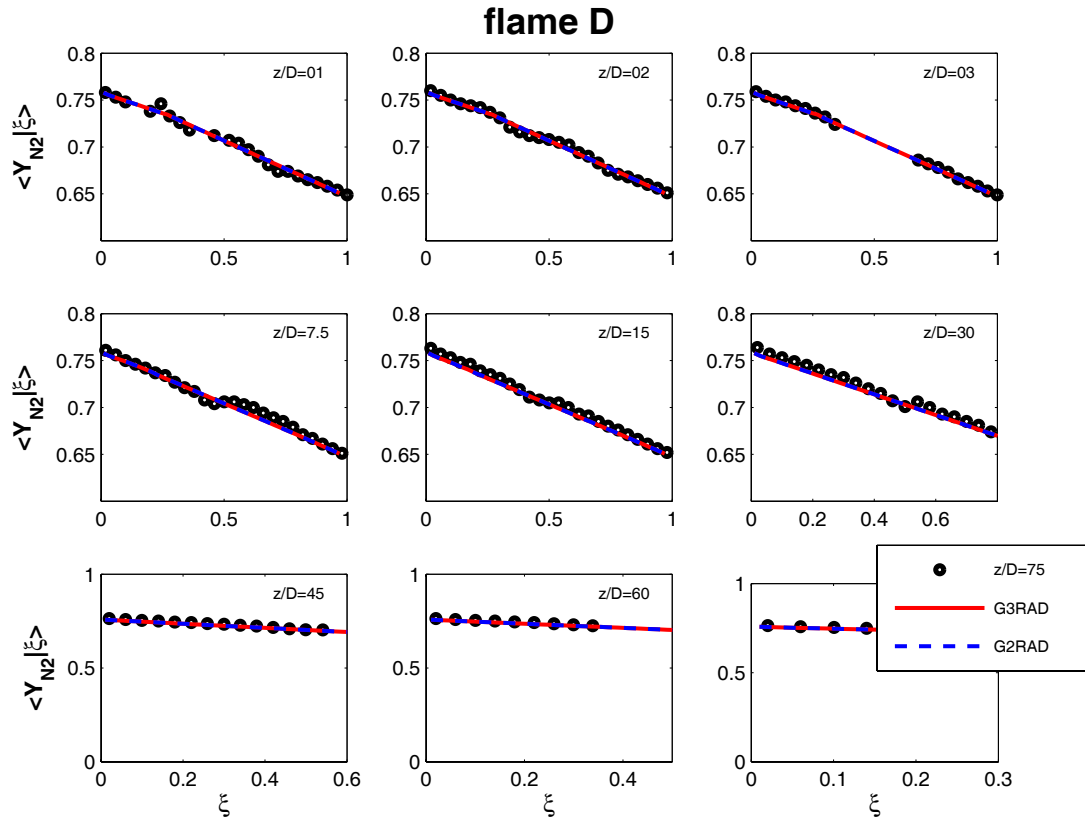


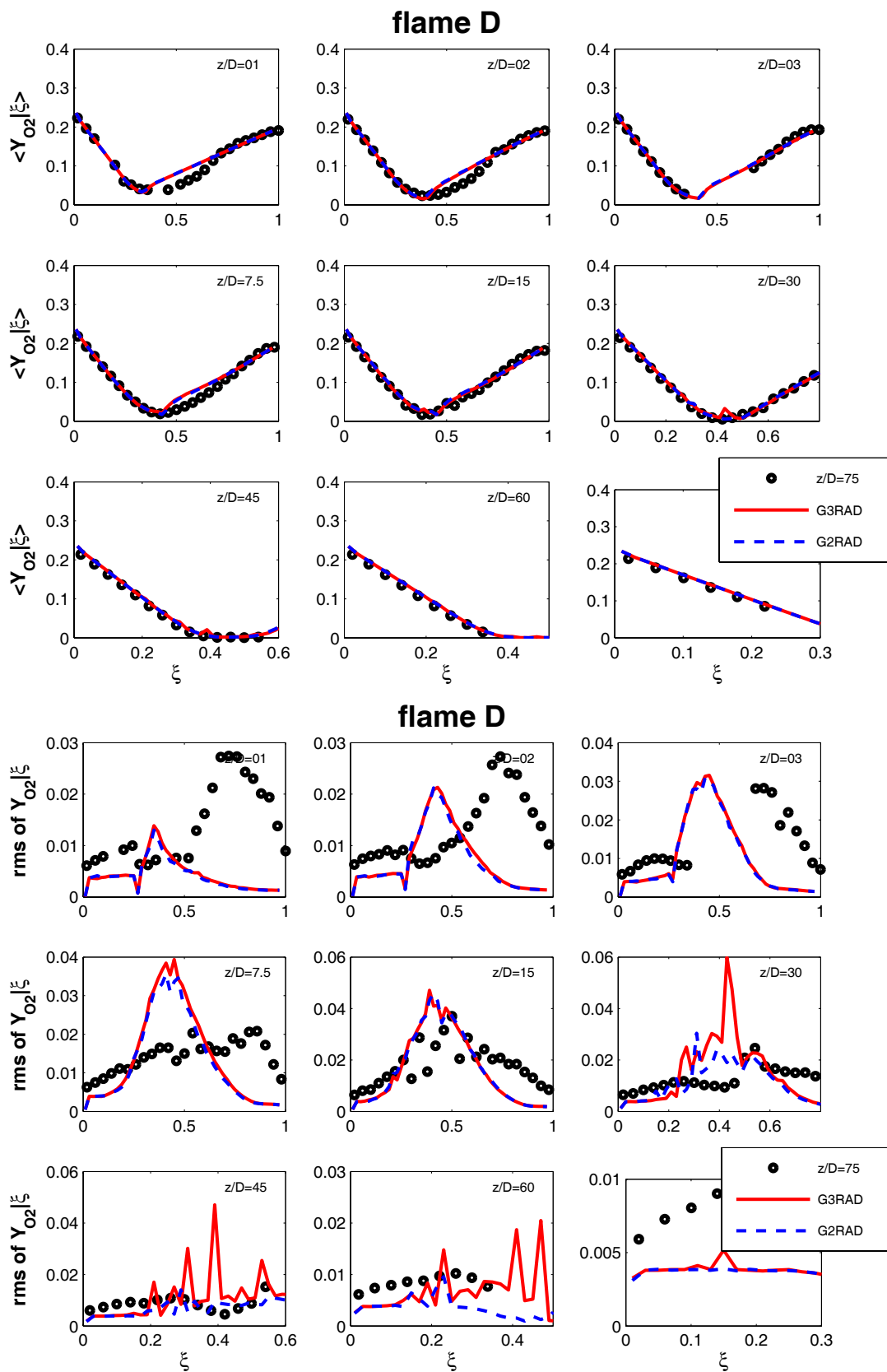
(3) Flame D

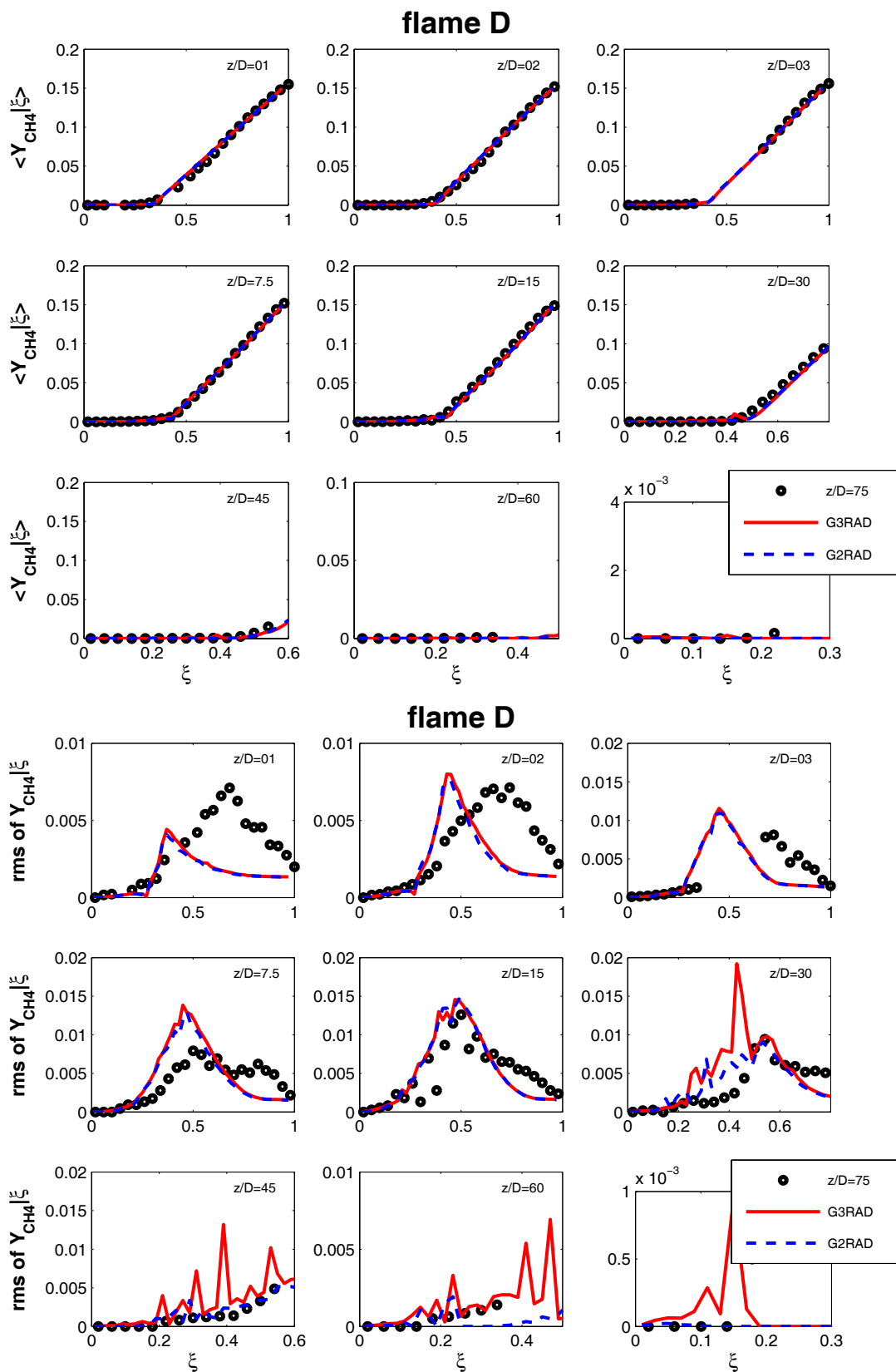


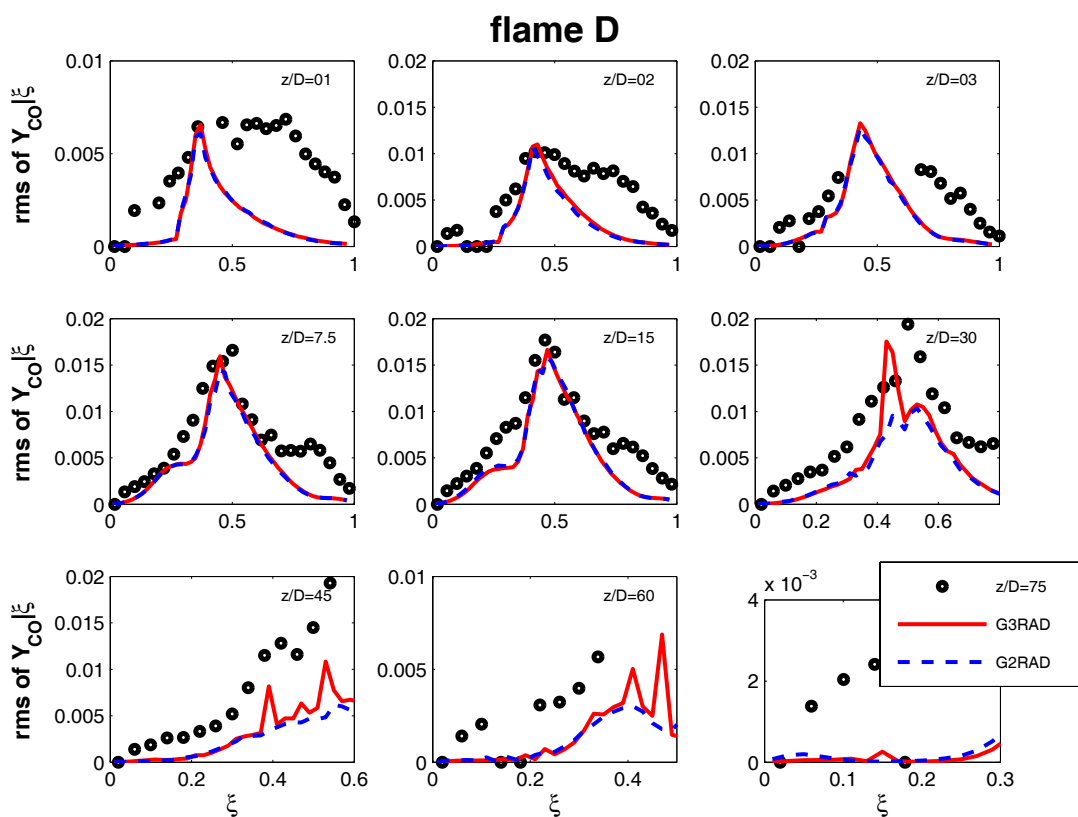
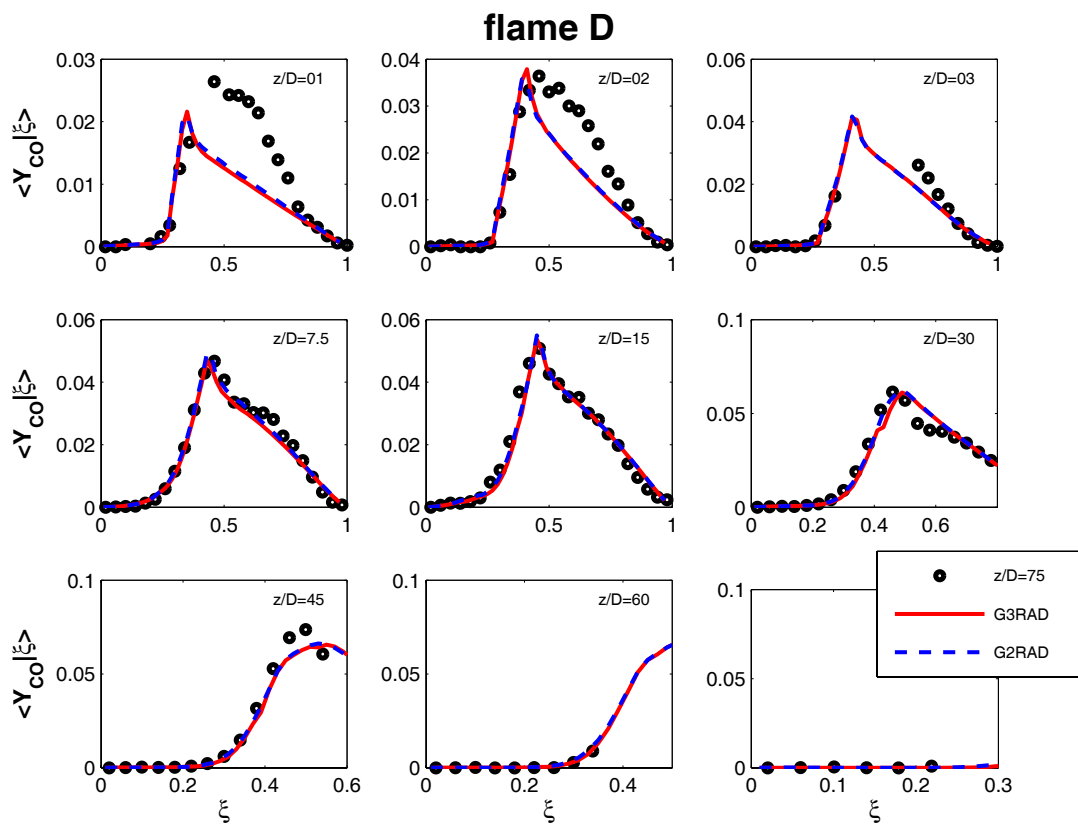


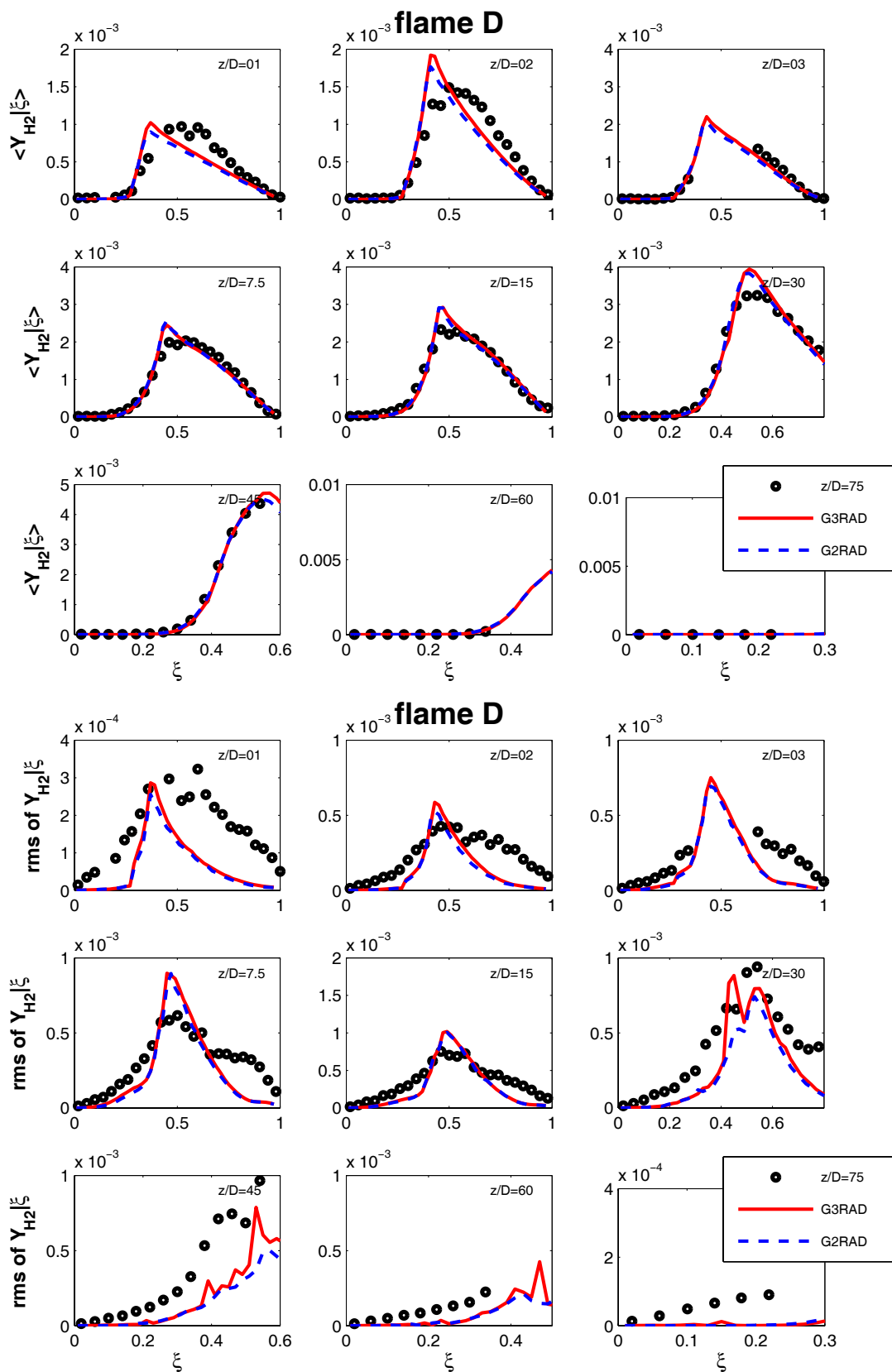


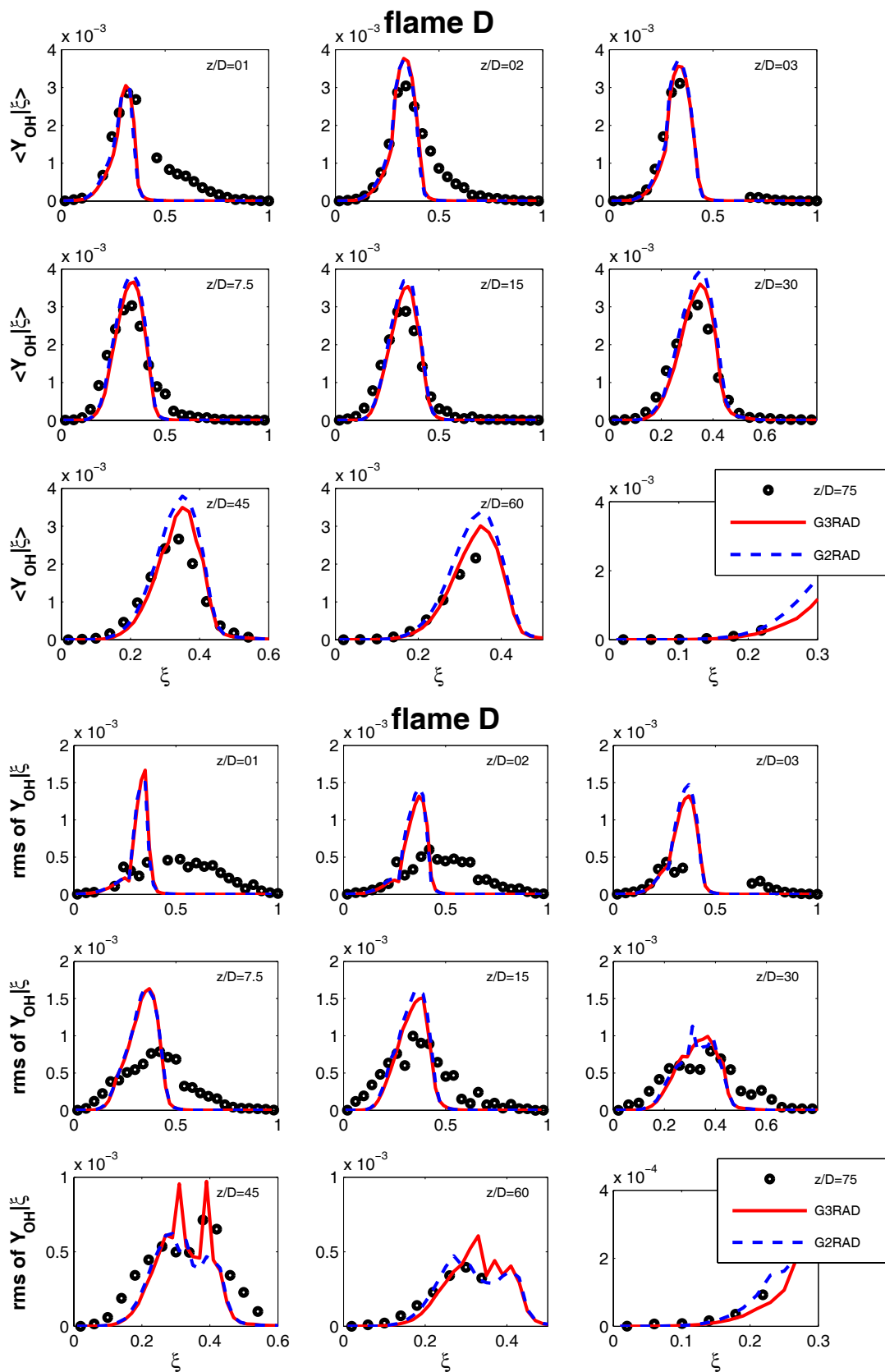


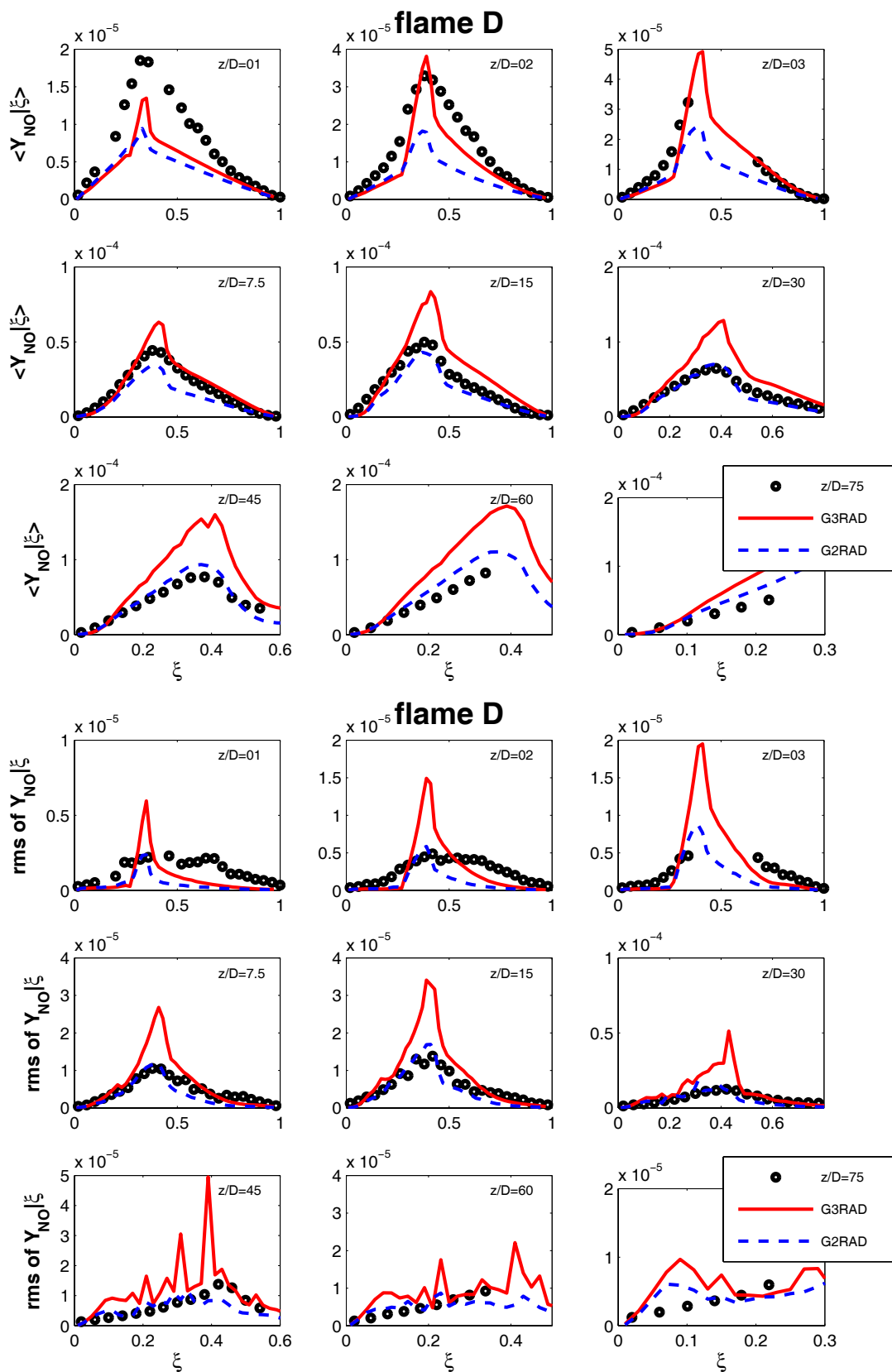






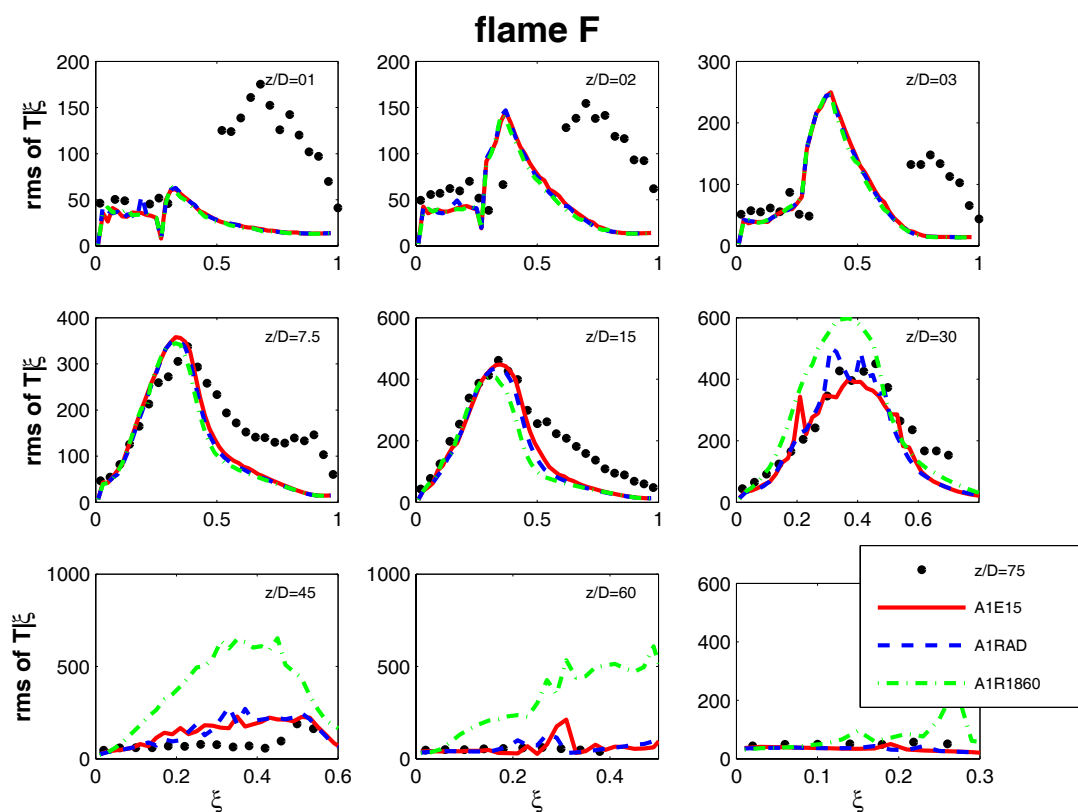
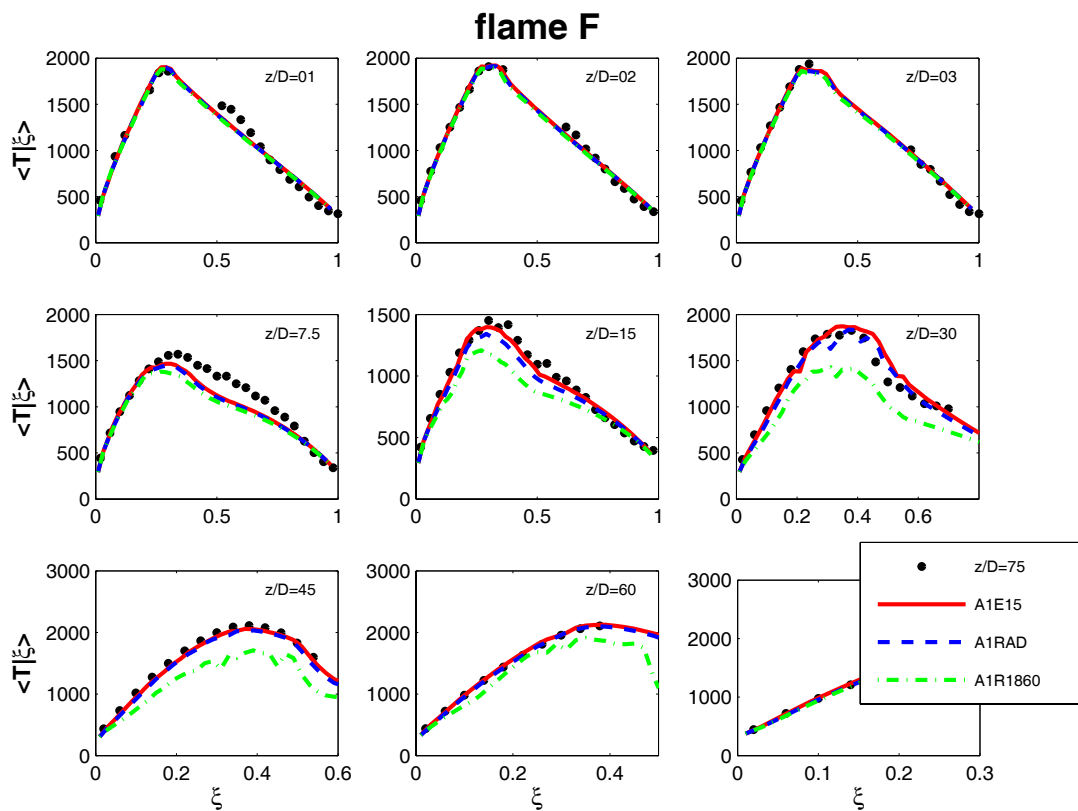


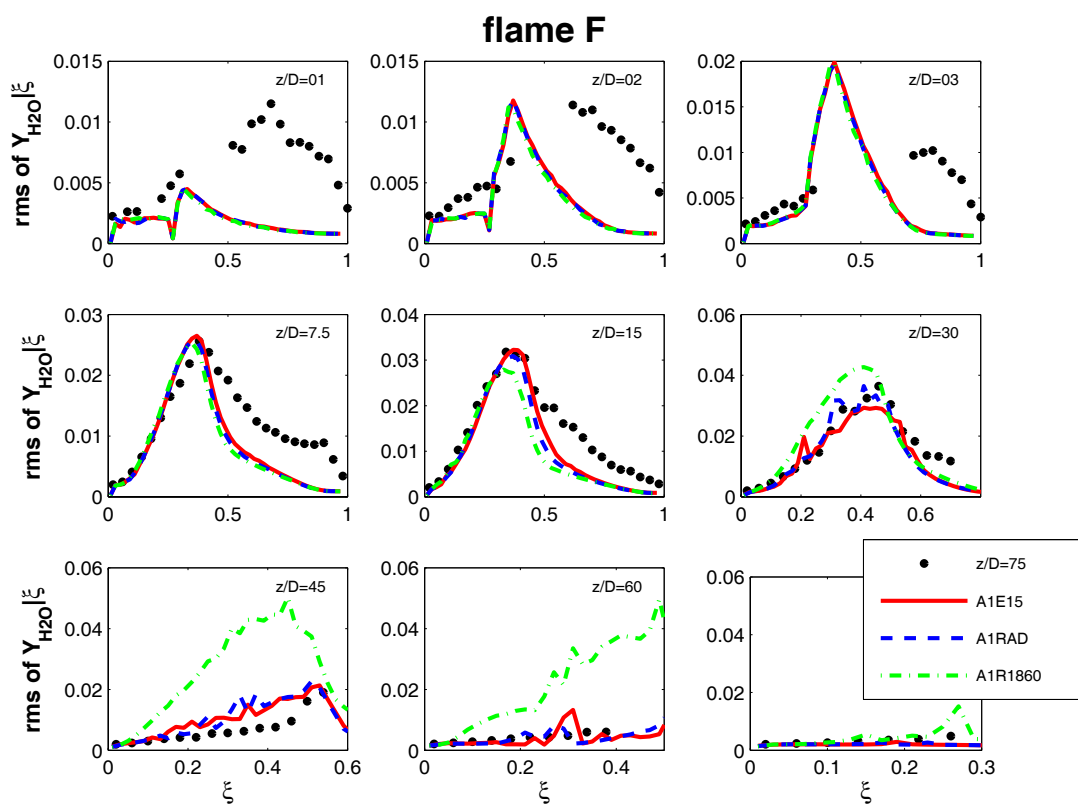
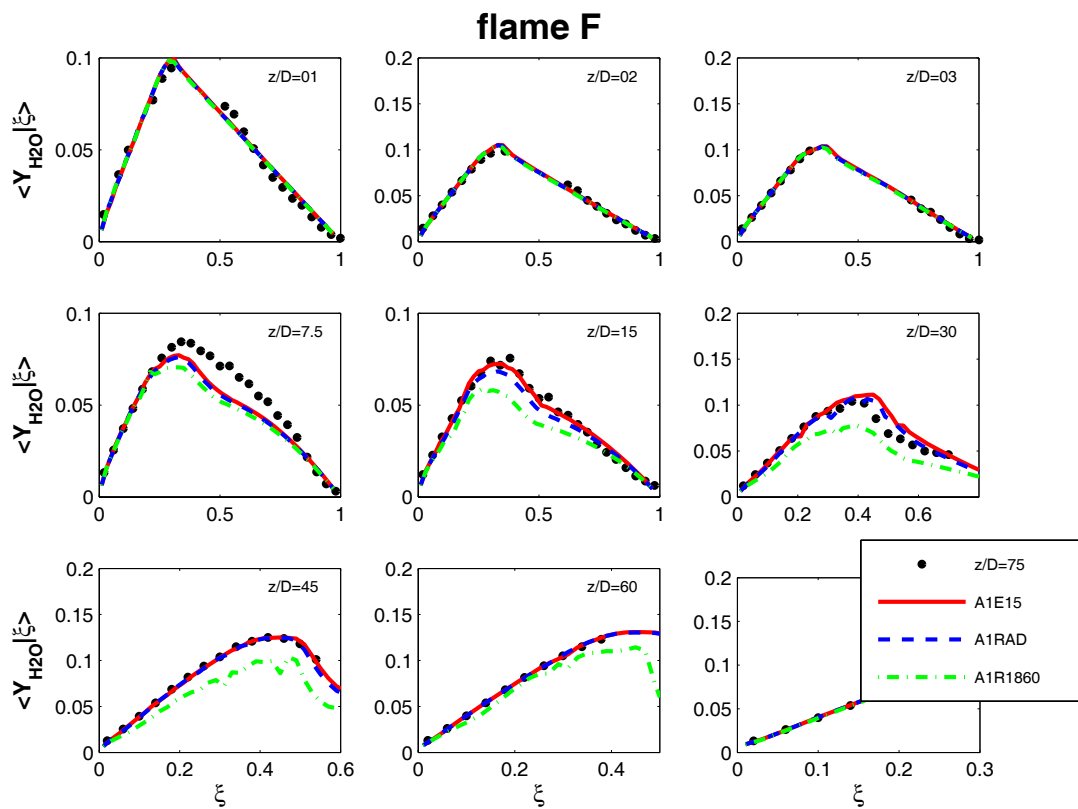


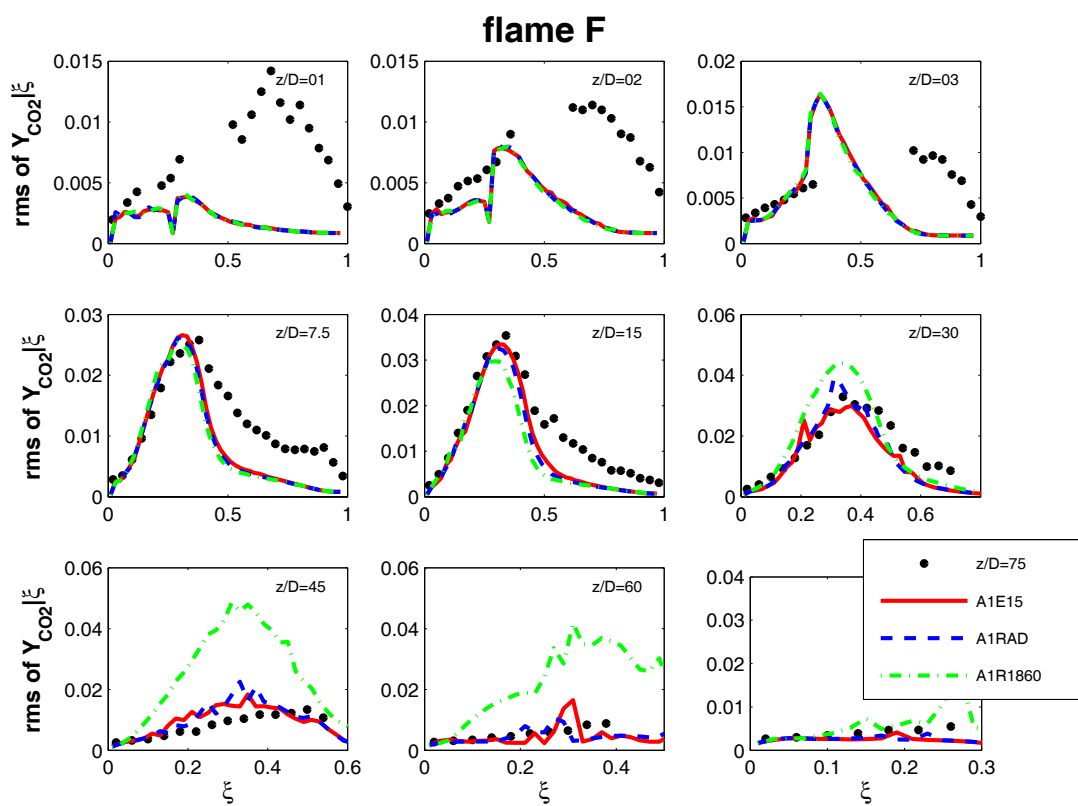
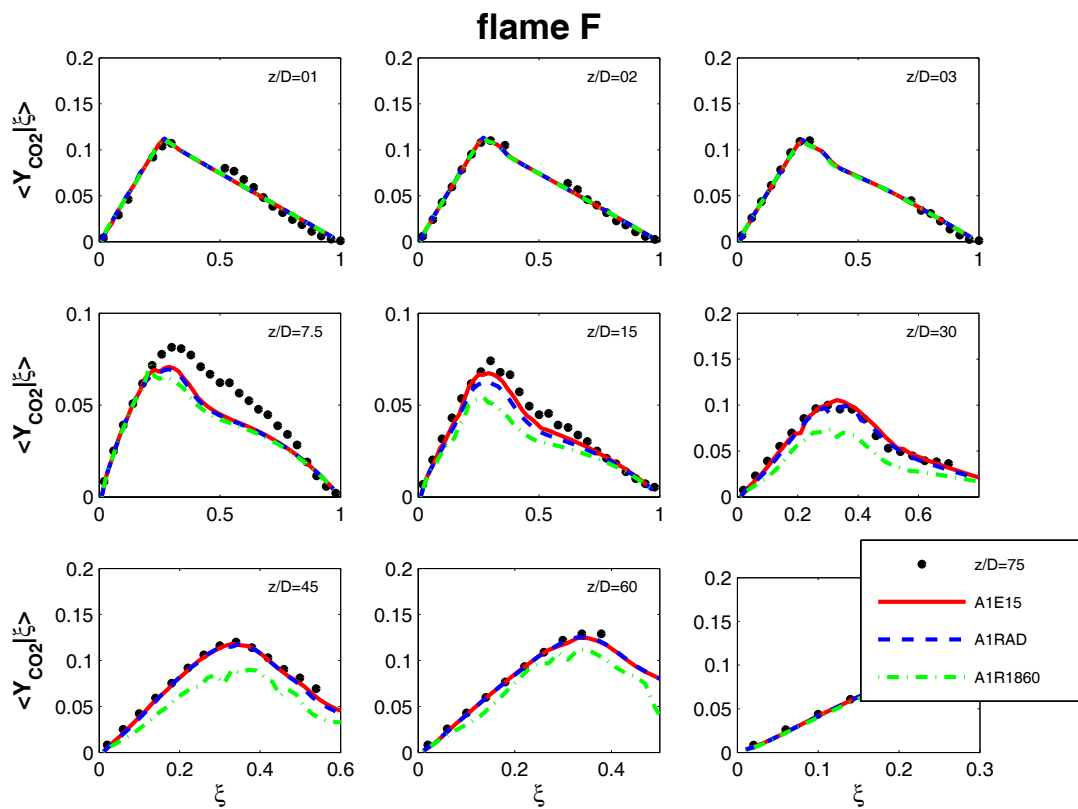


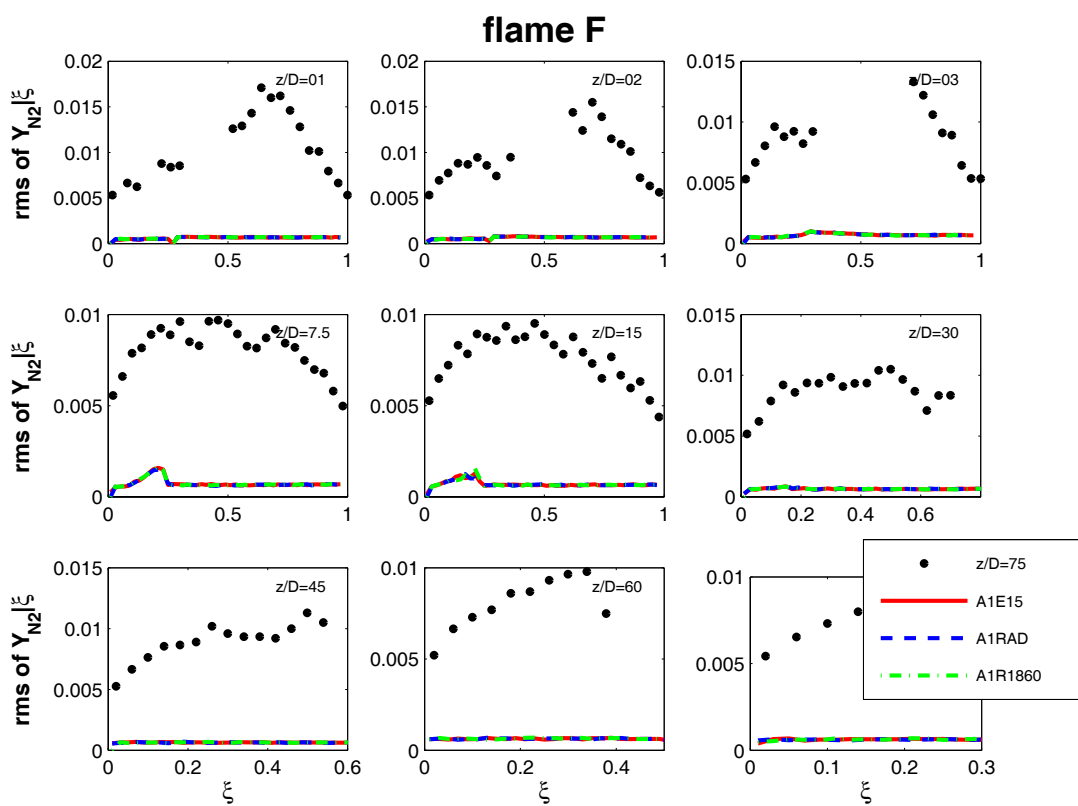
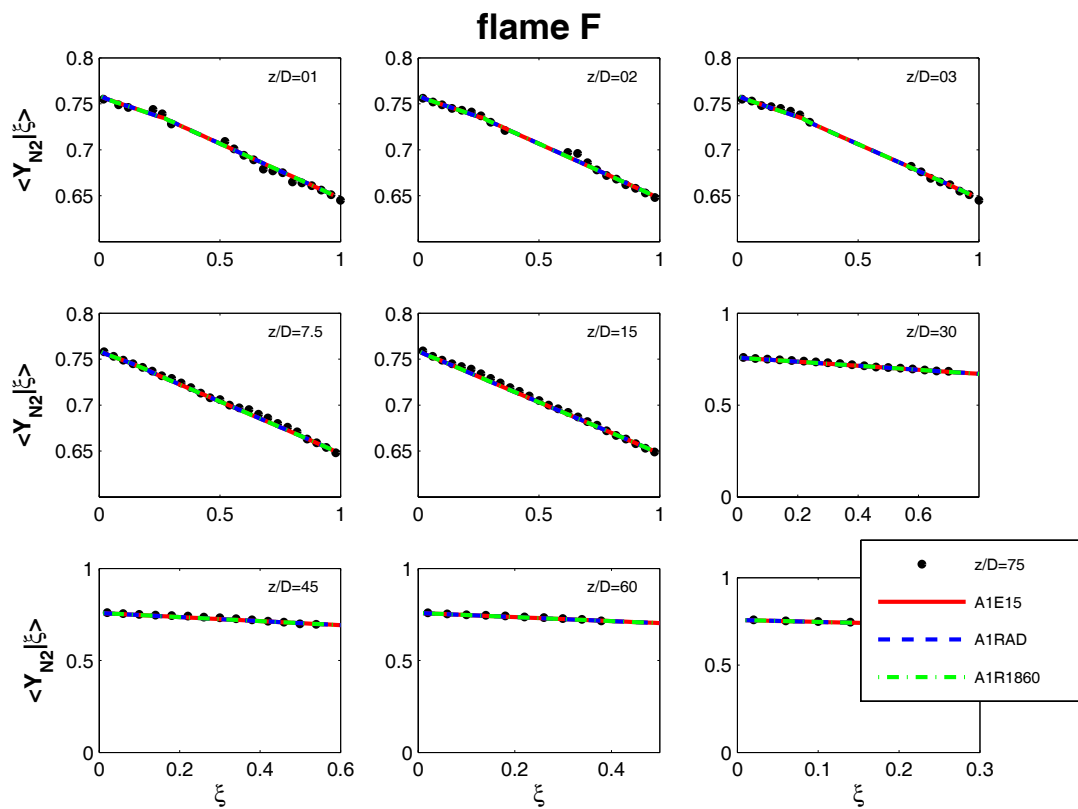
B-2 Flame F calculations

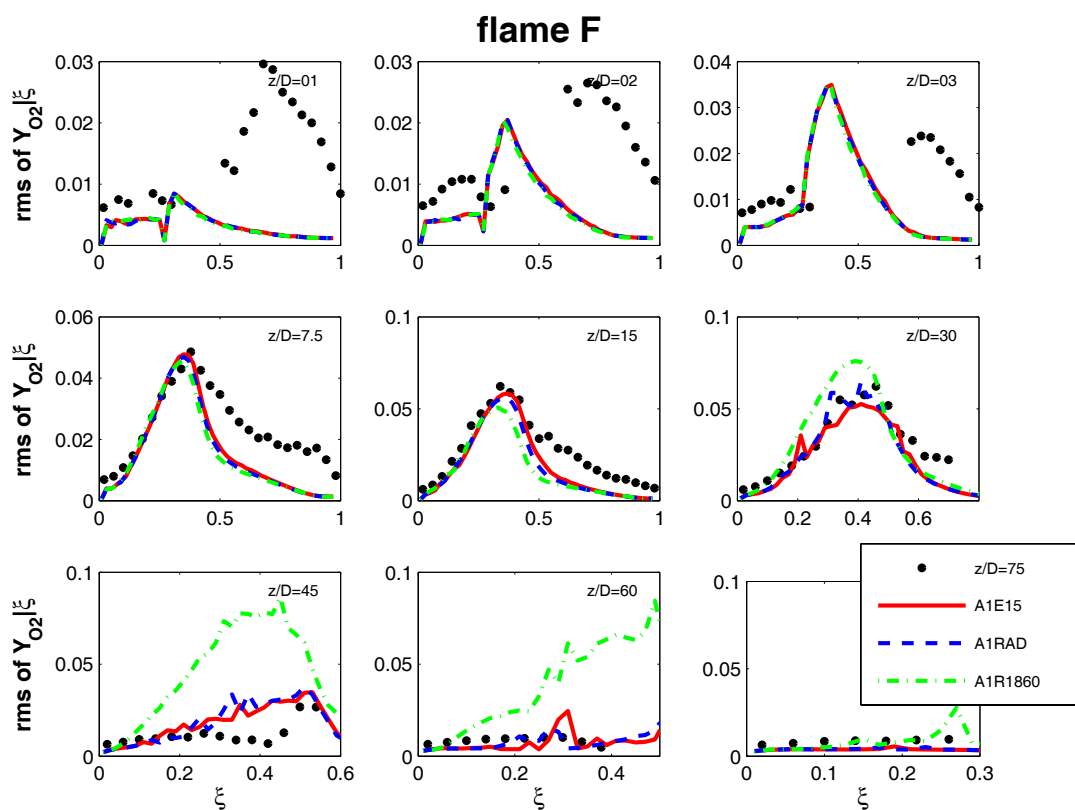
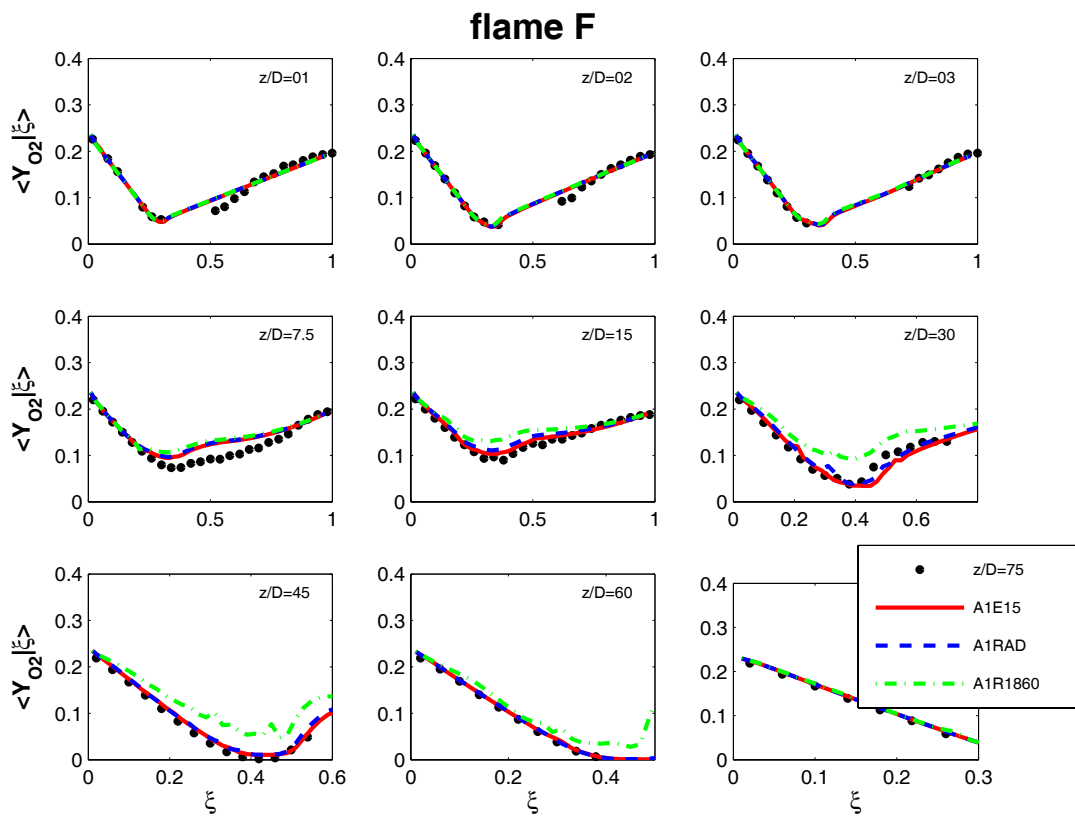
(1) A1E15, A1RAD and A1R1860

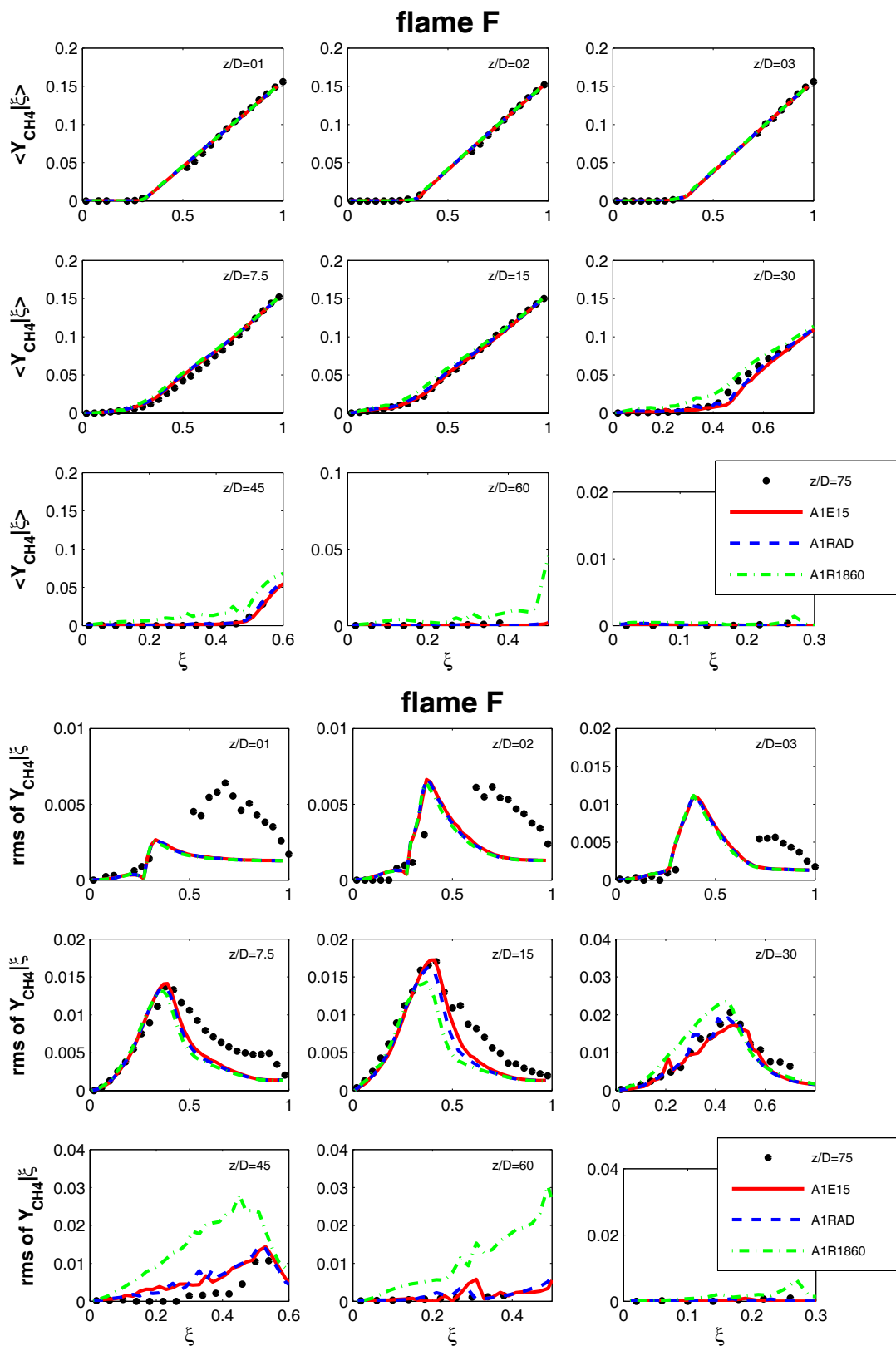


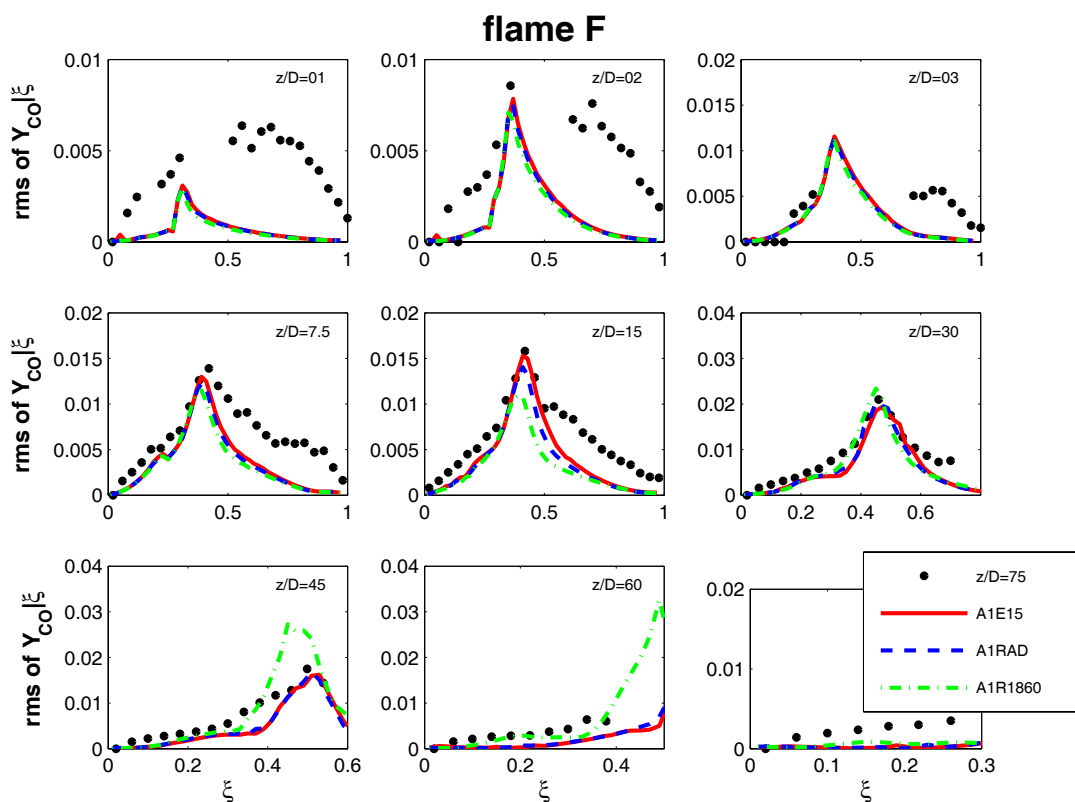
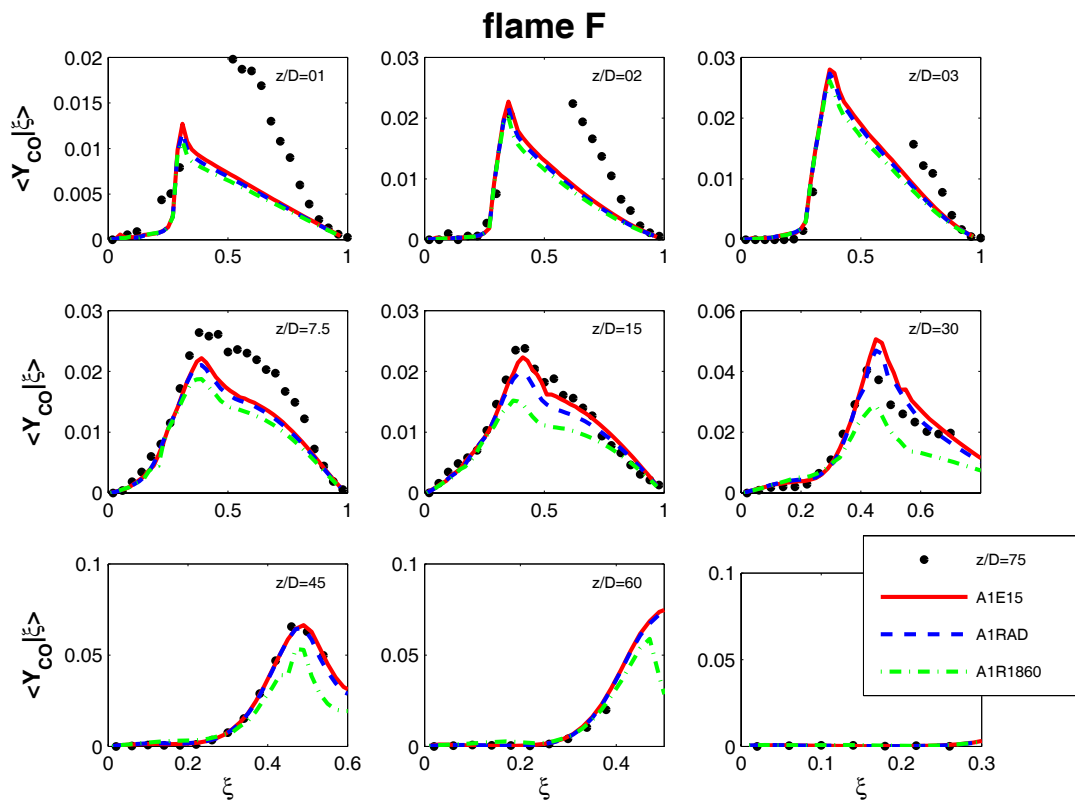


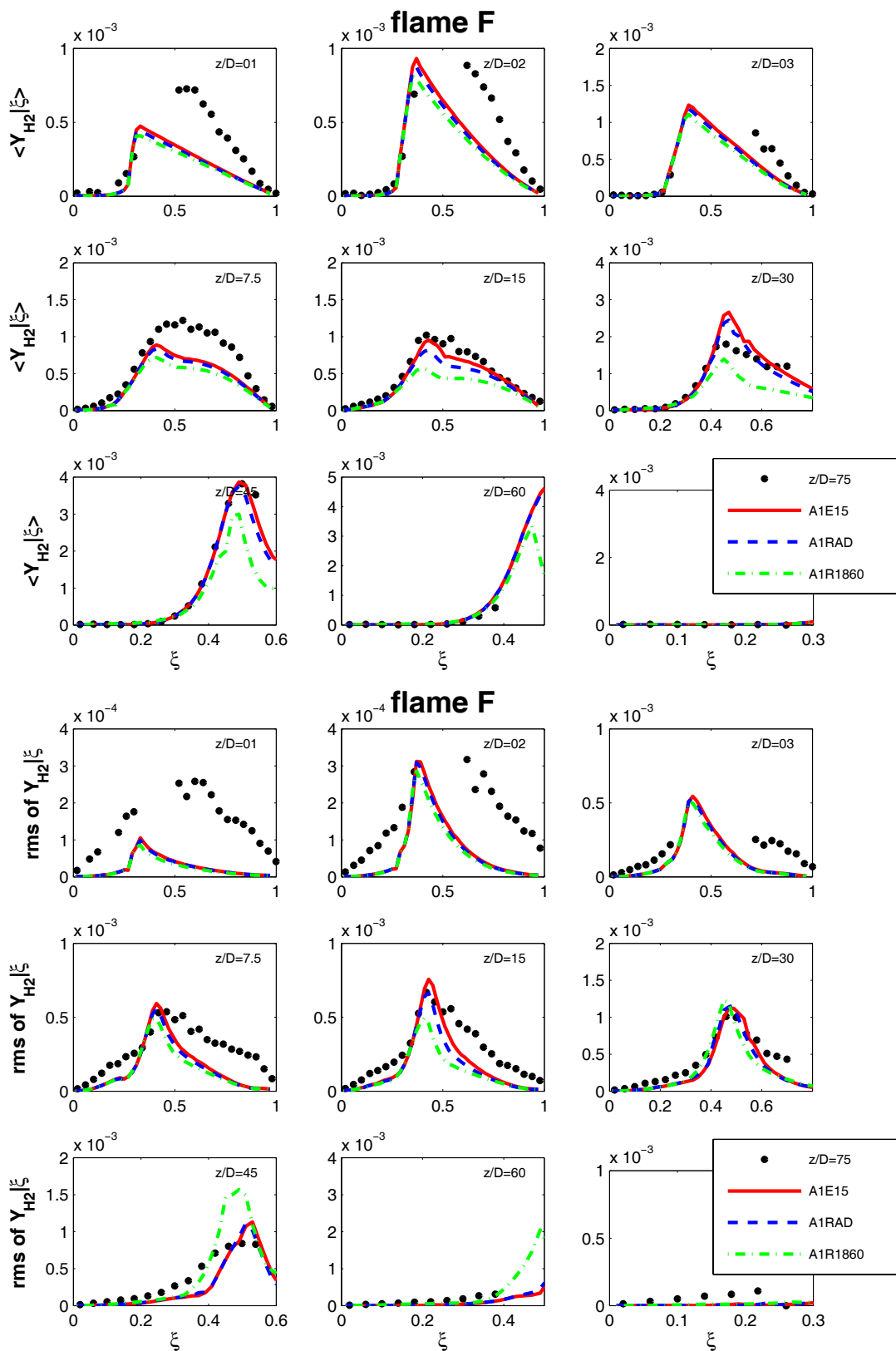


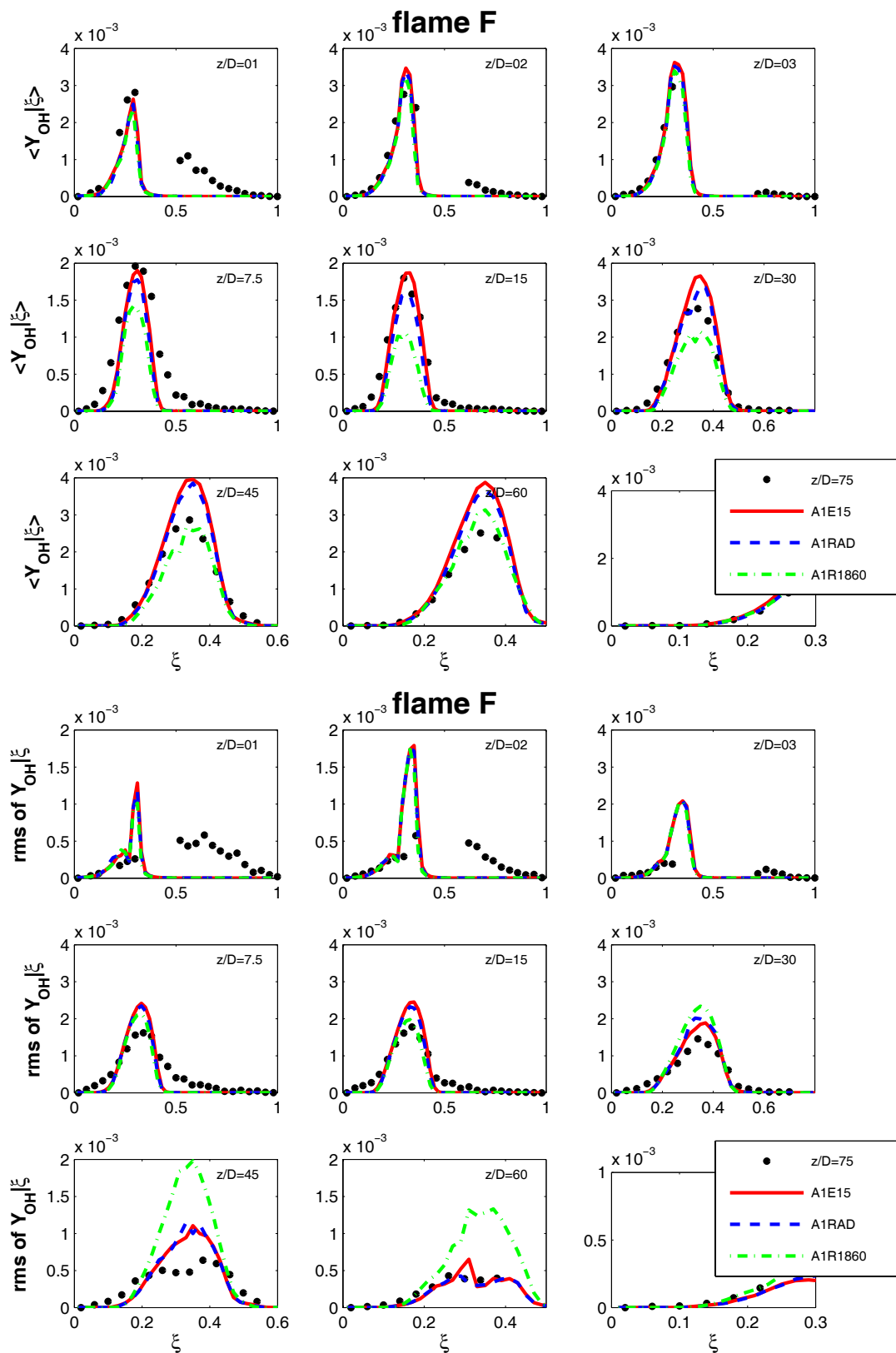




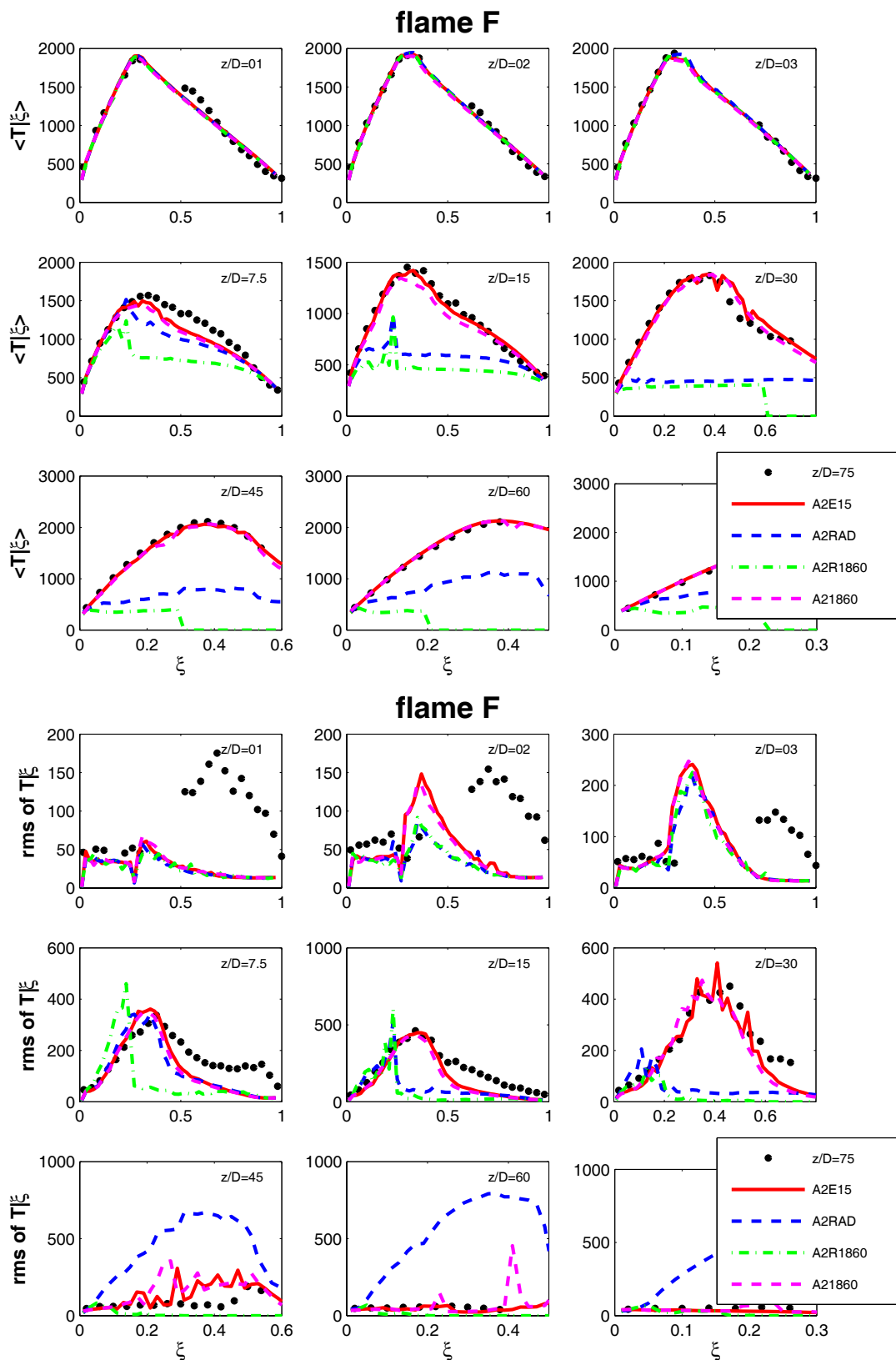


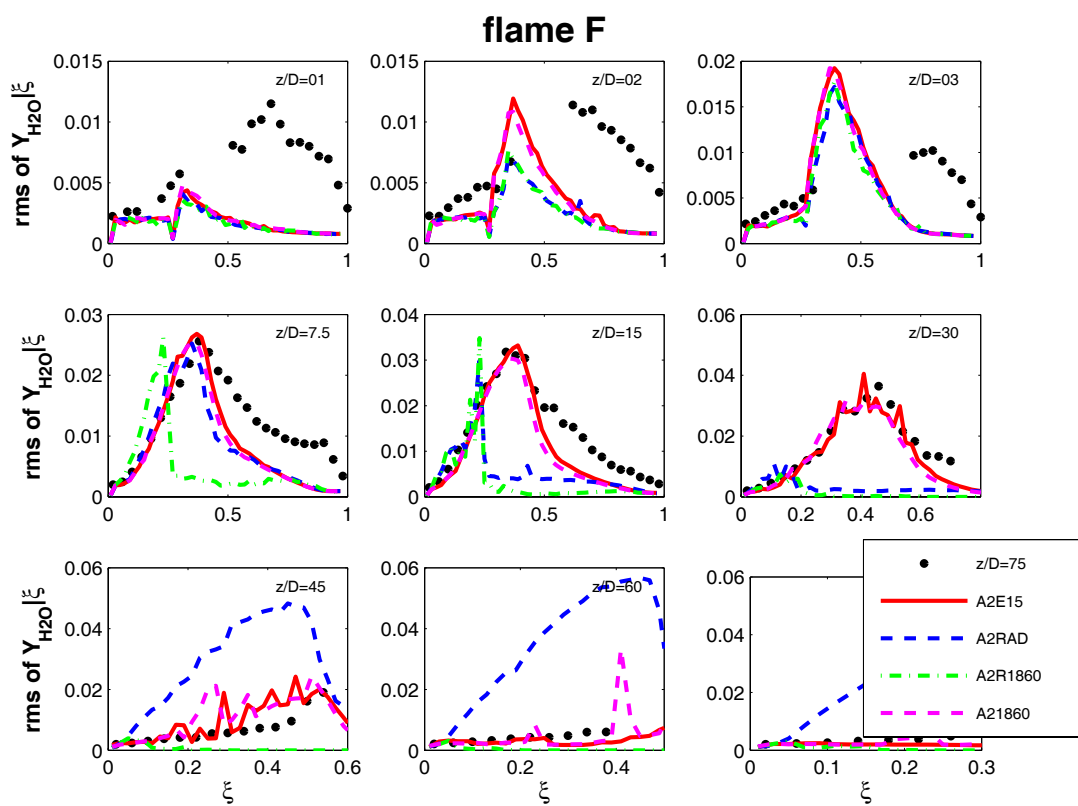
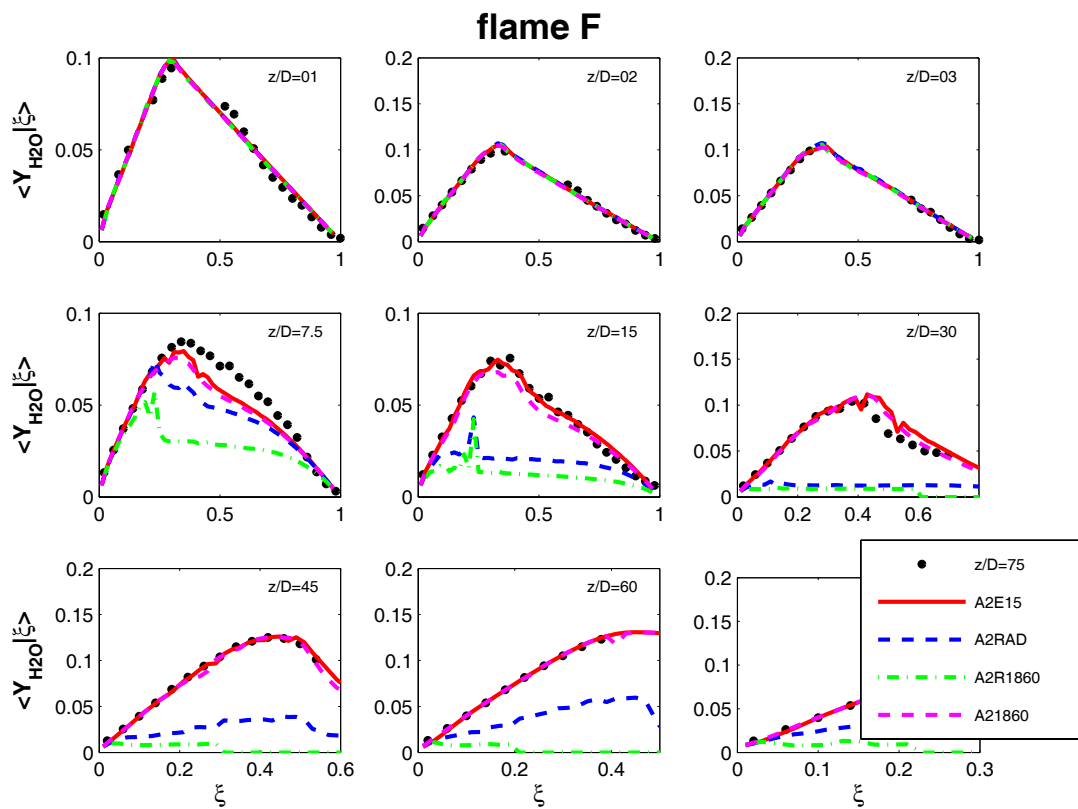


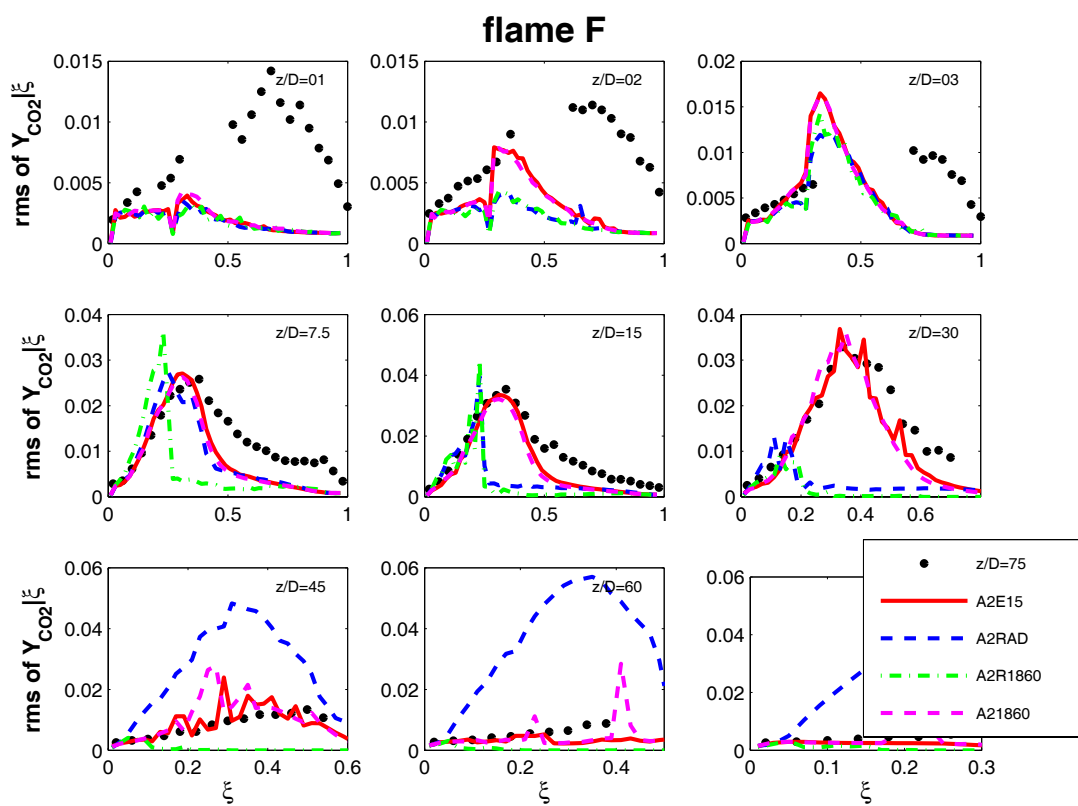
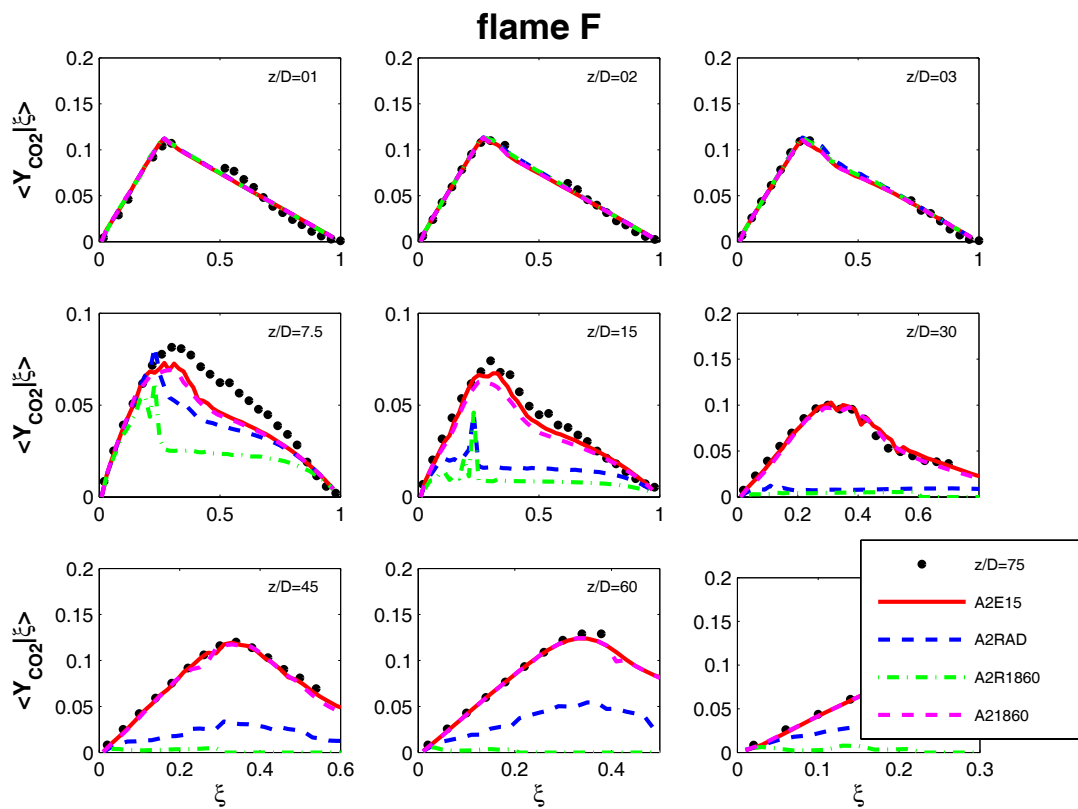


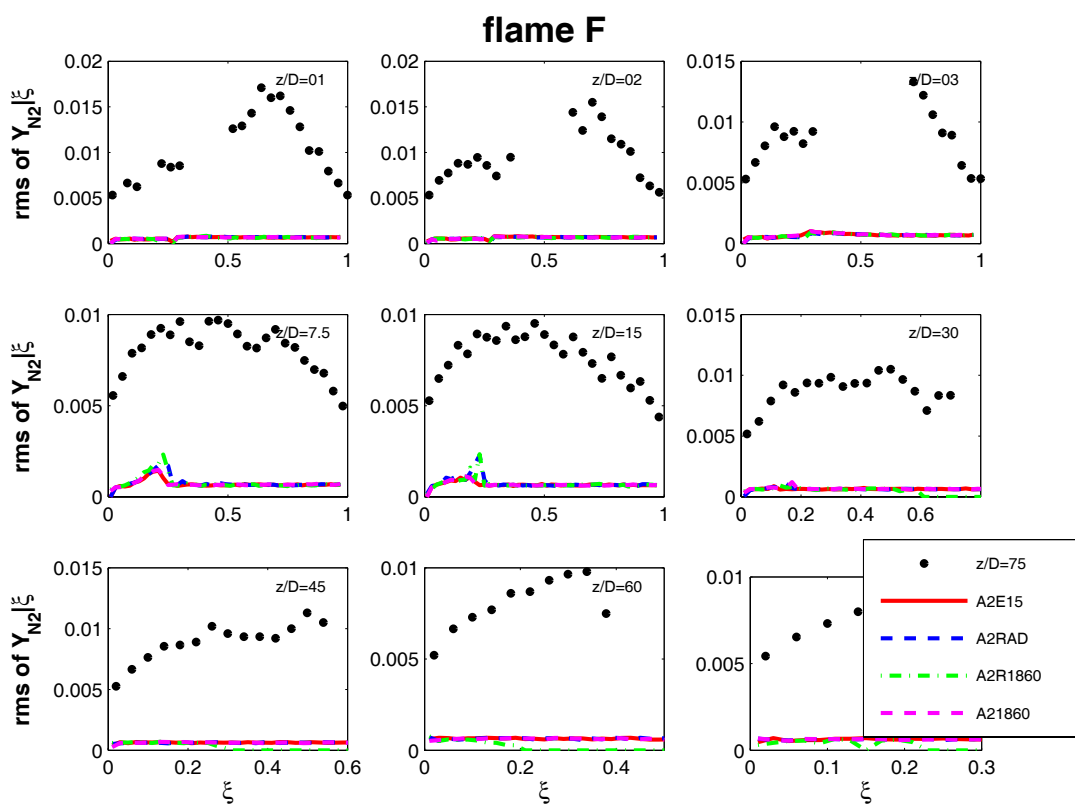
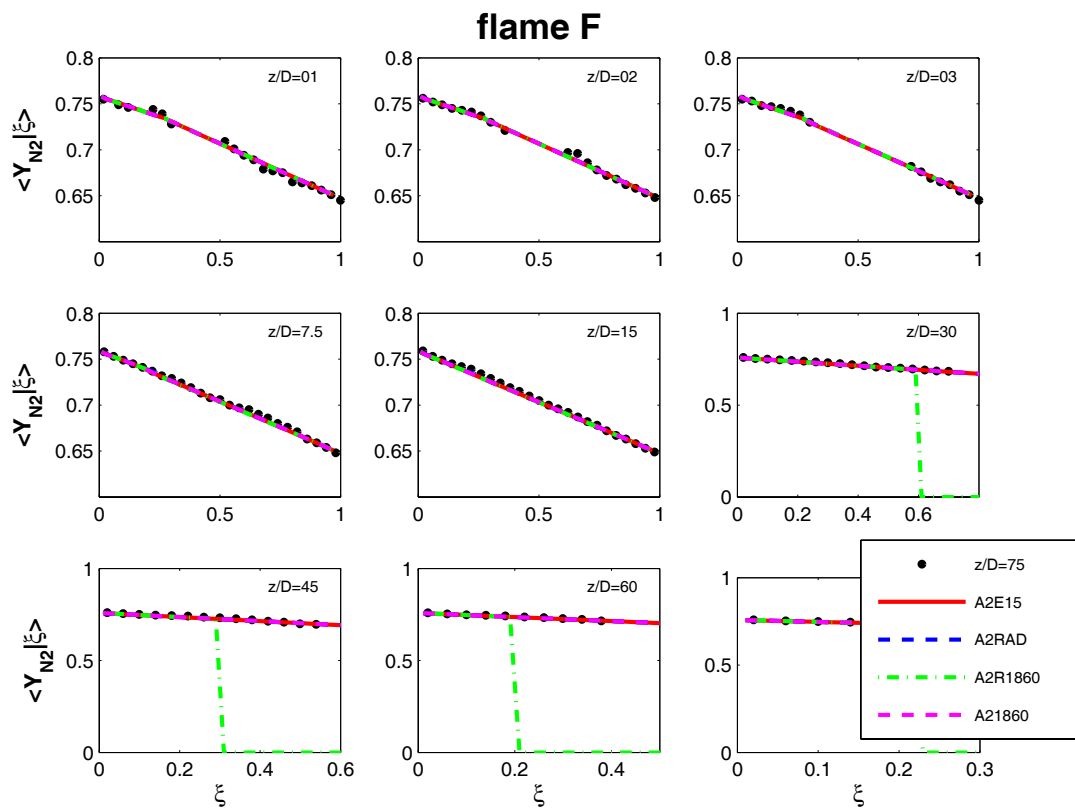


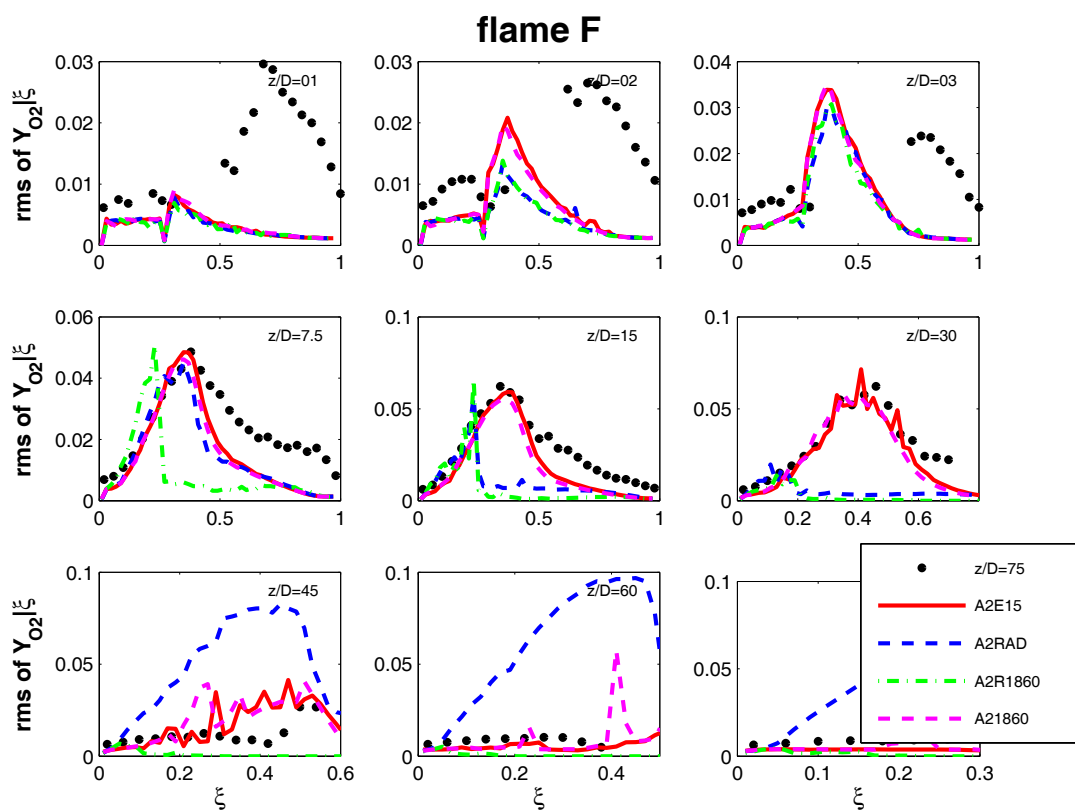
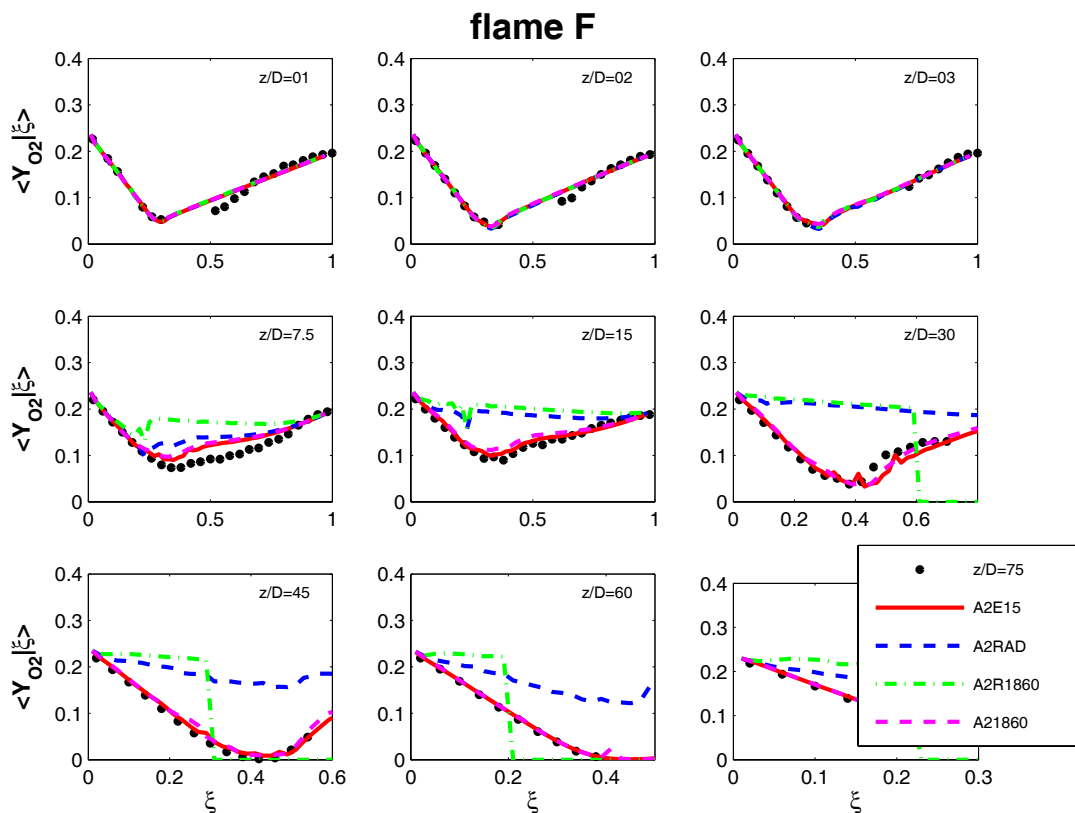
(2) A2E15, A2RAD, A21860 and A2R1860

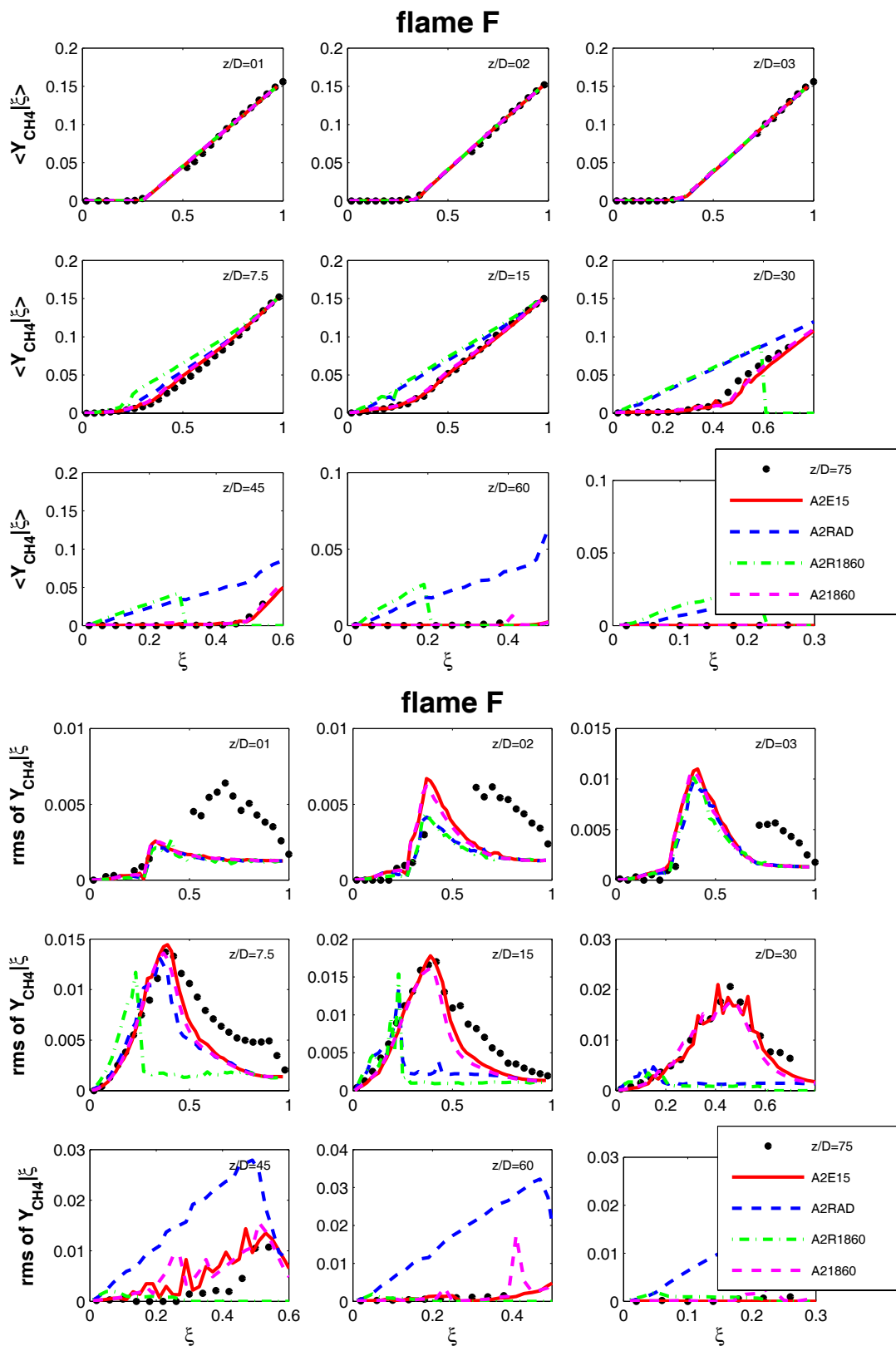


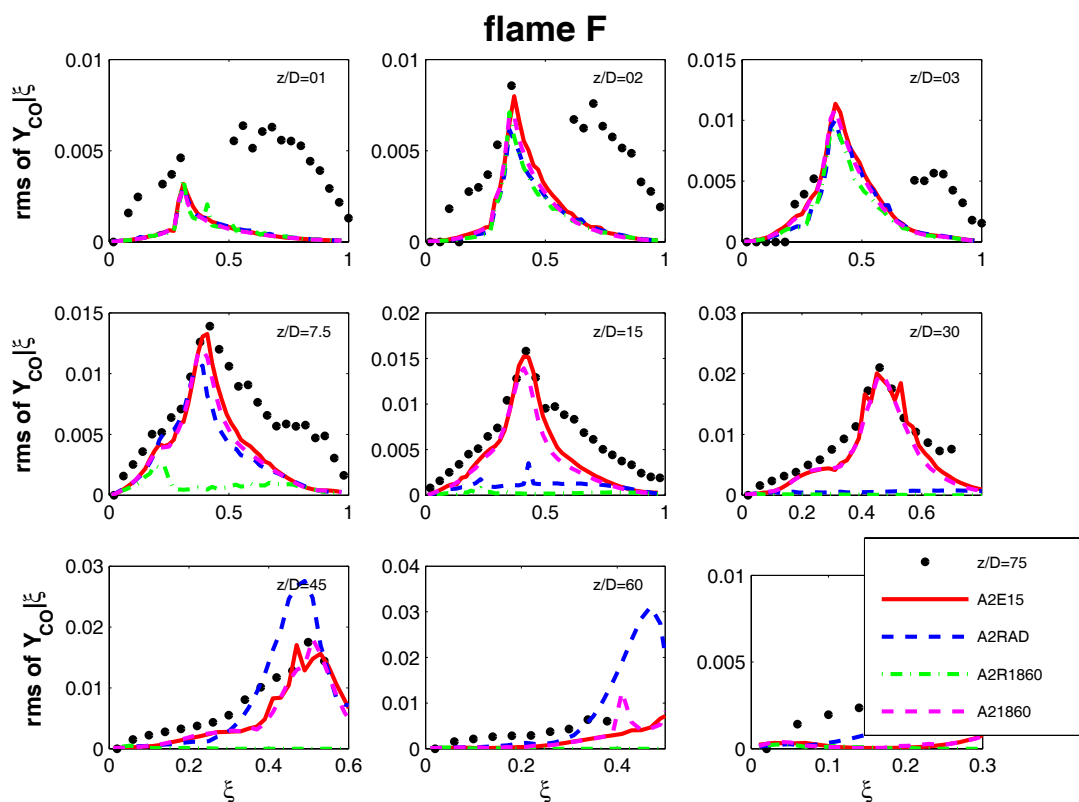
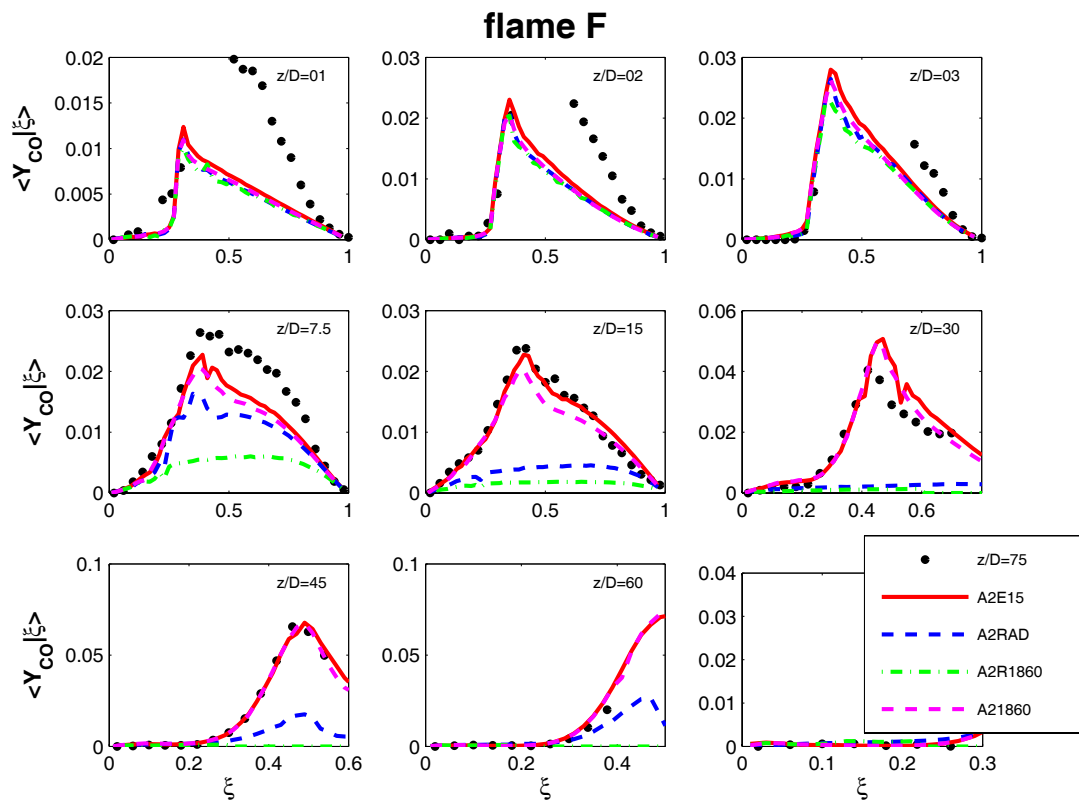


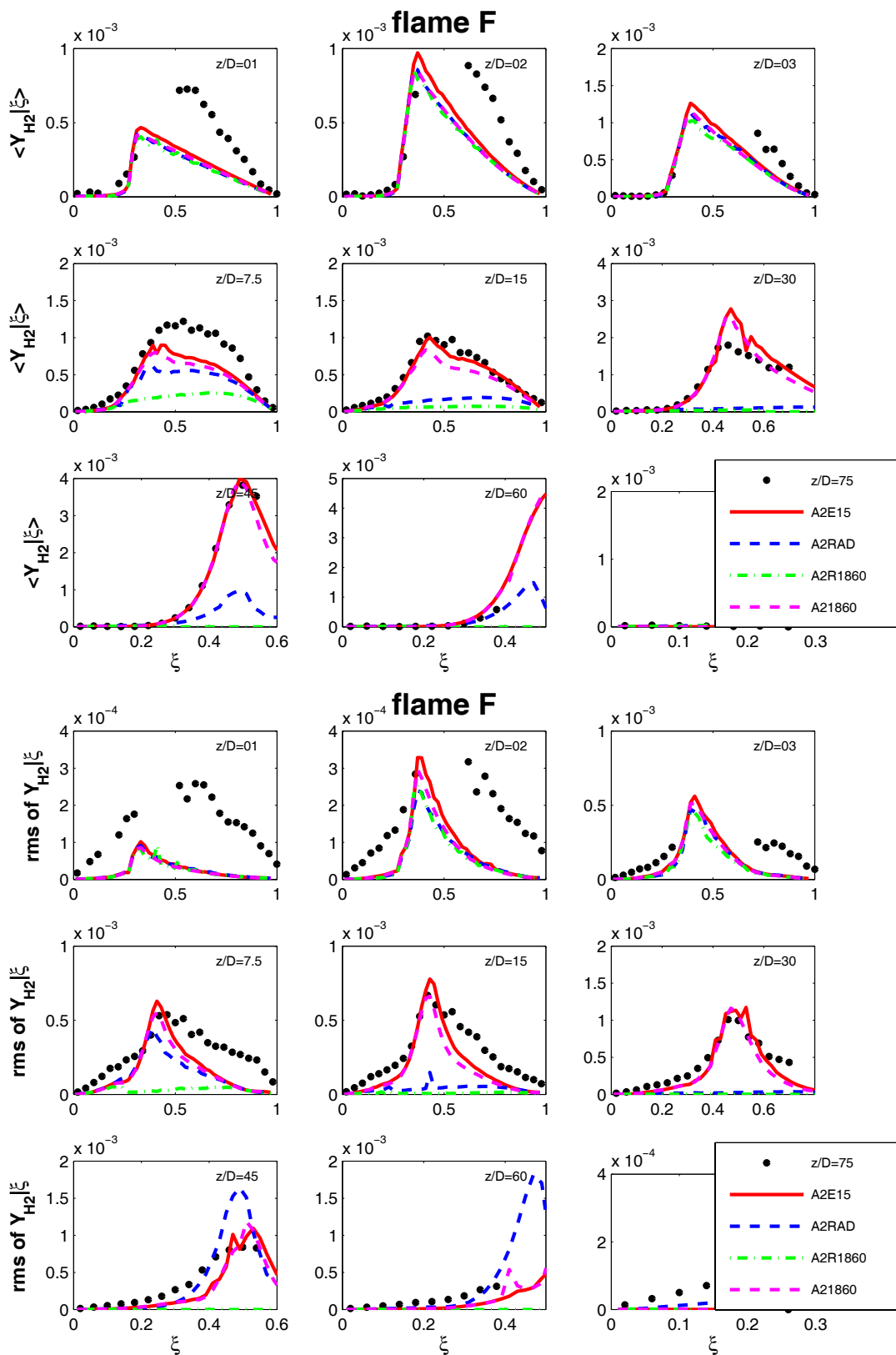


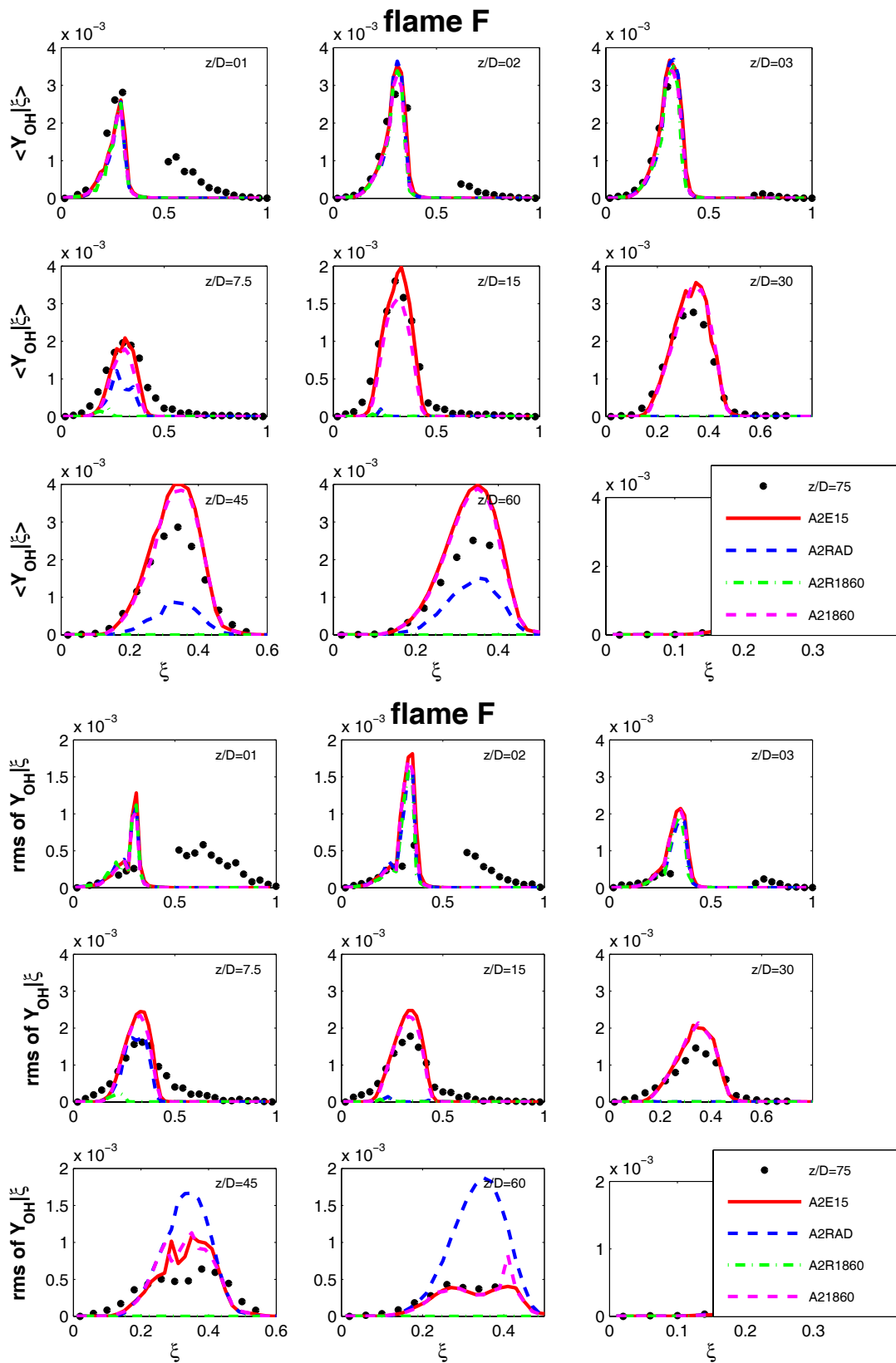


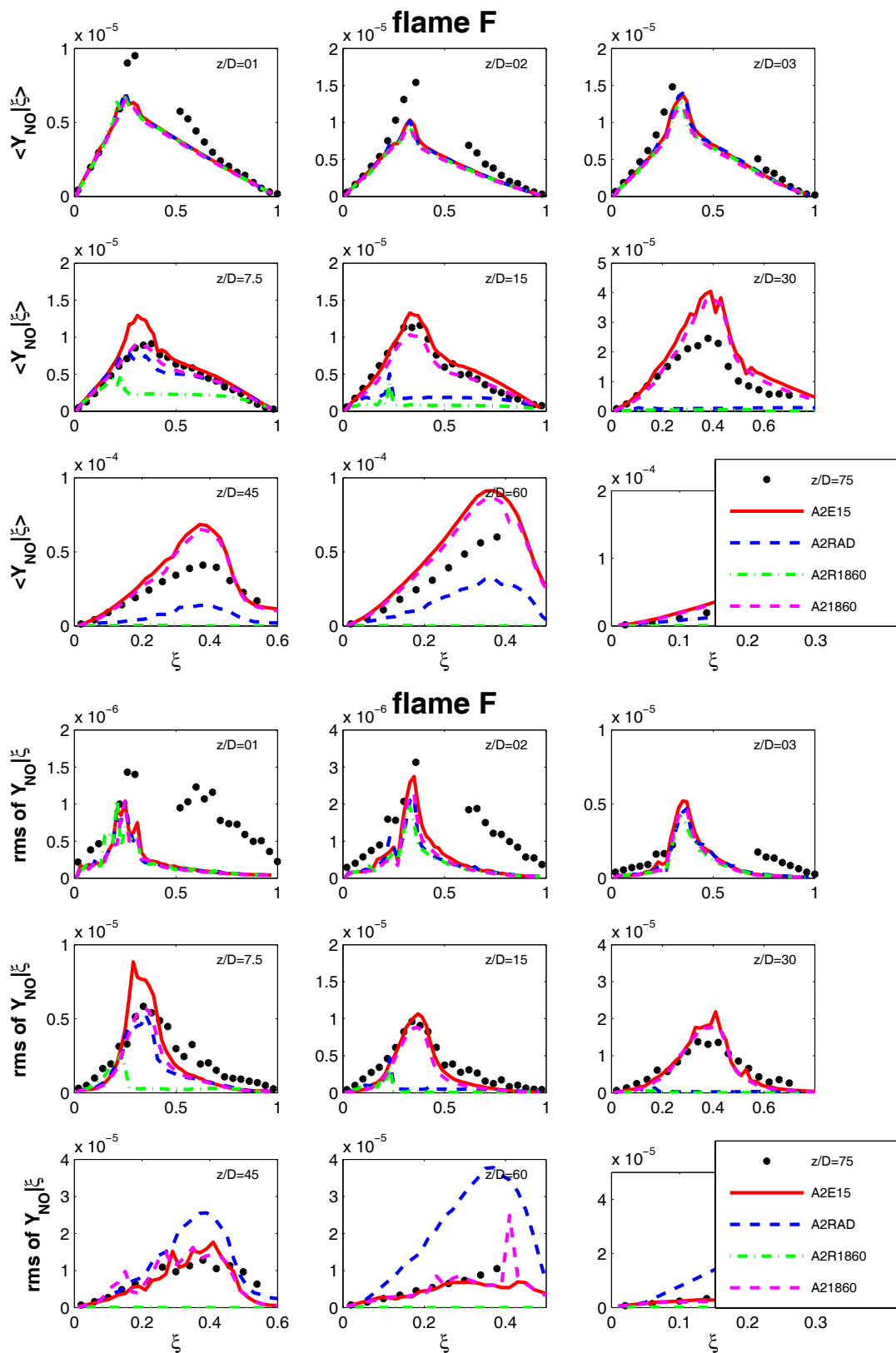




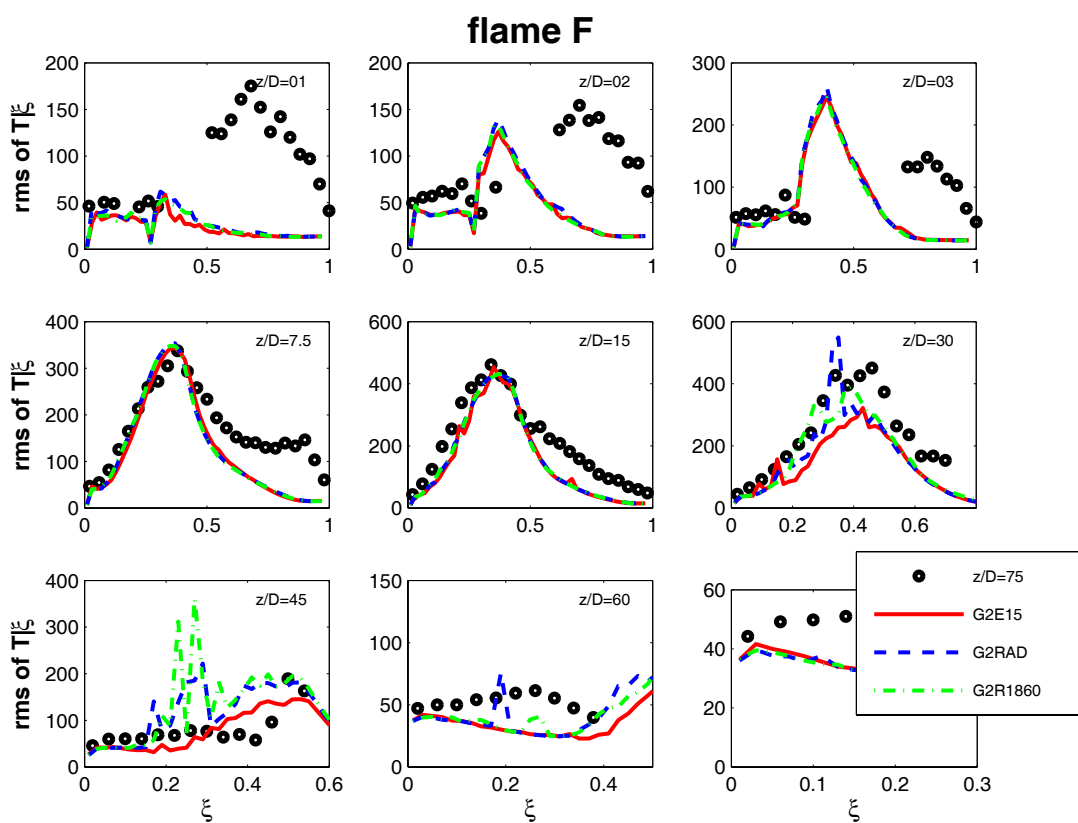
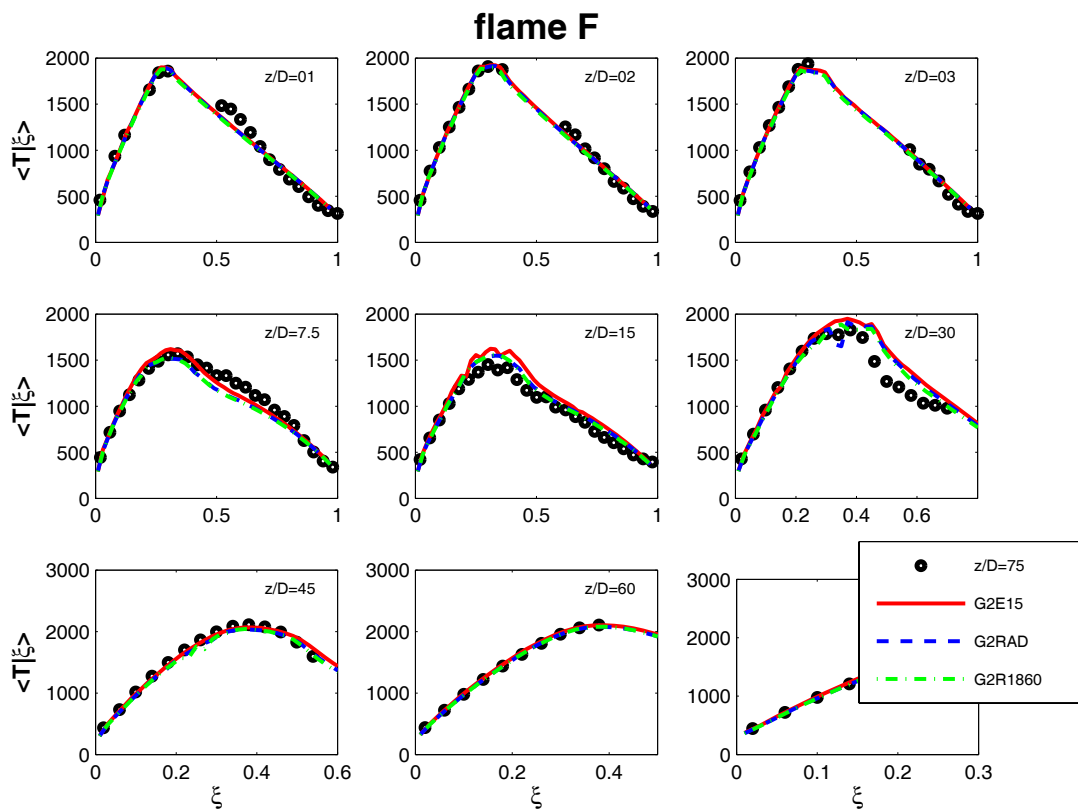


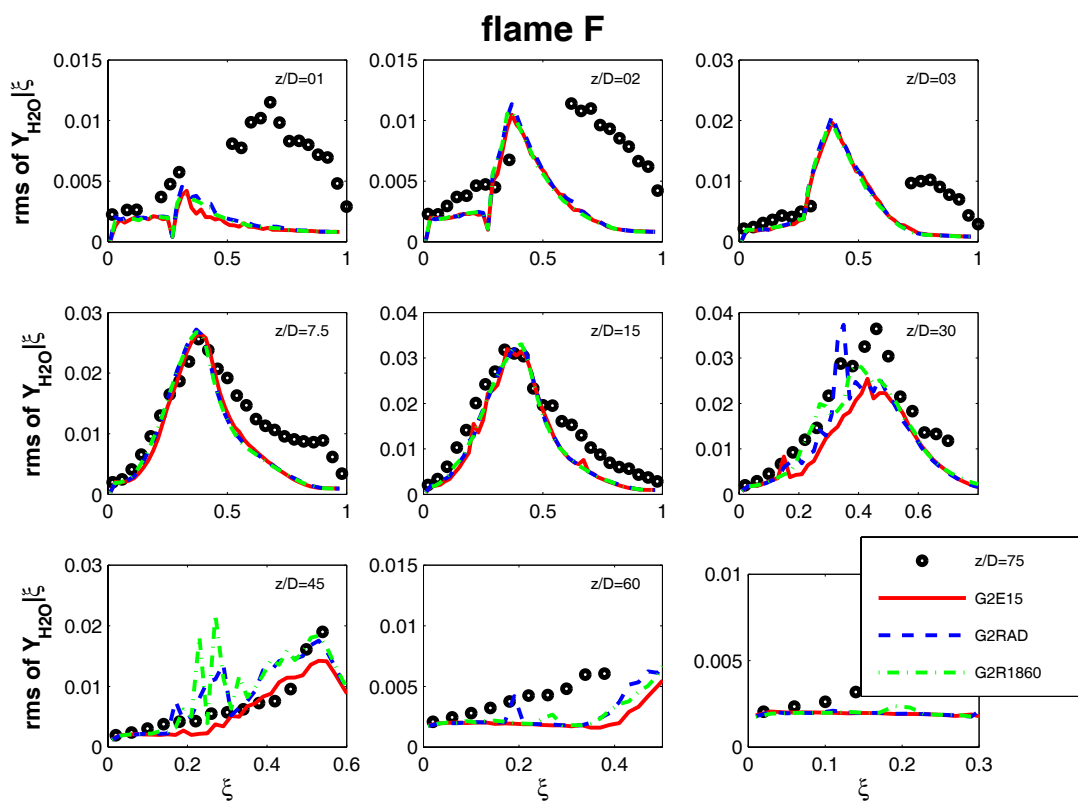
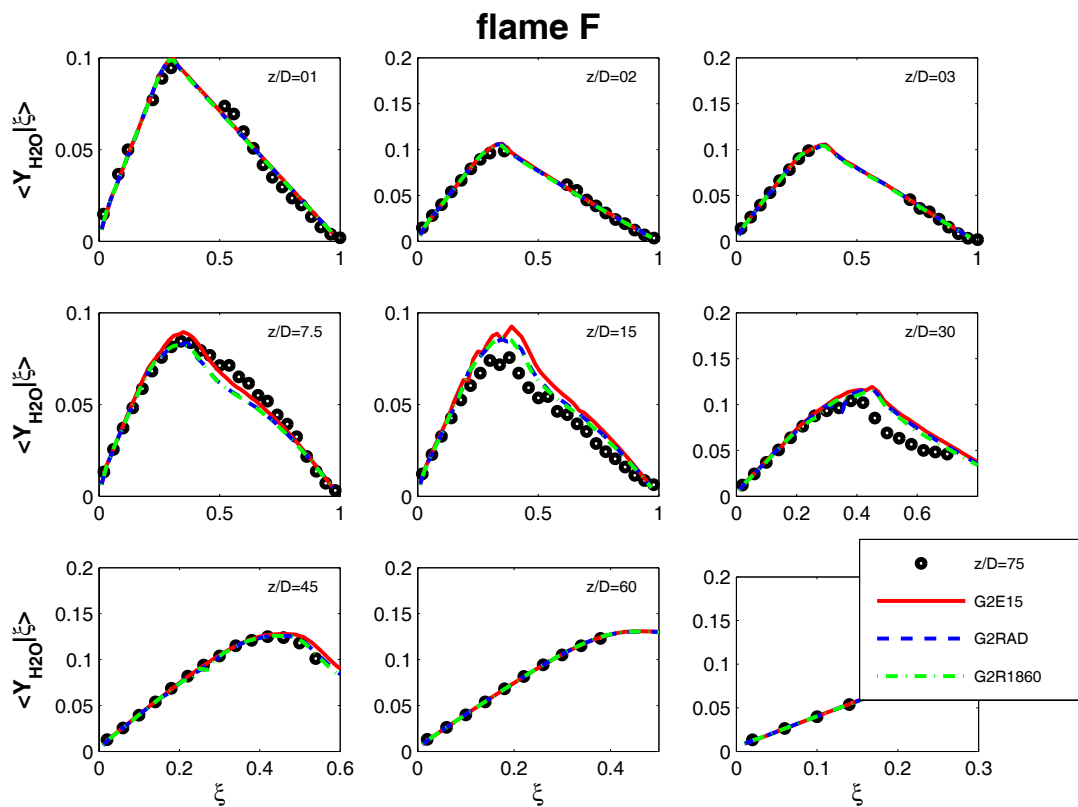


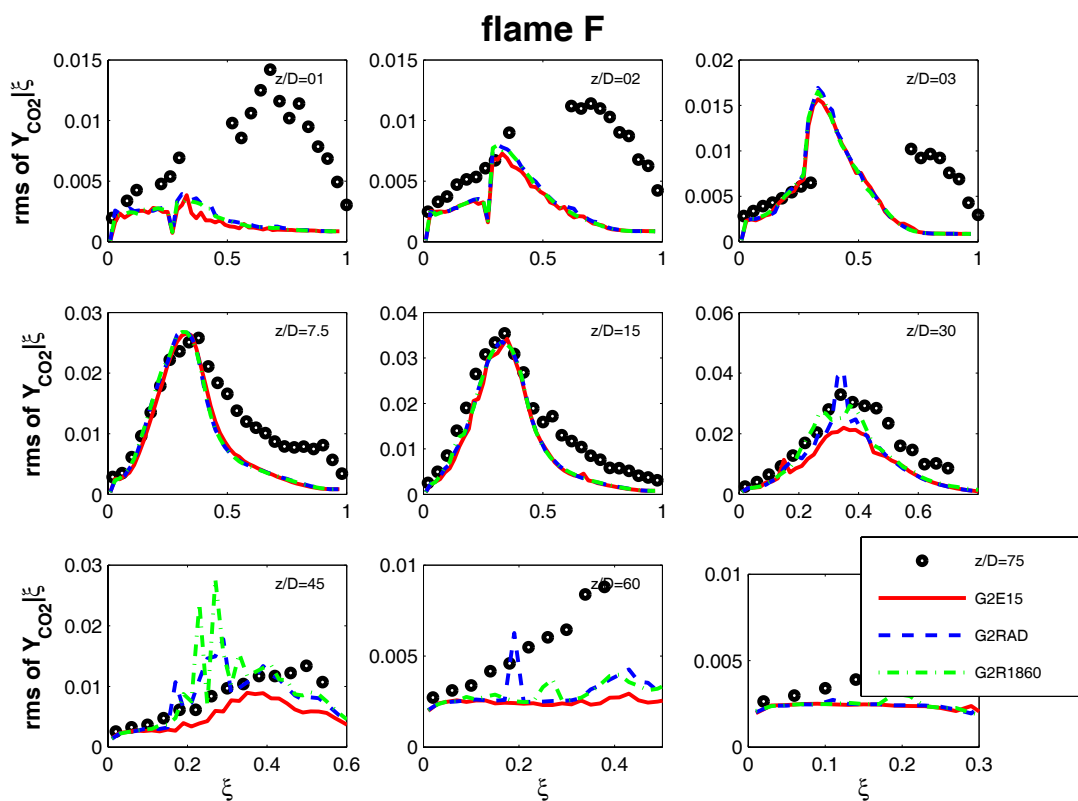
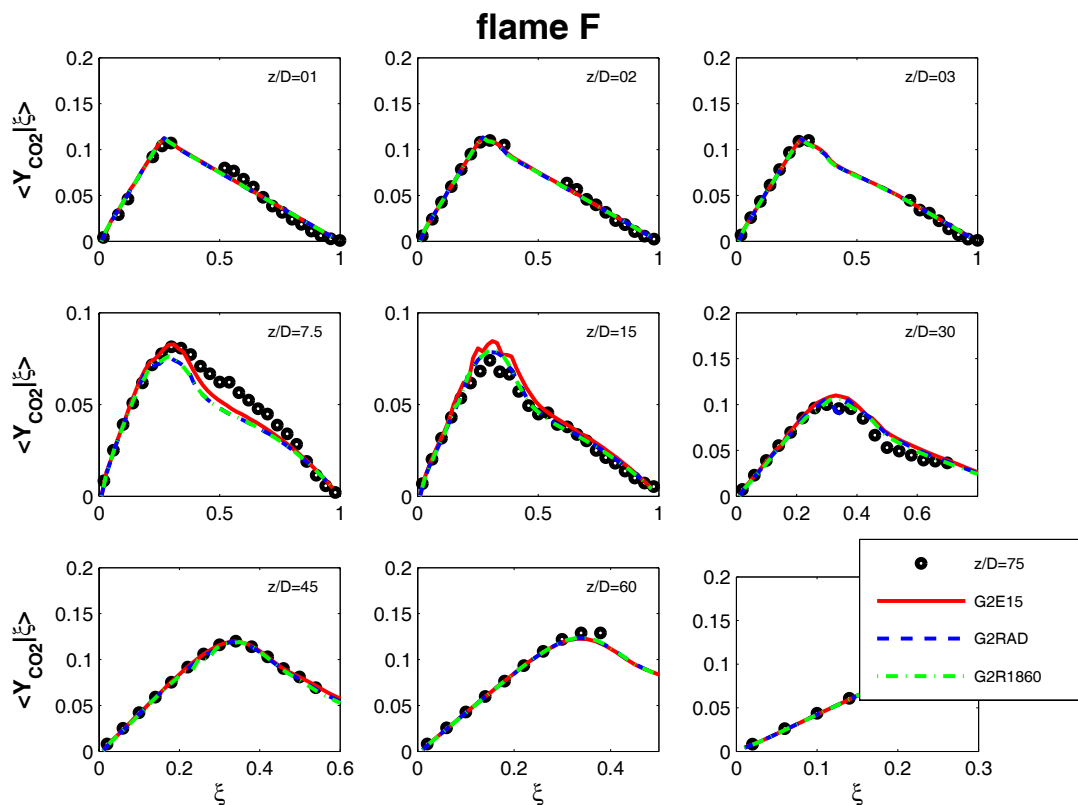


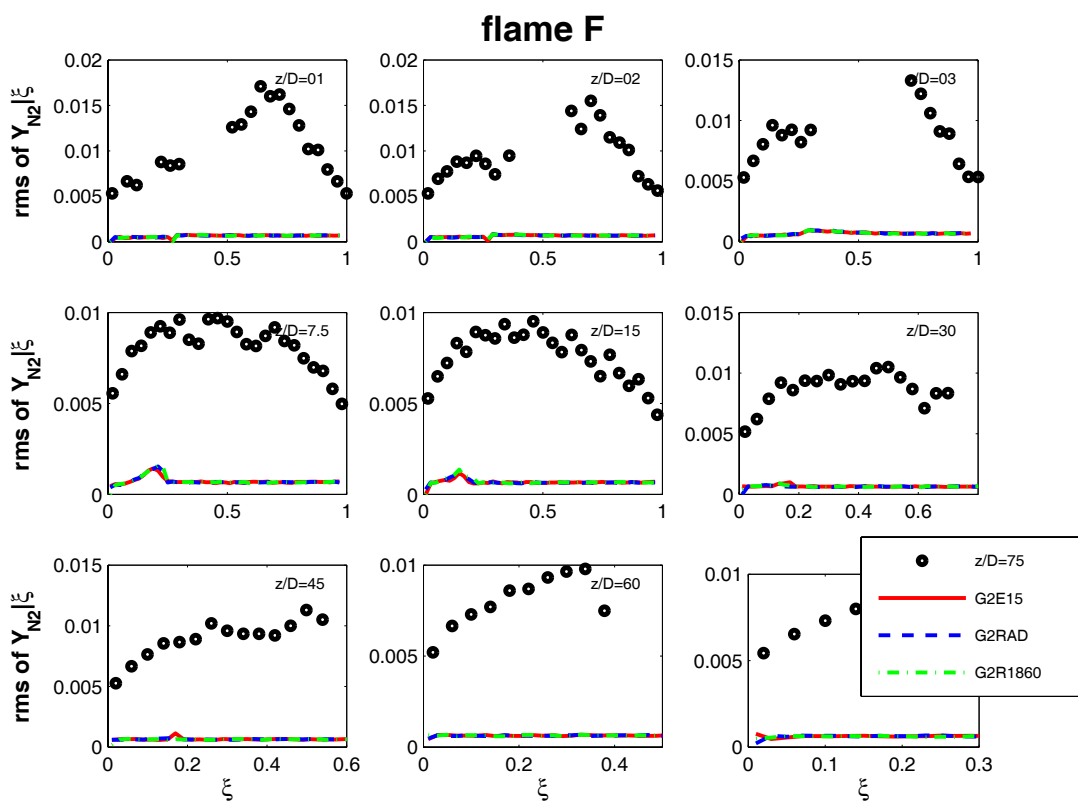
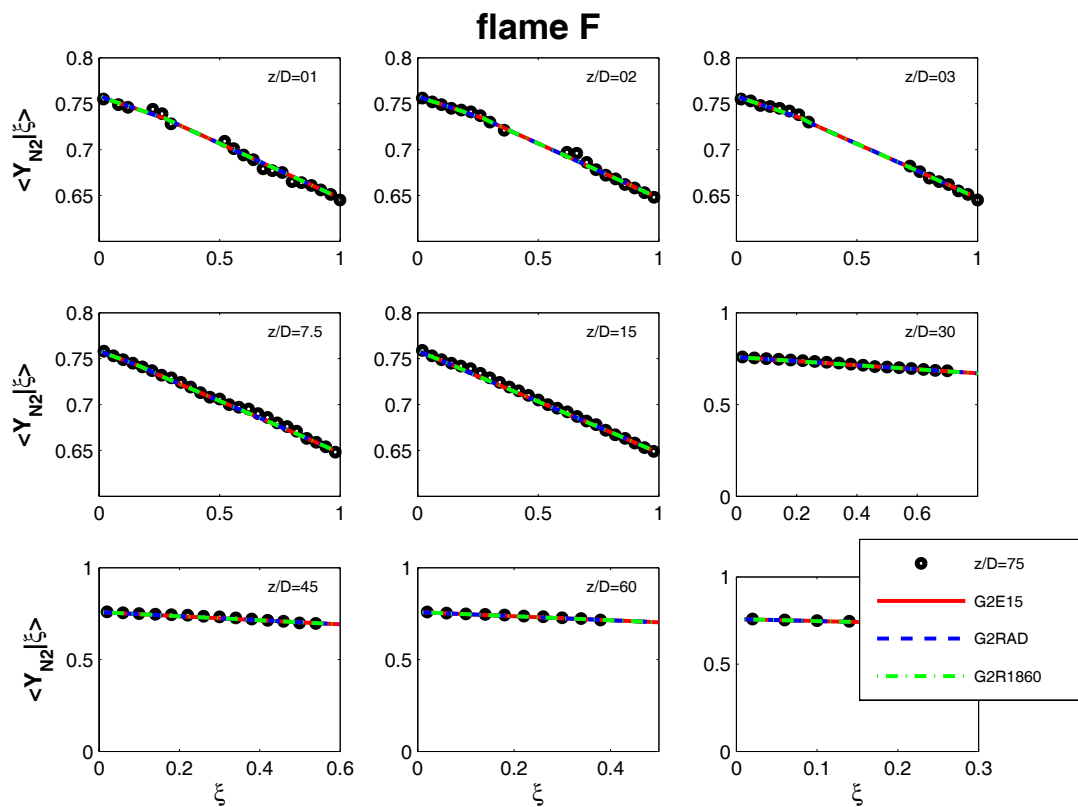


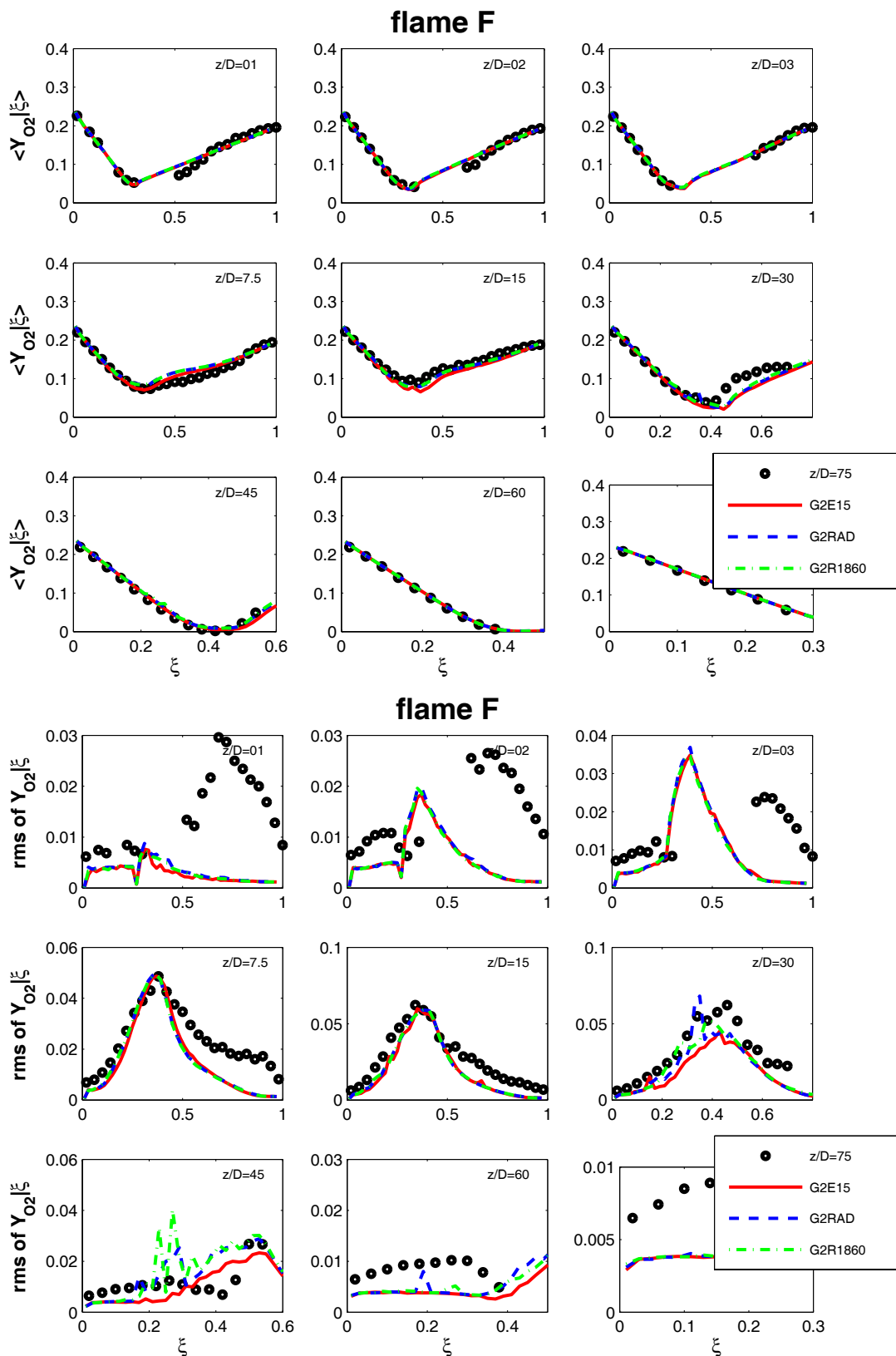
(3) G2E15, G2RAD, and G2R1860

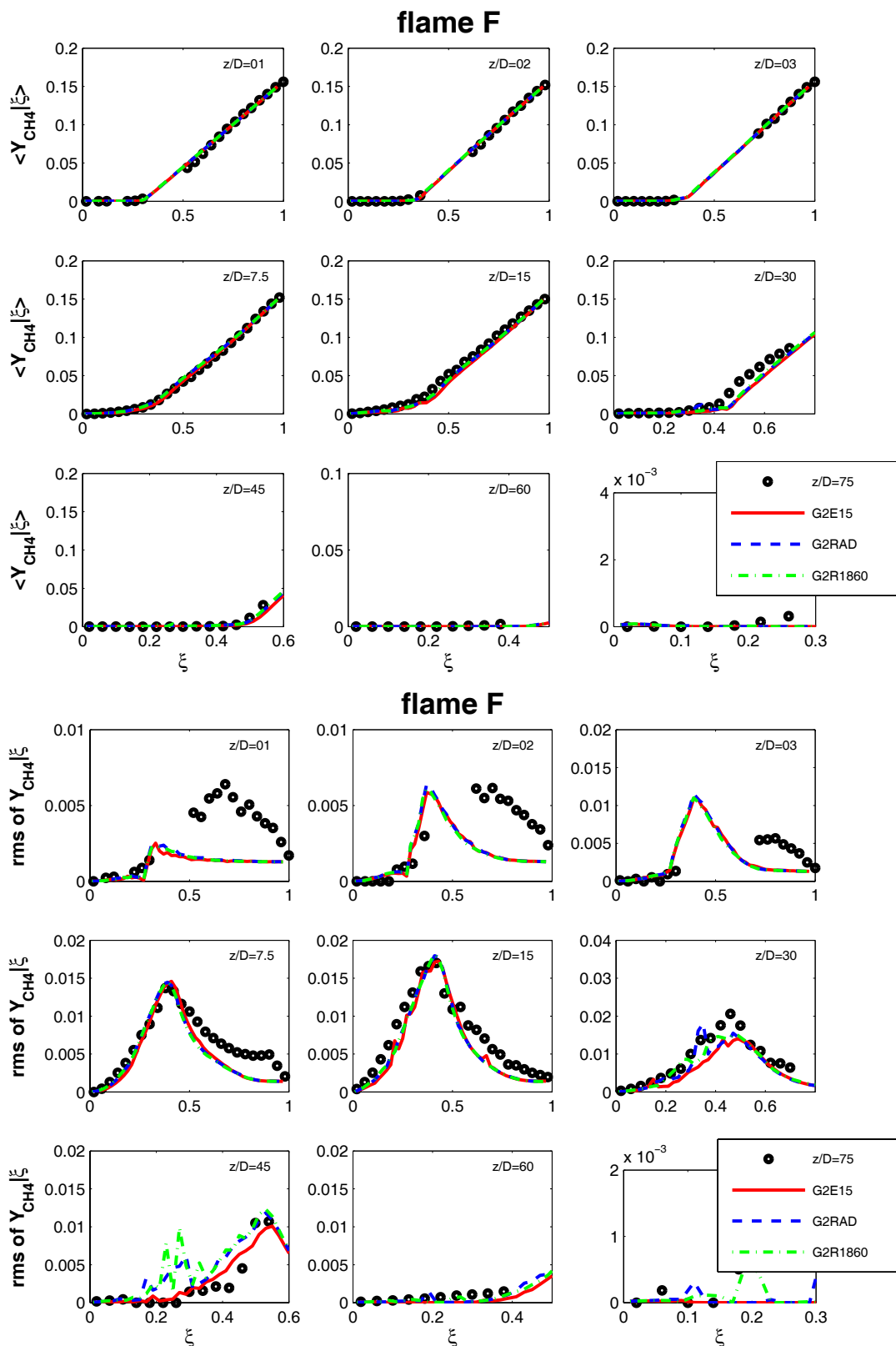


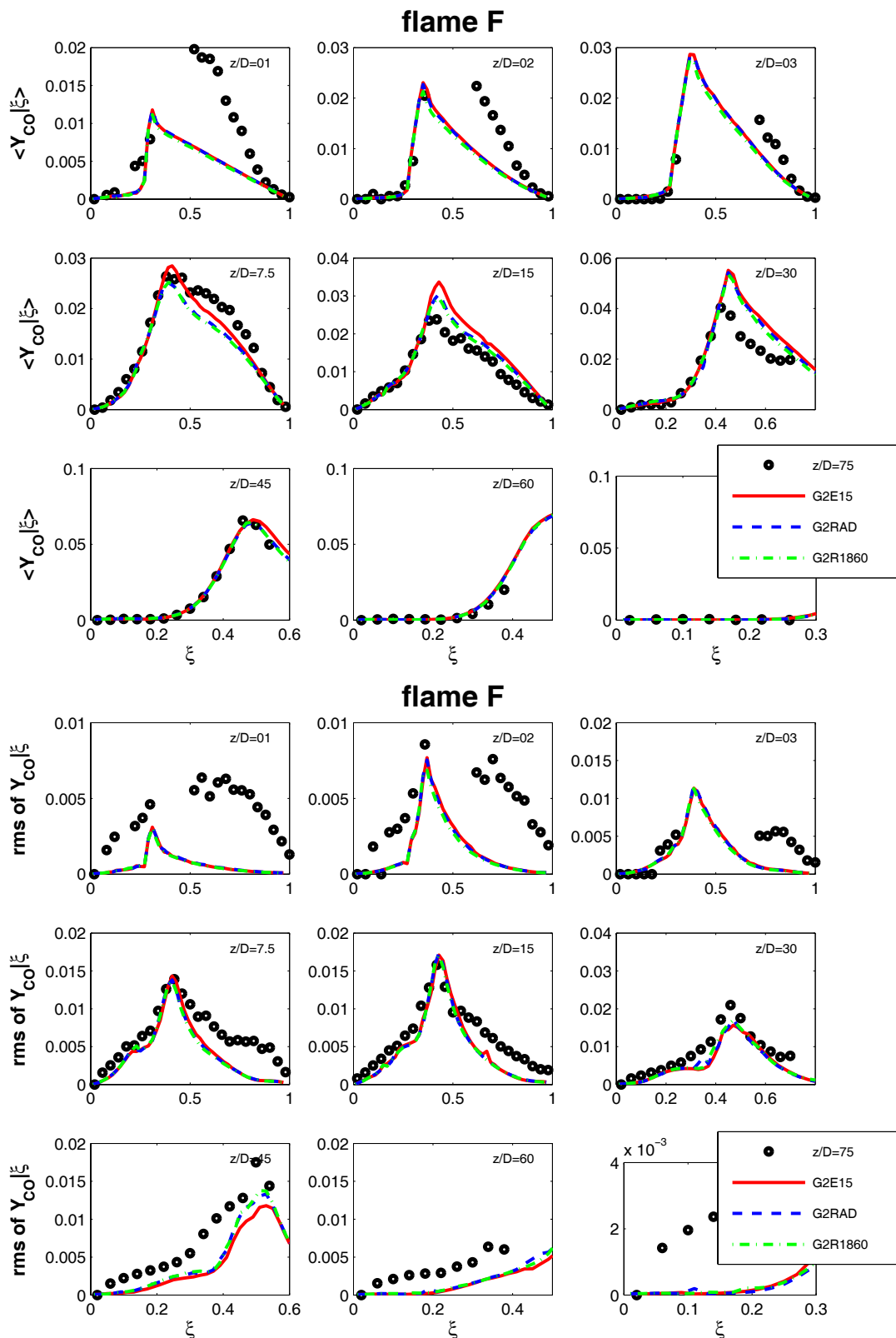


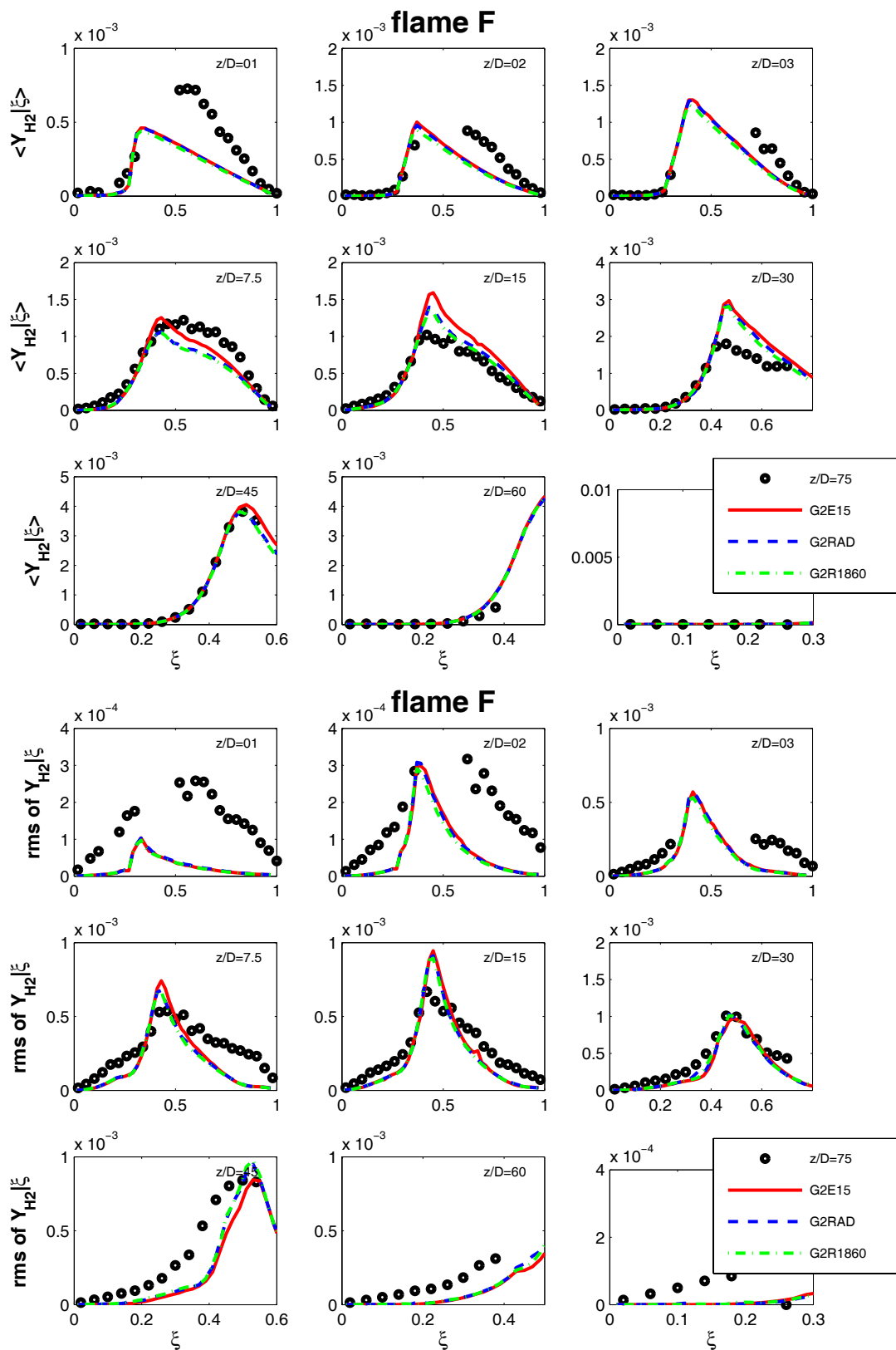


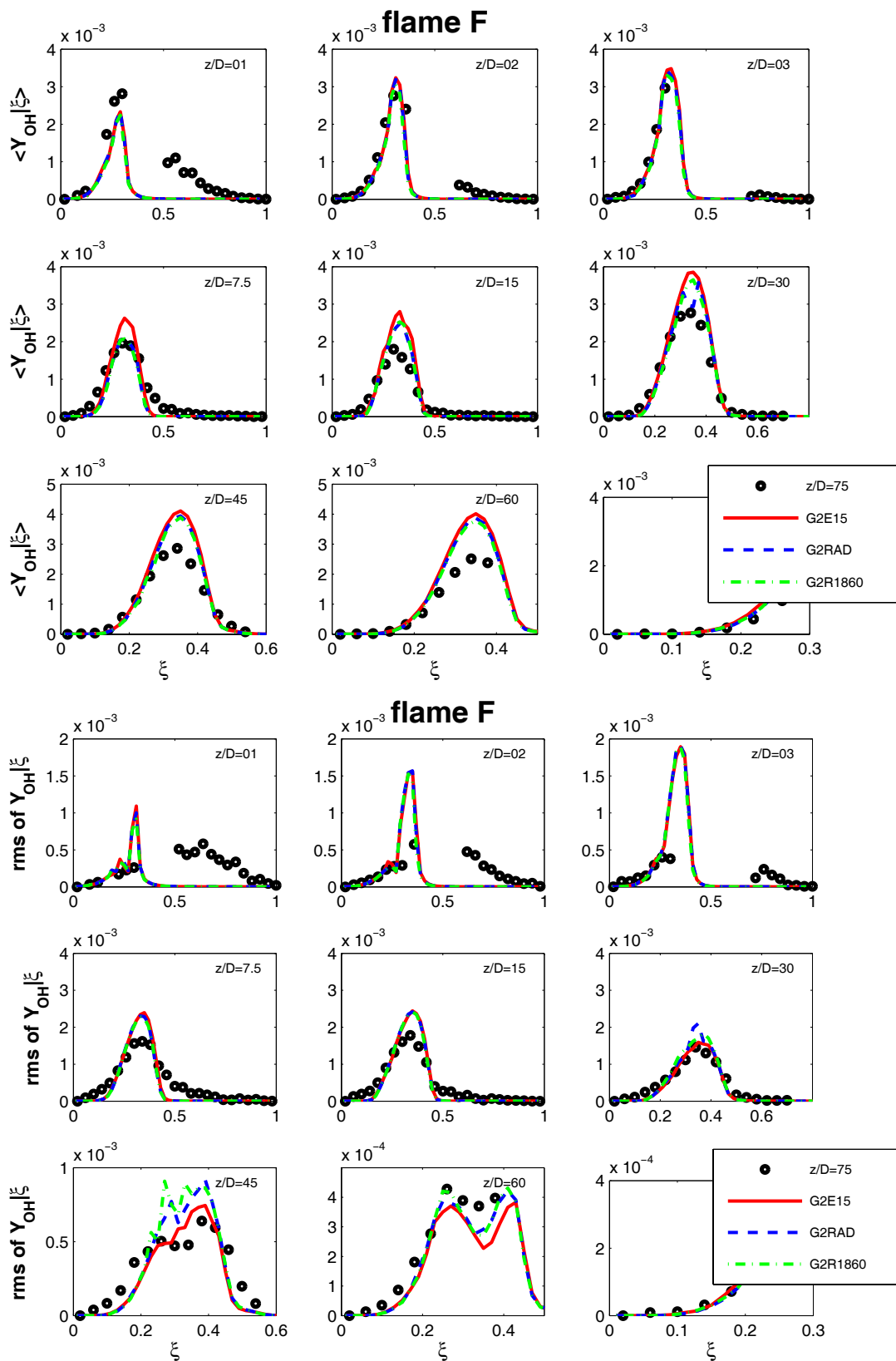


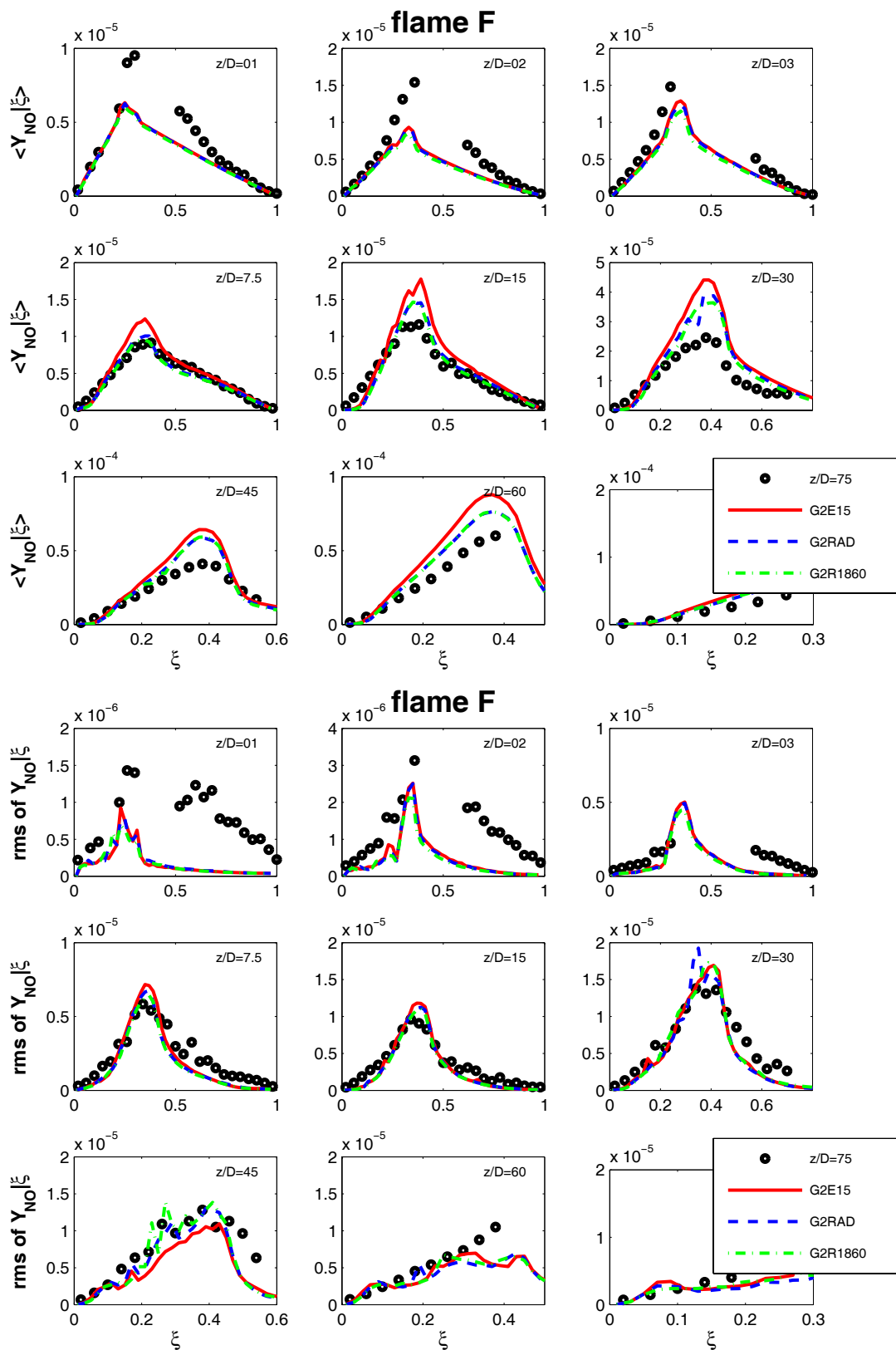




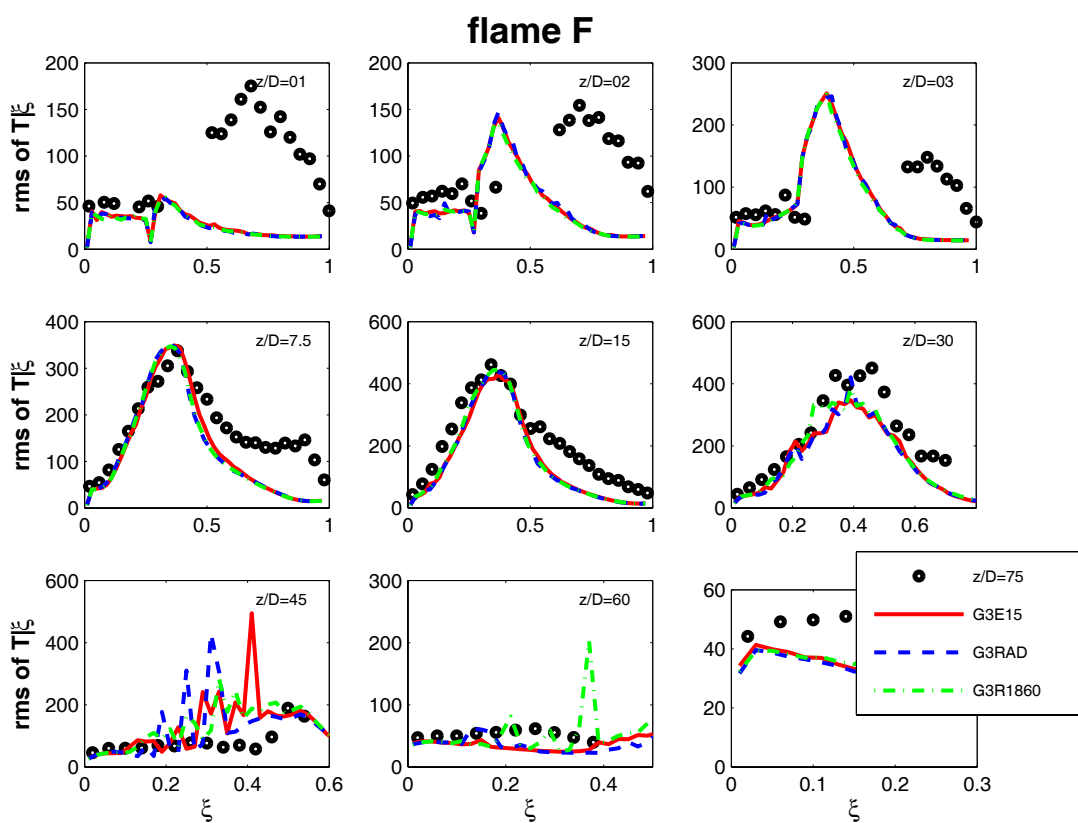
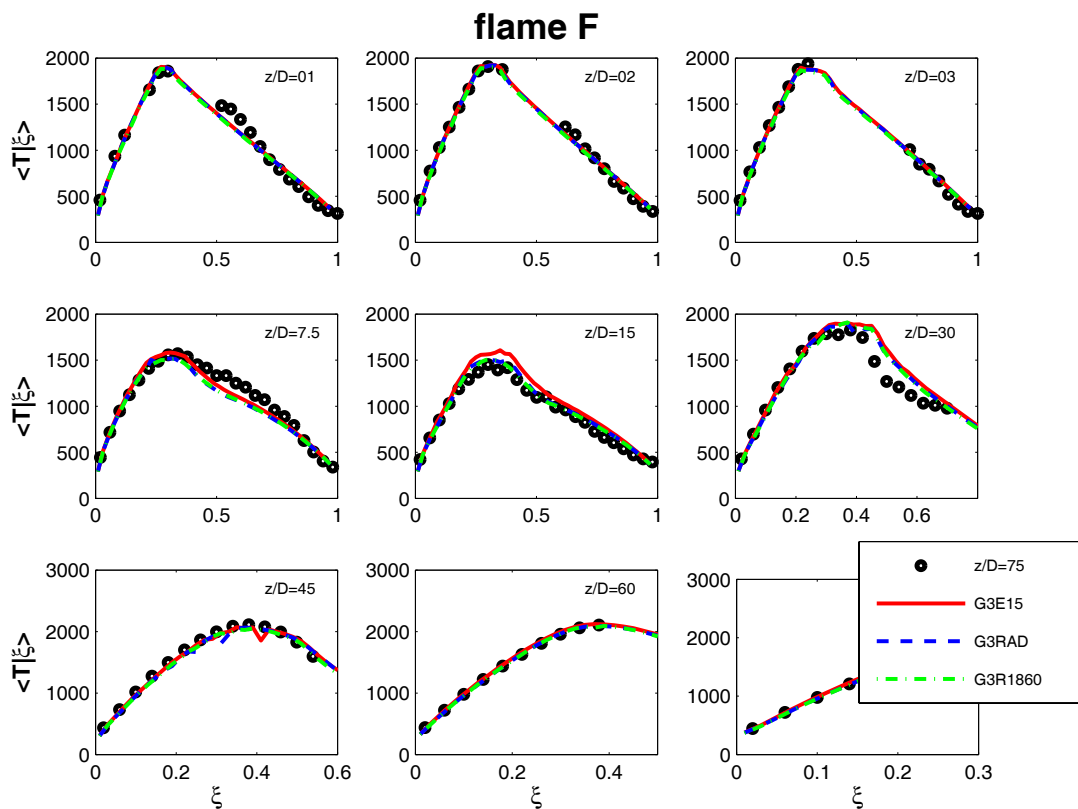


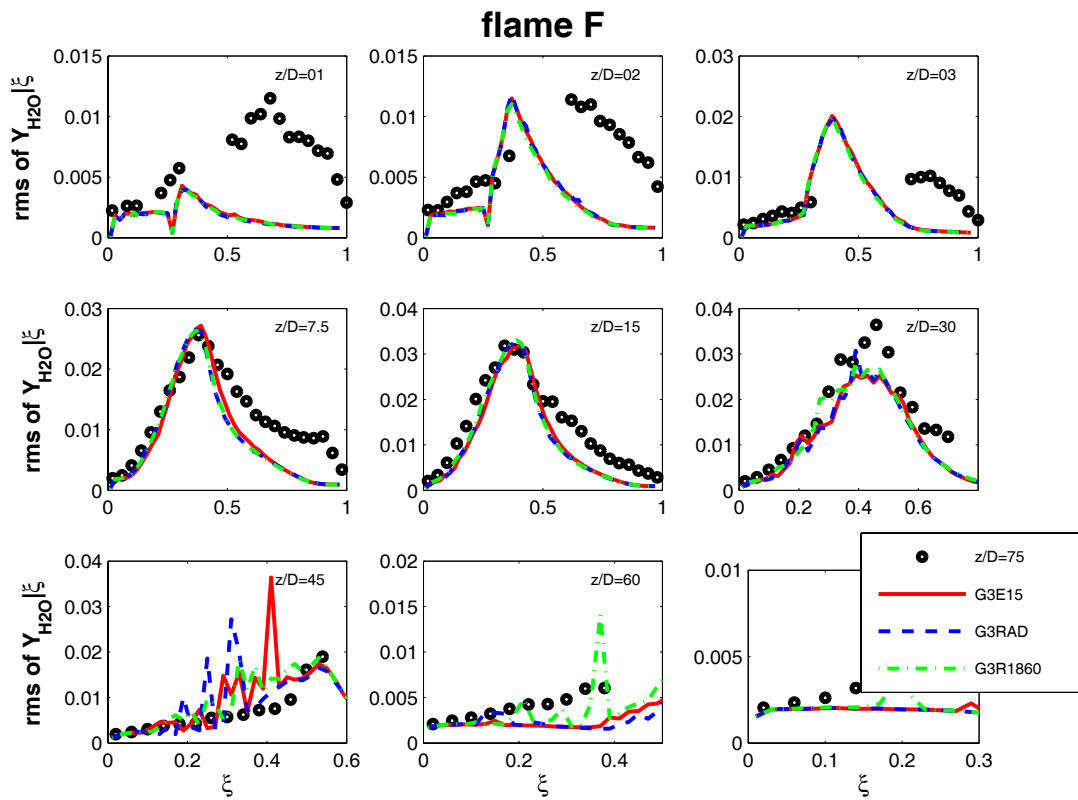
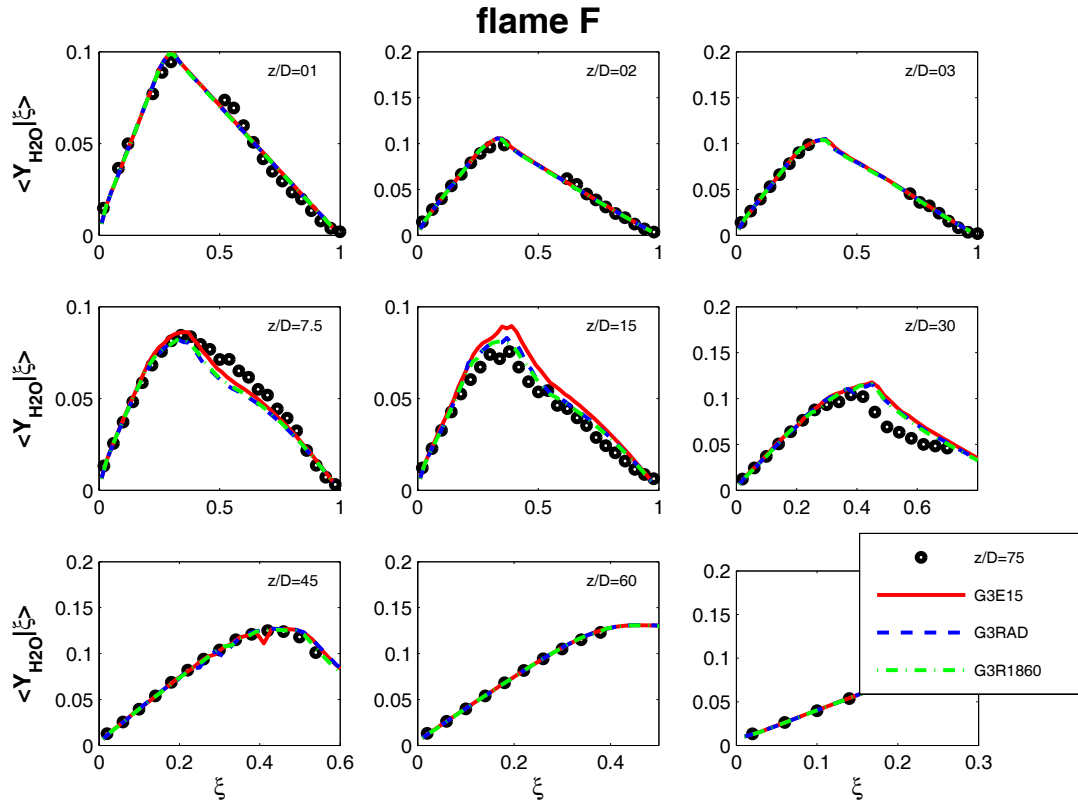


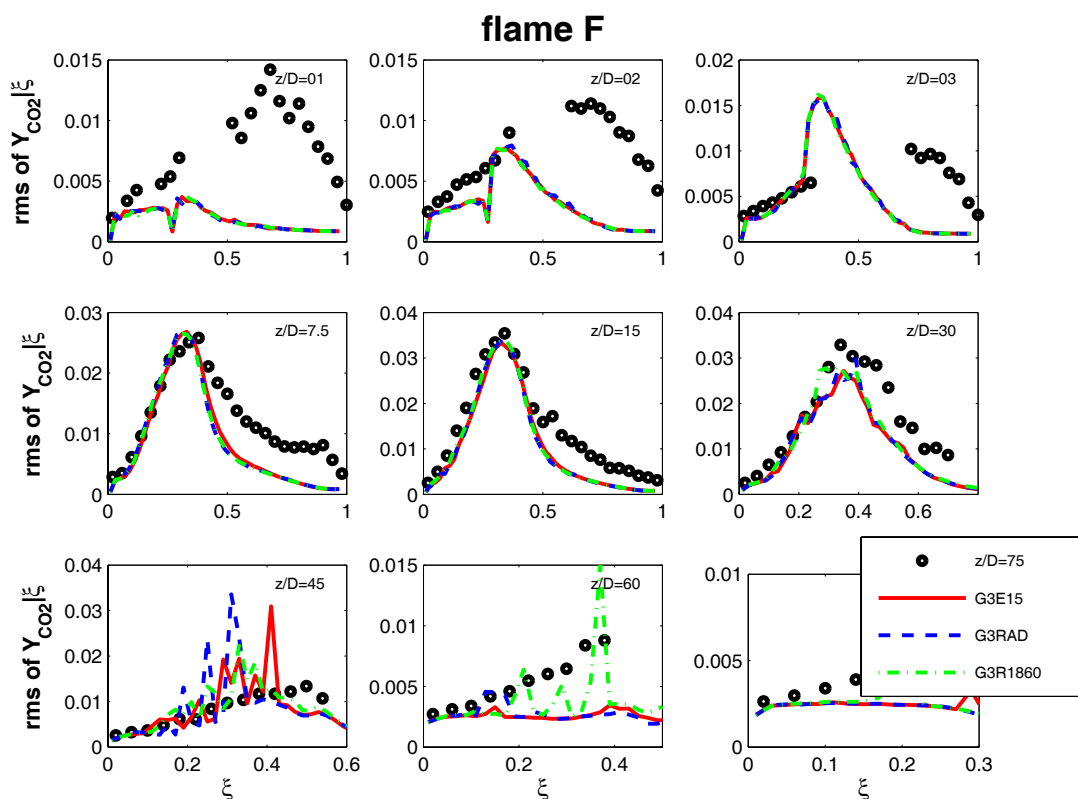
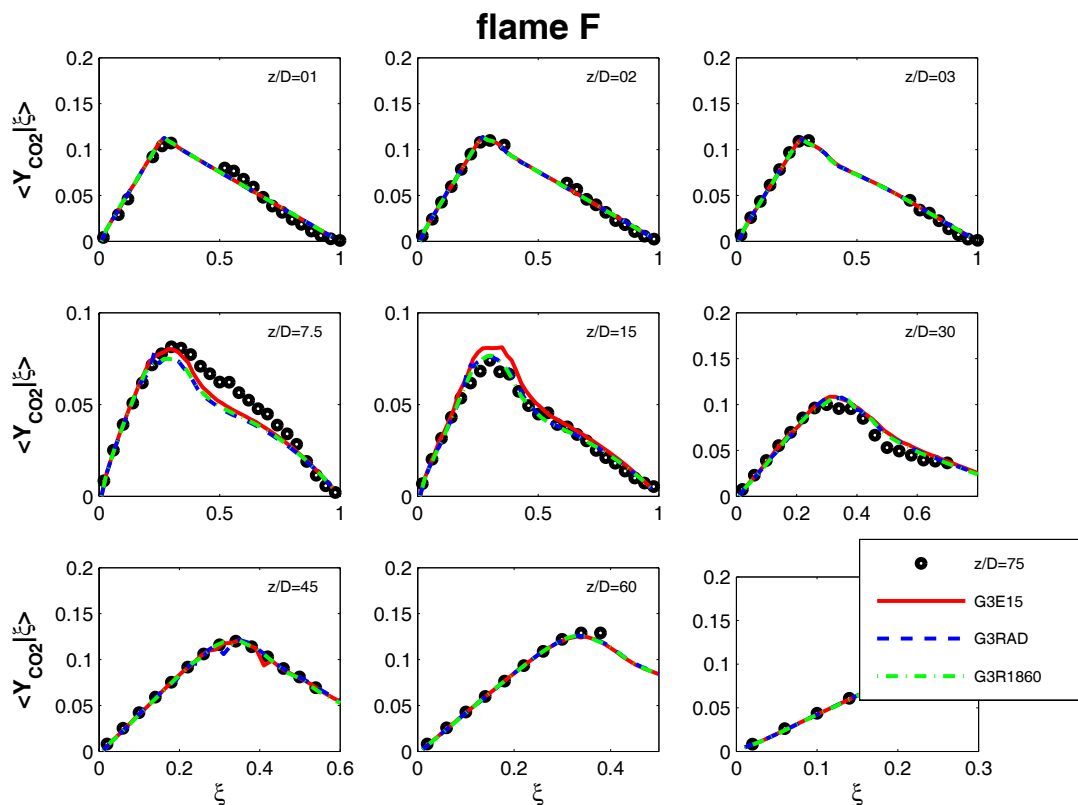


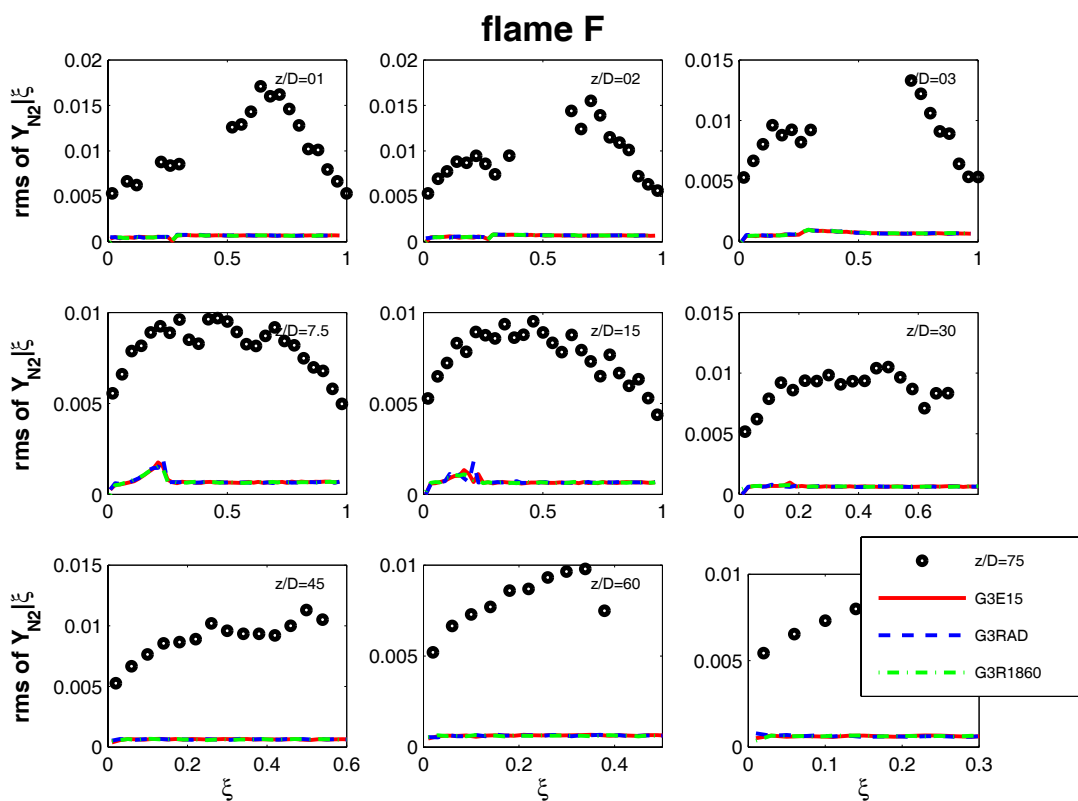
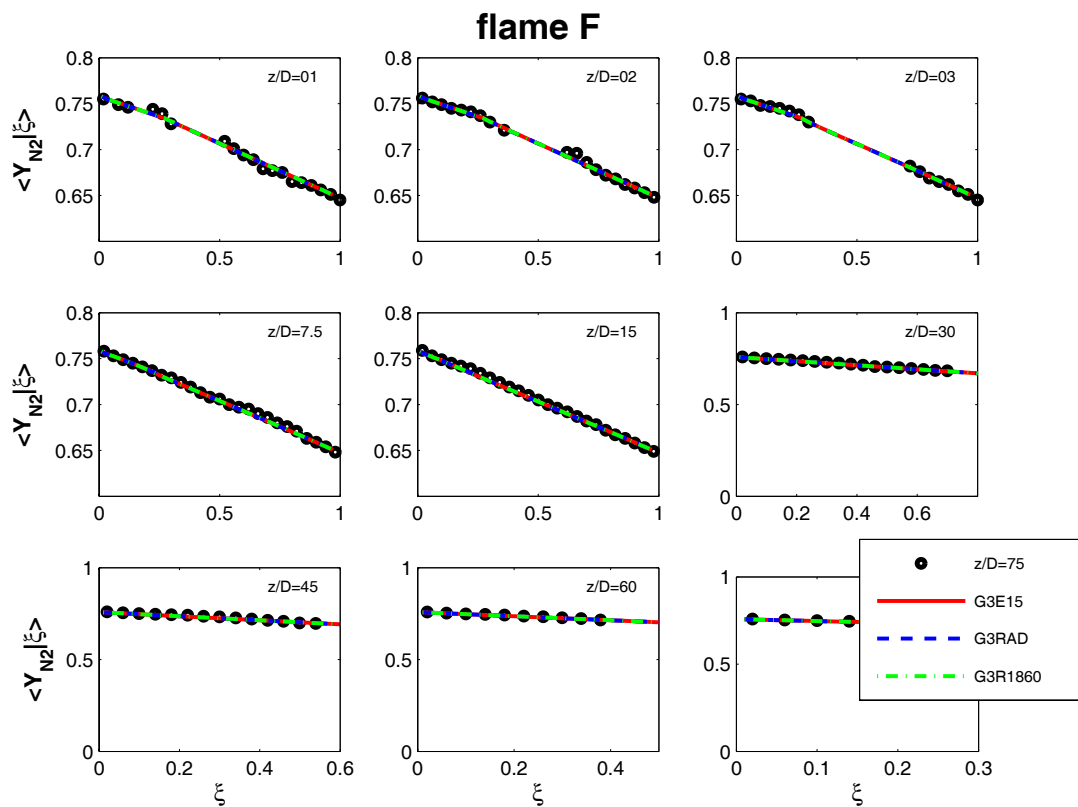


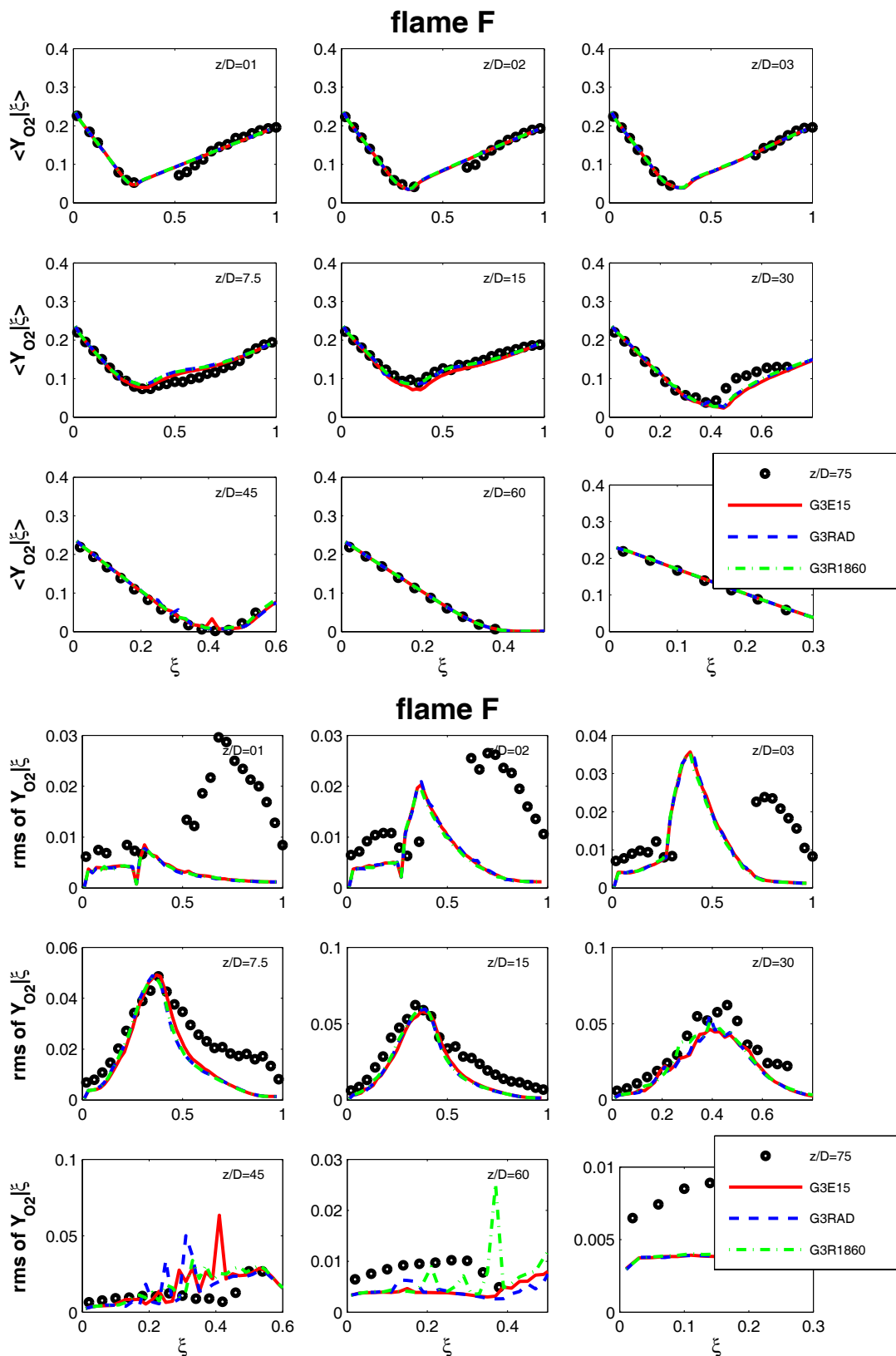
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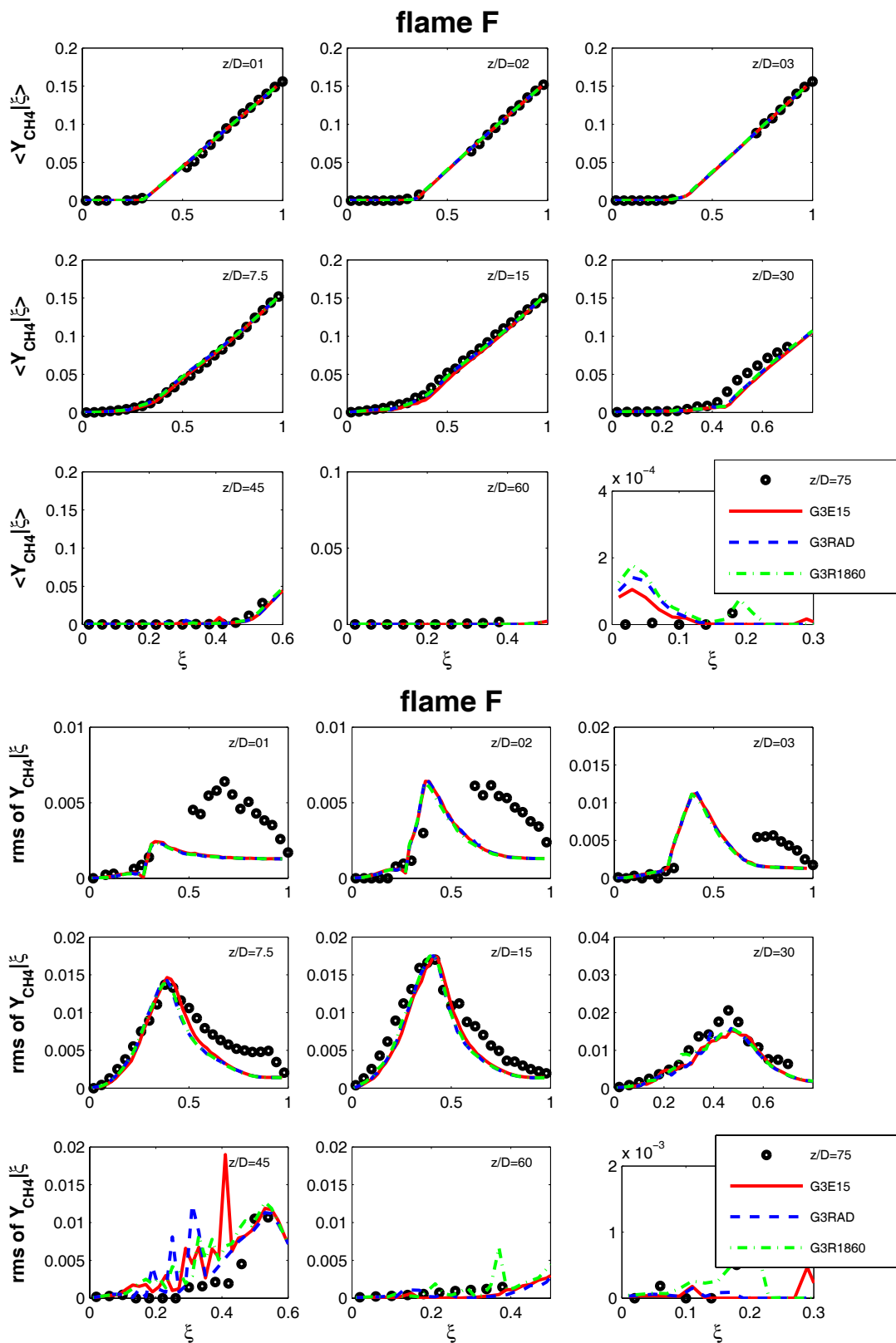


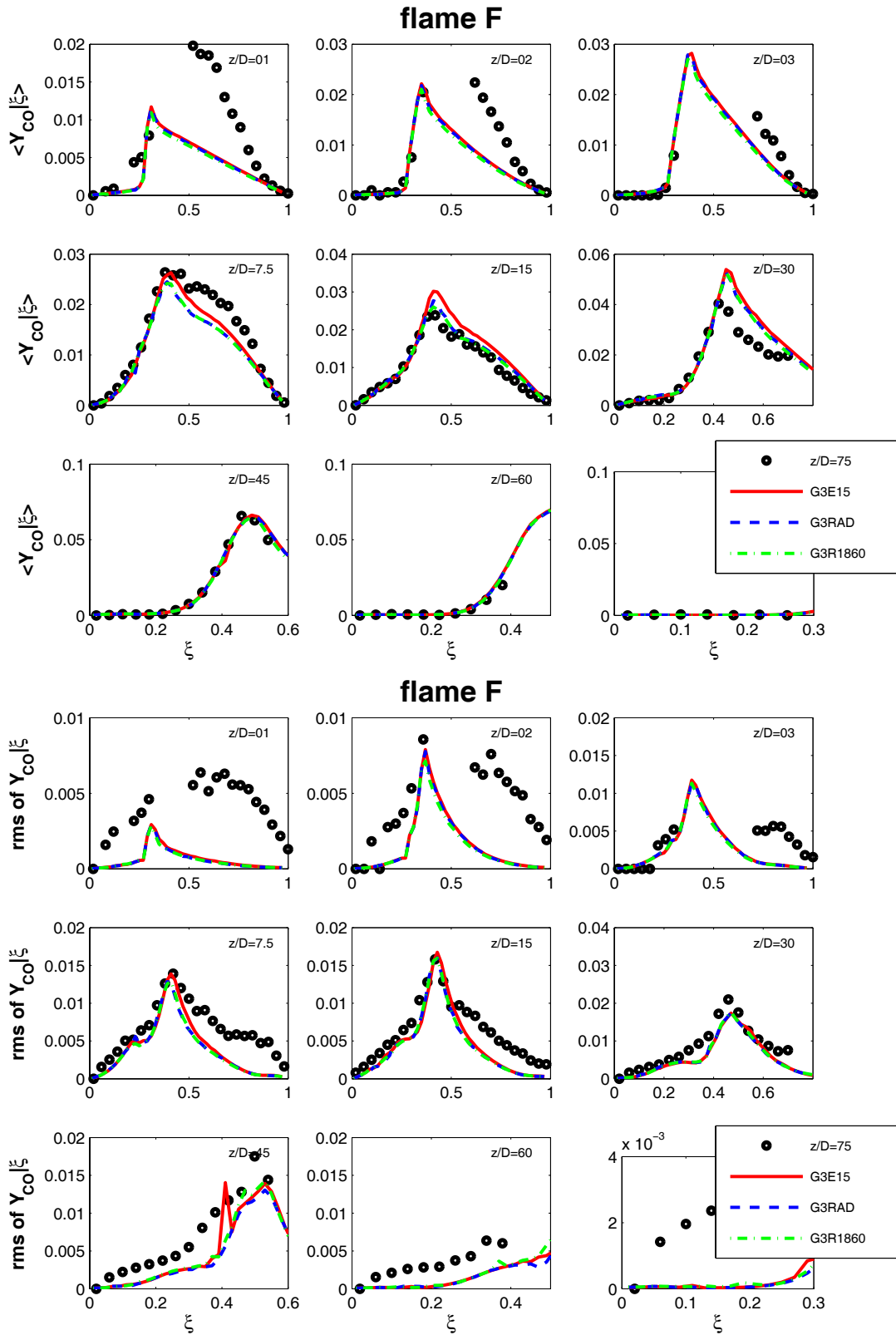


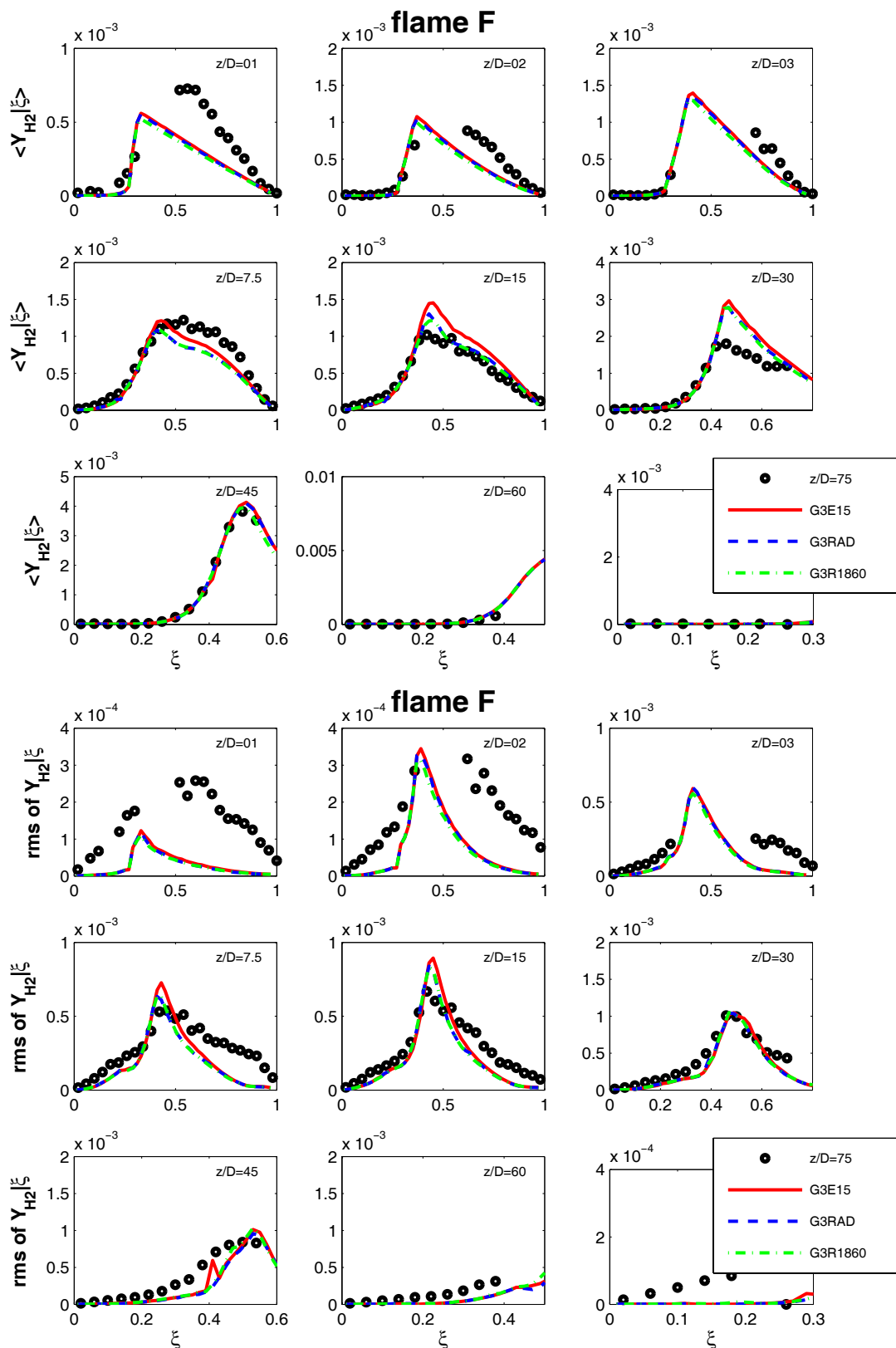


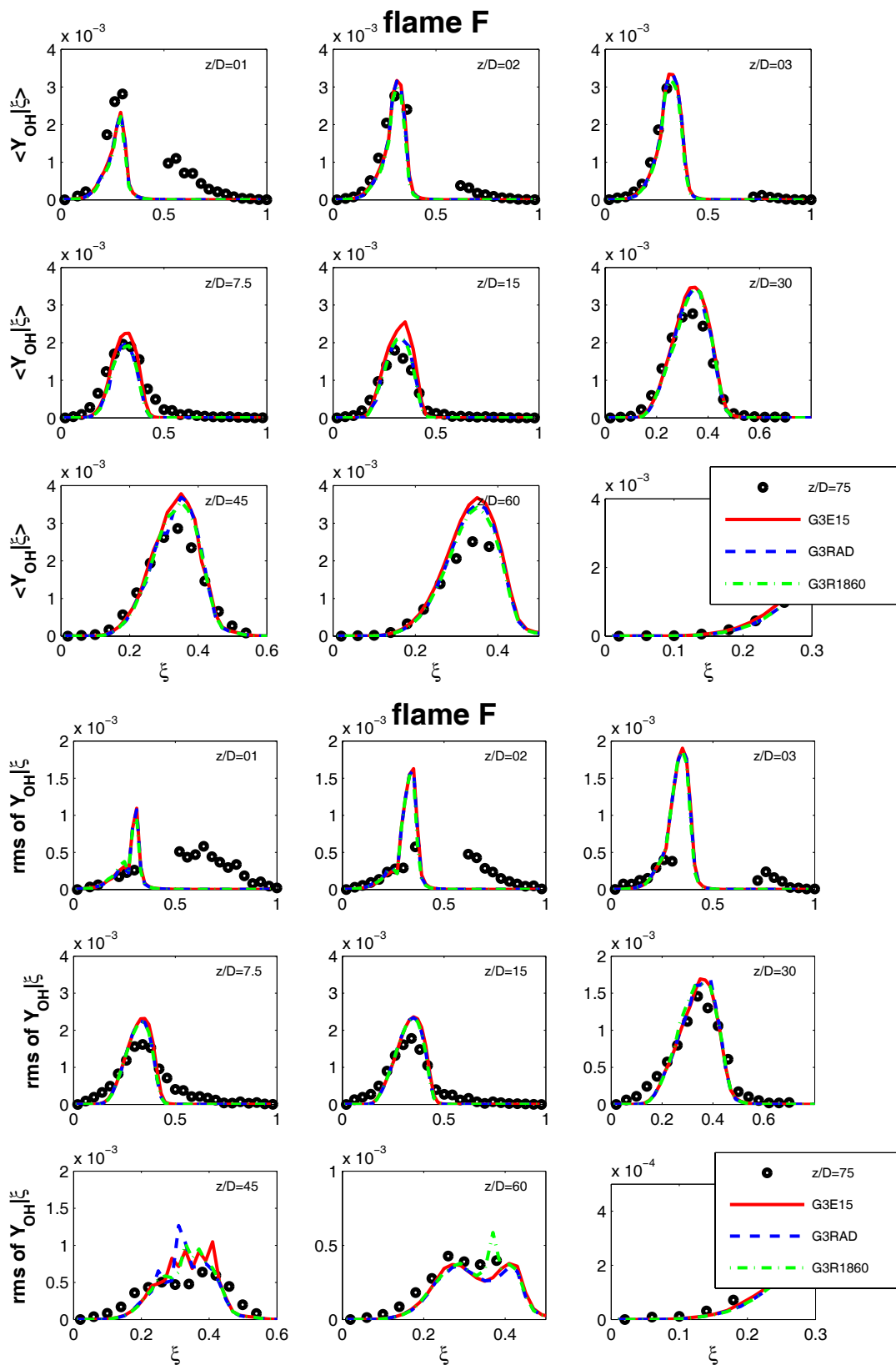


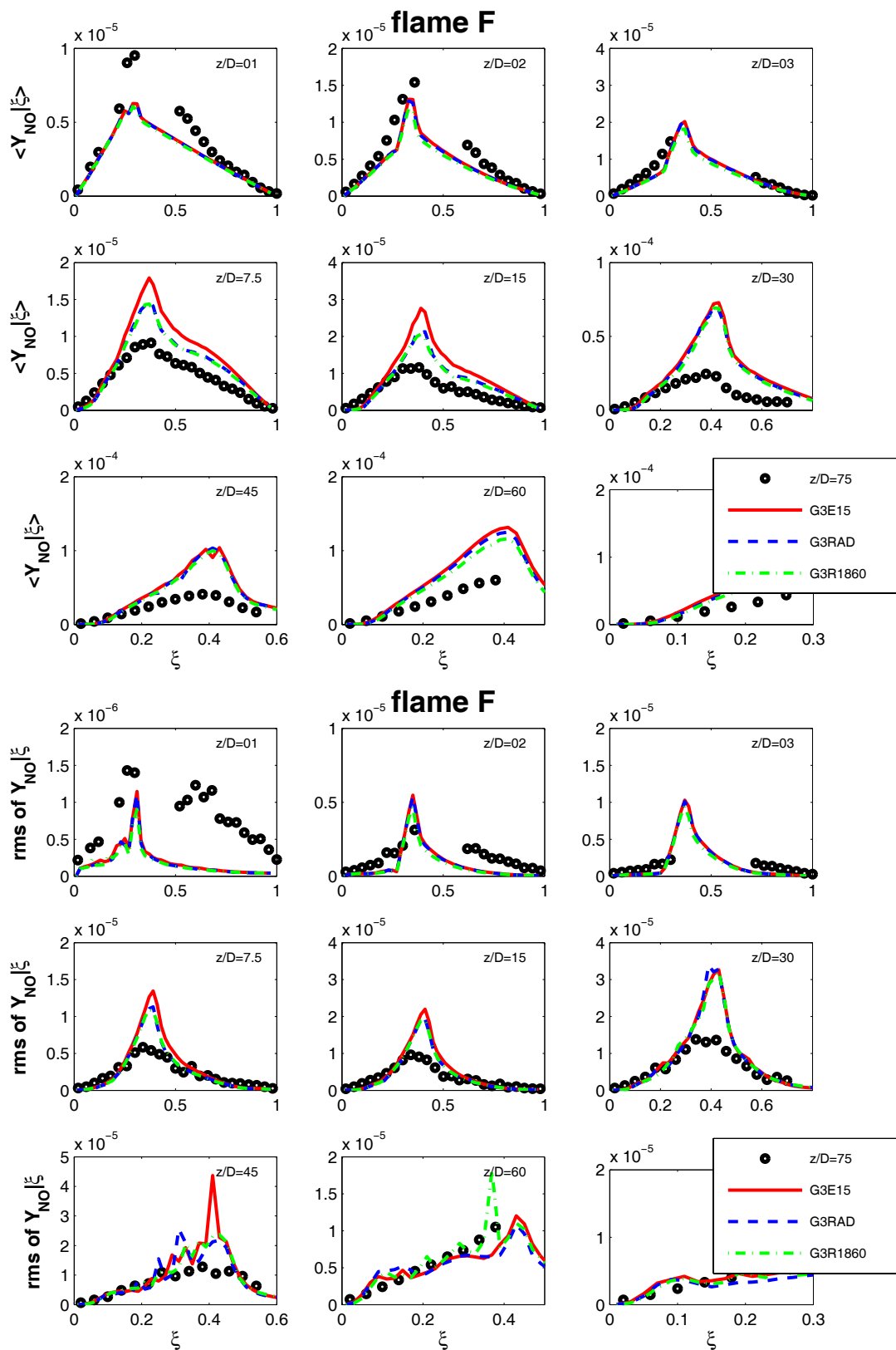




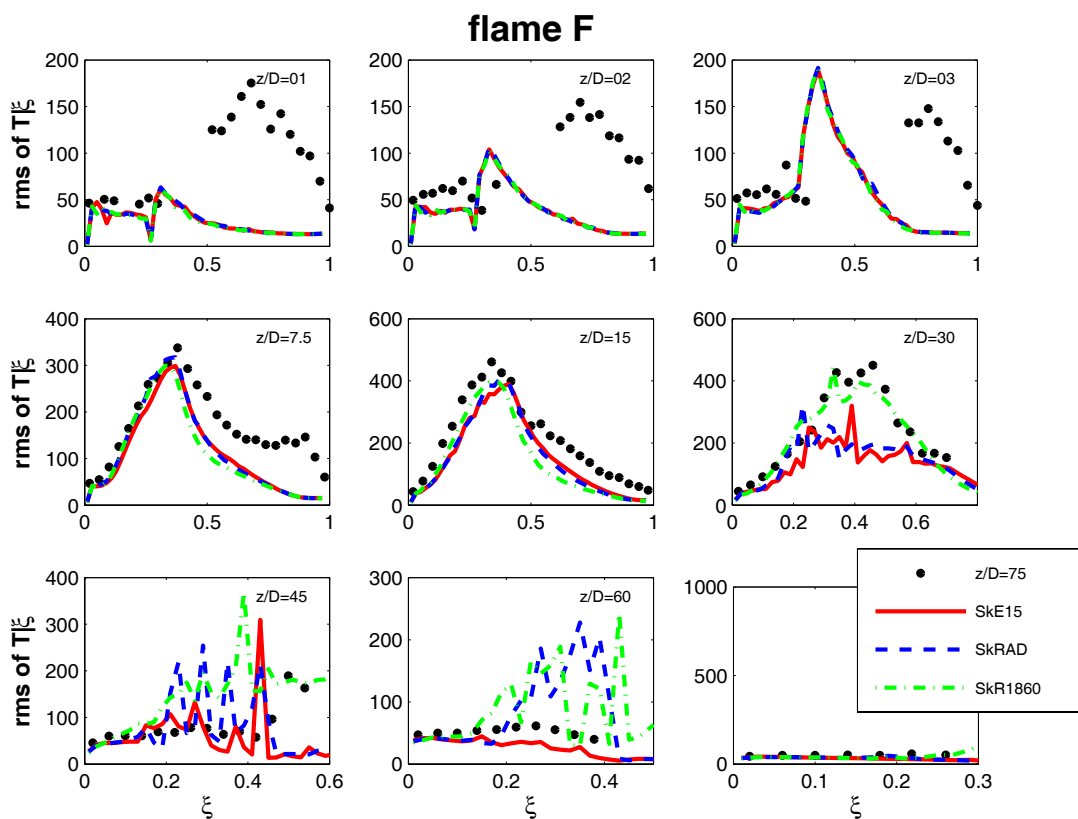
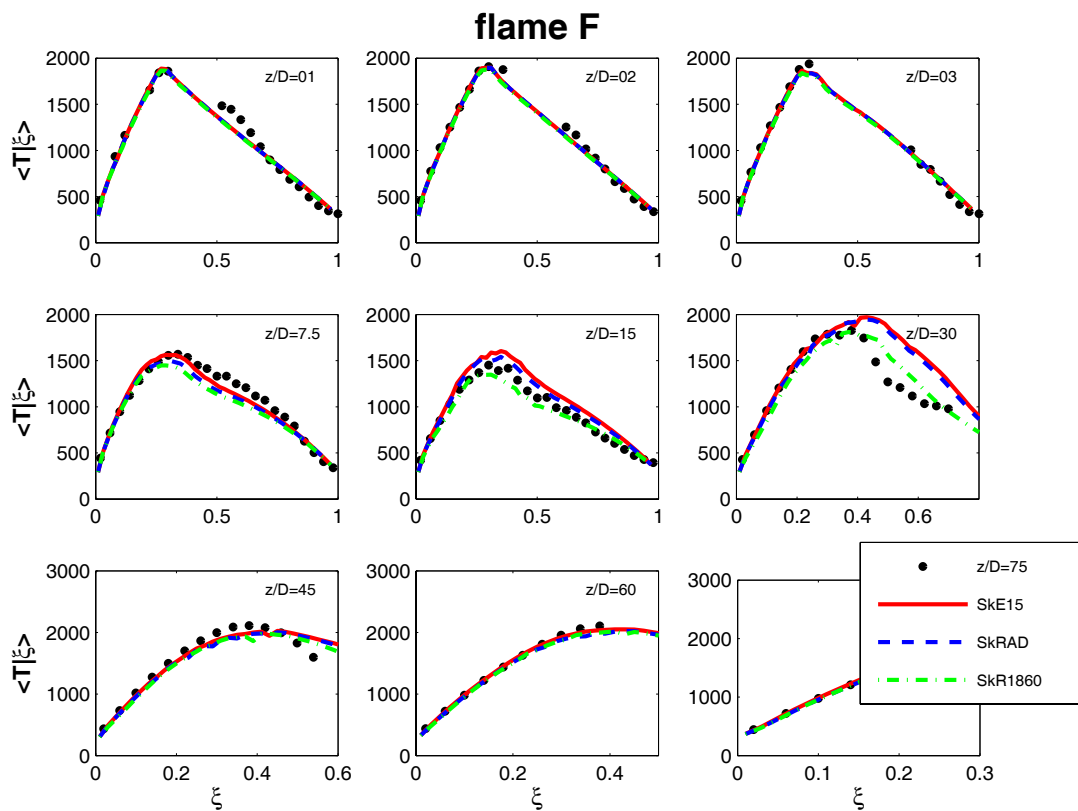


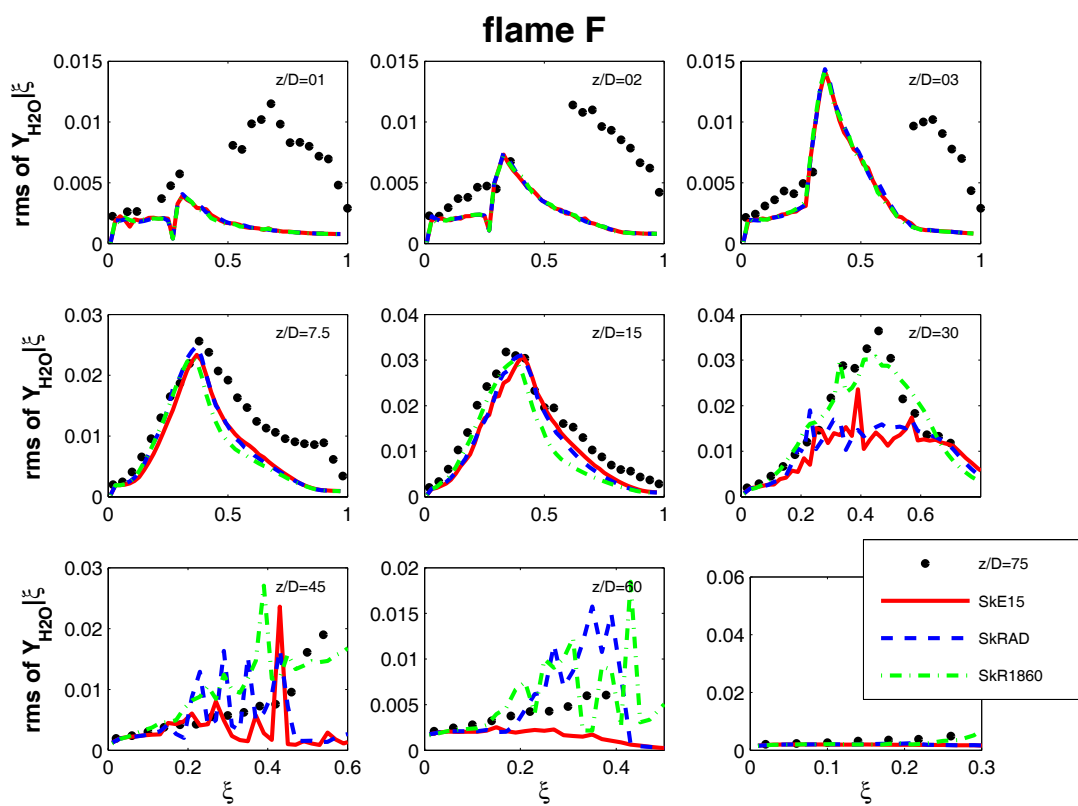
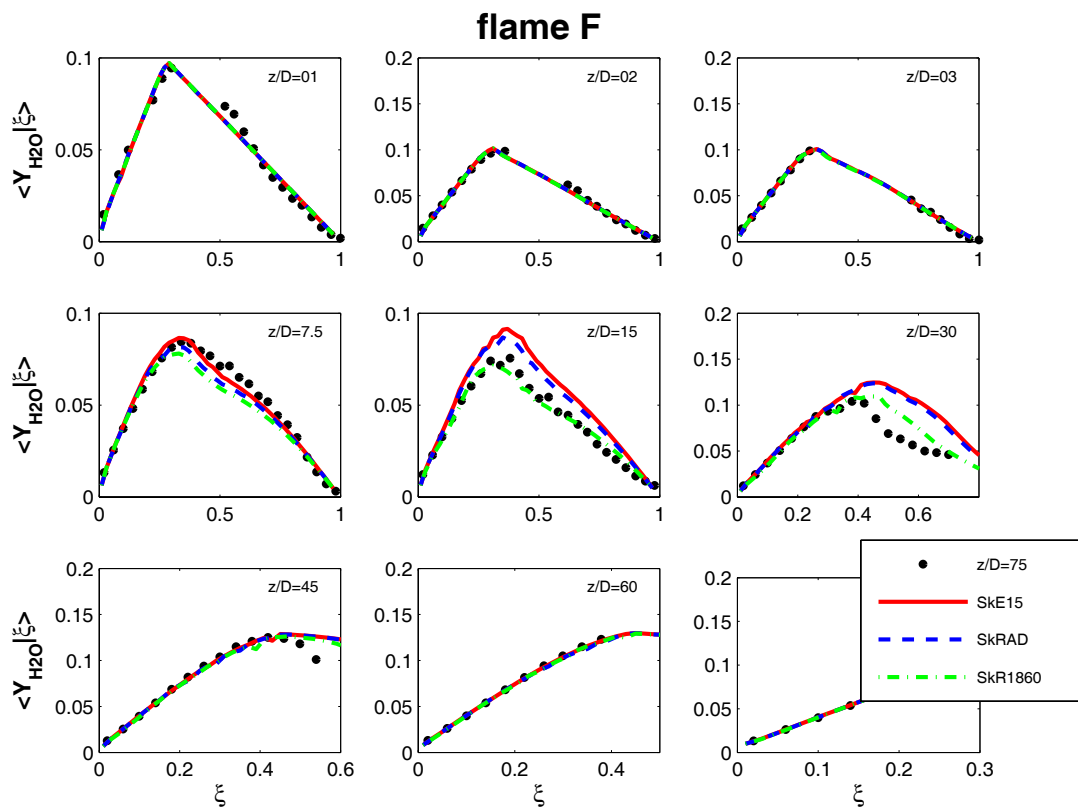


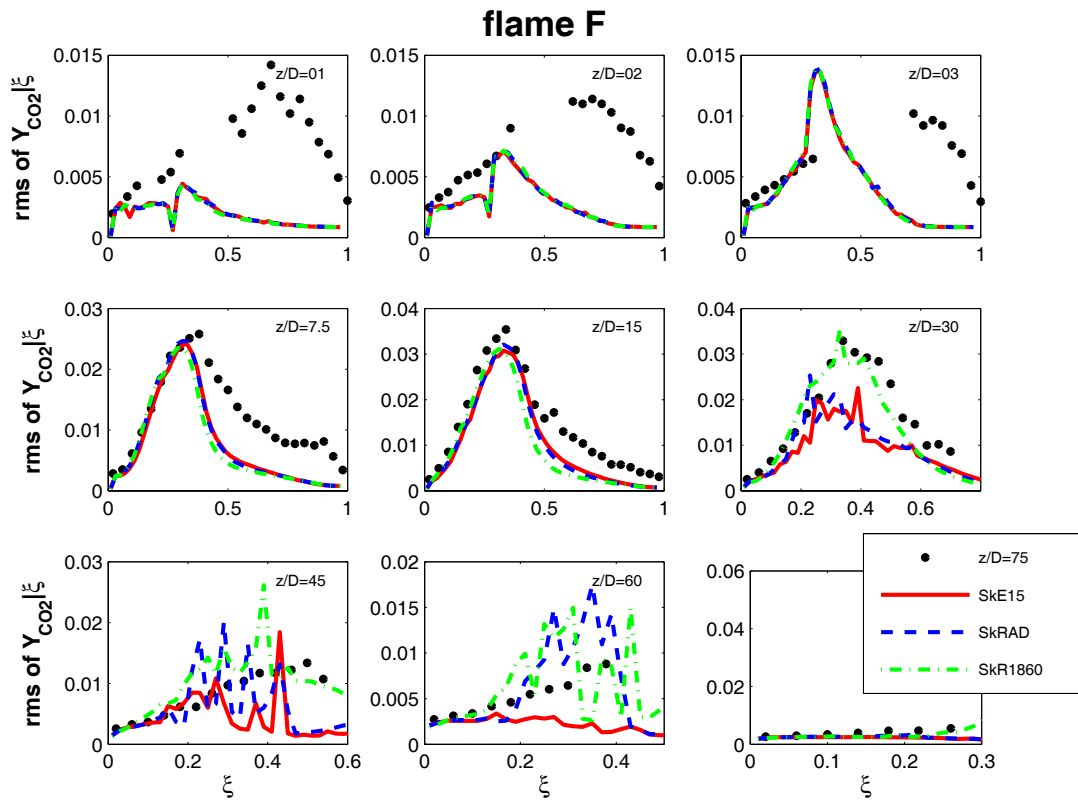
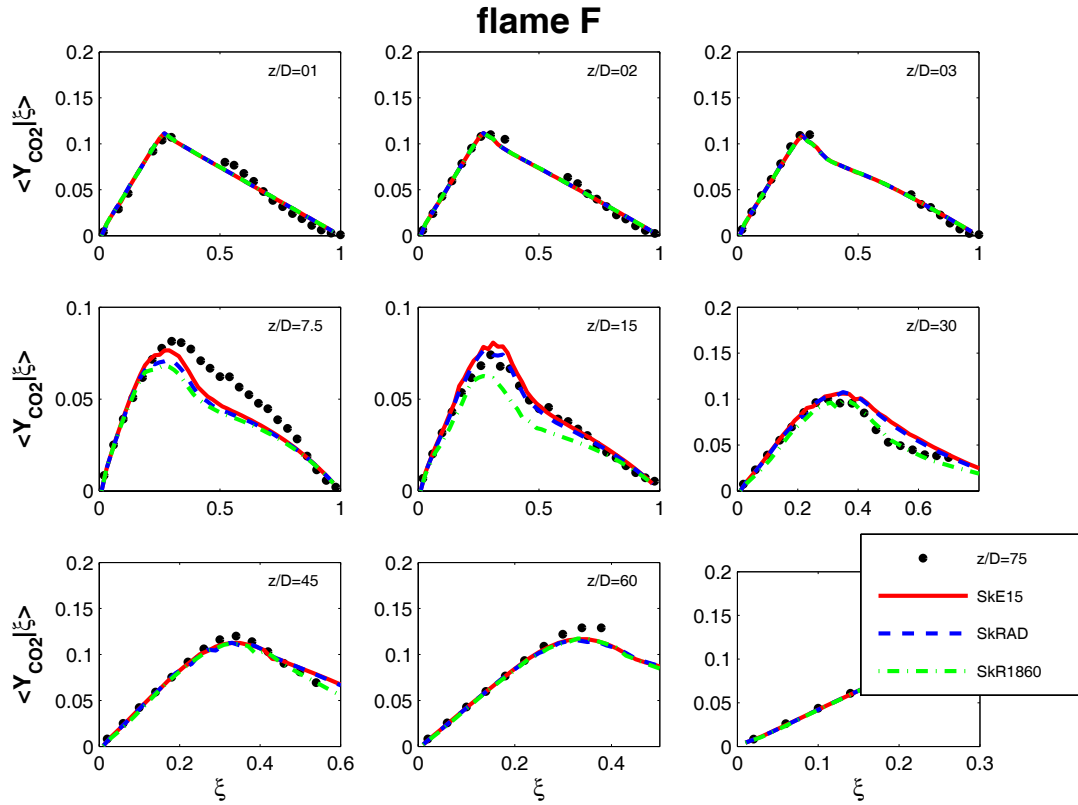


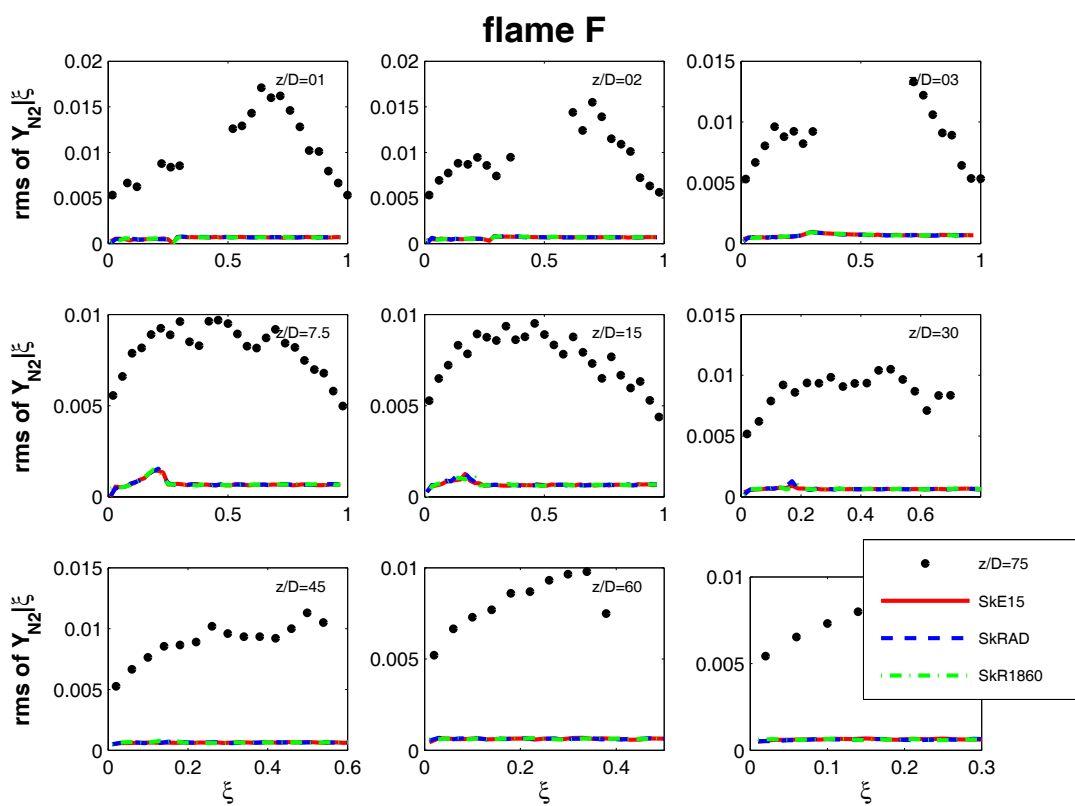
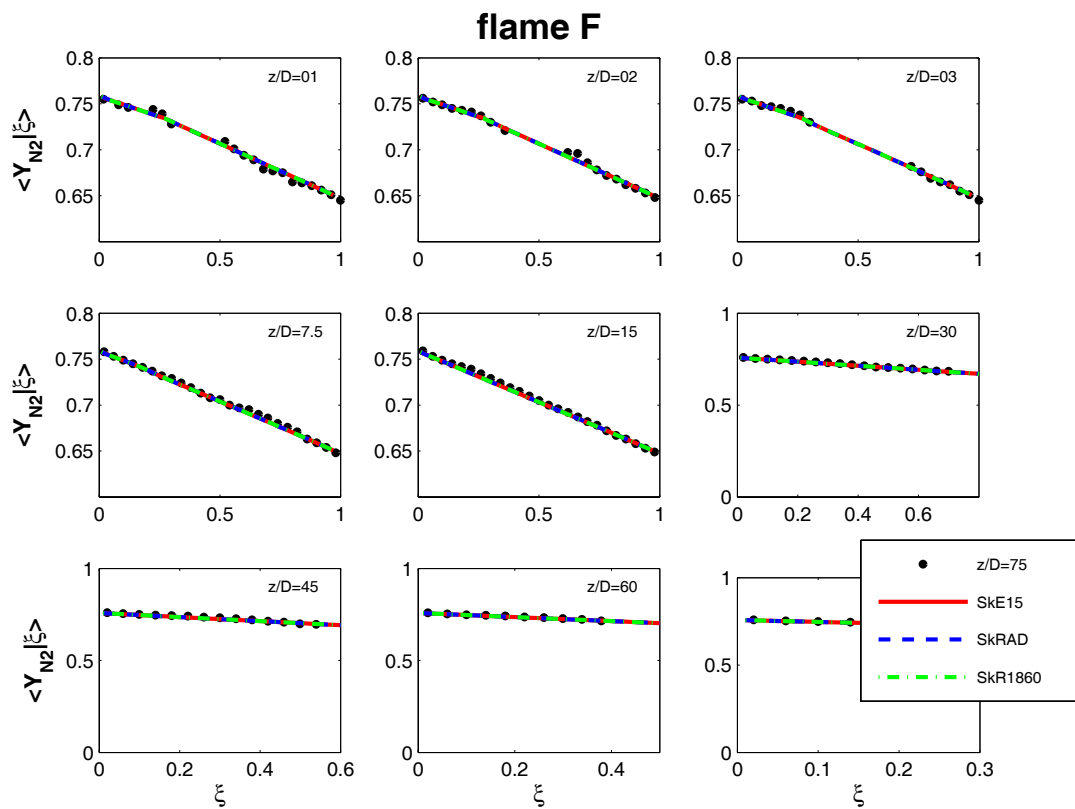


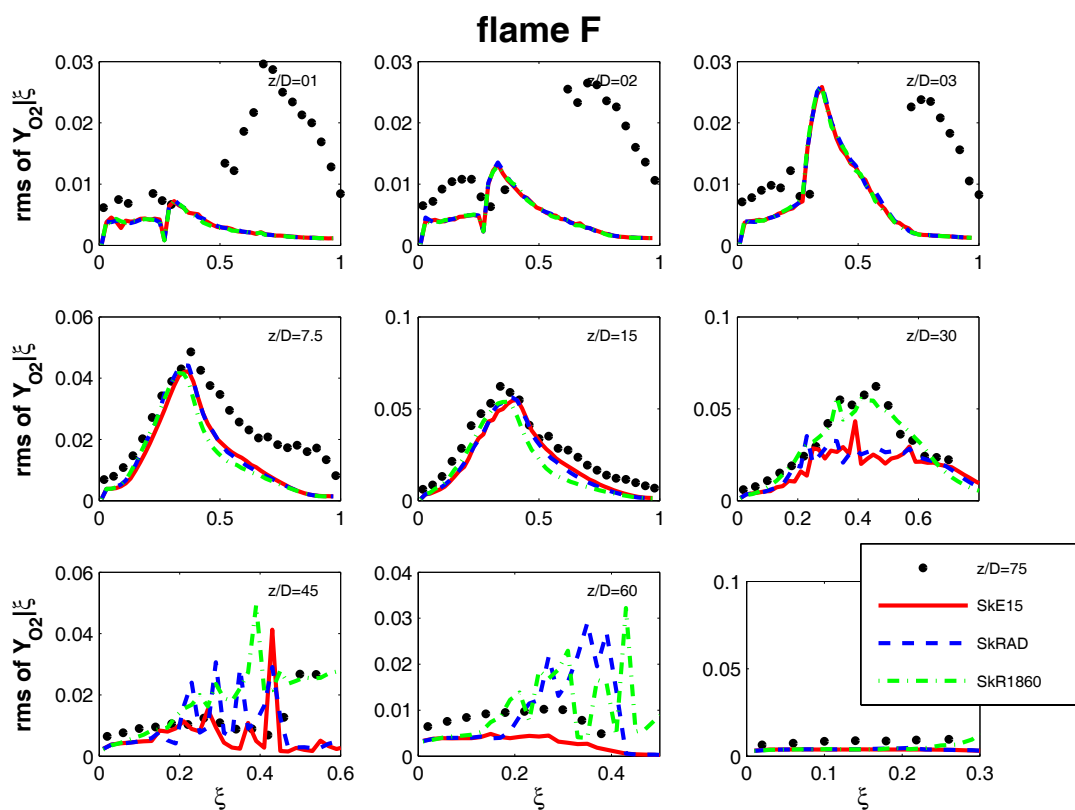
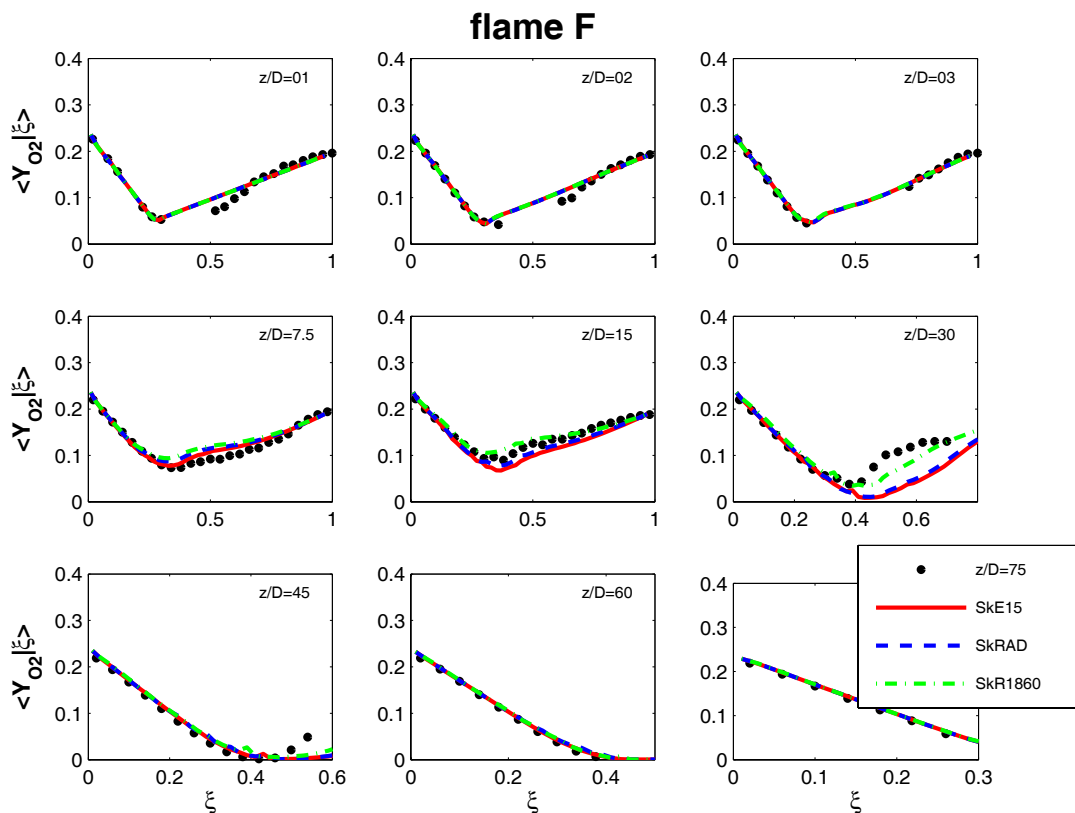
(5) SkE15, SkRAD, and SkR`1860

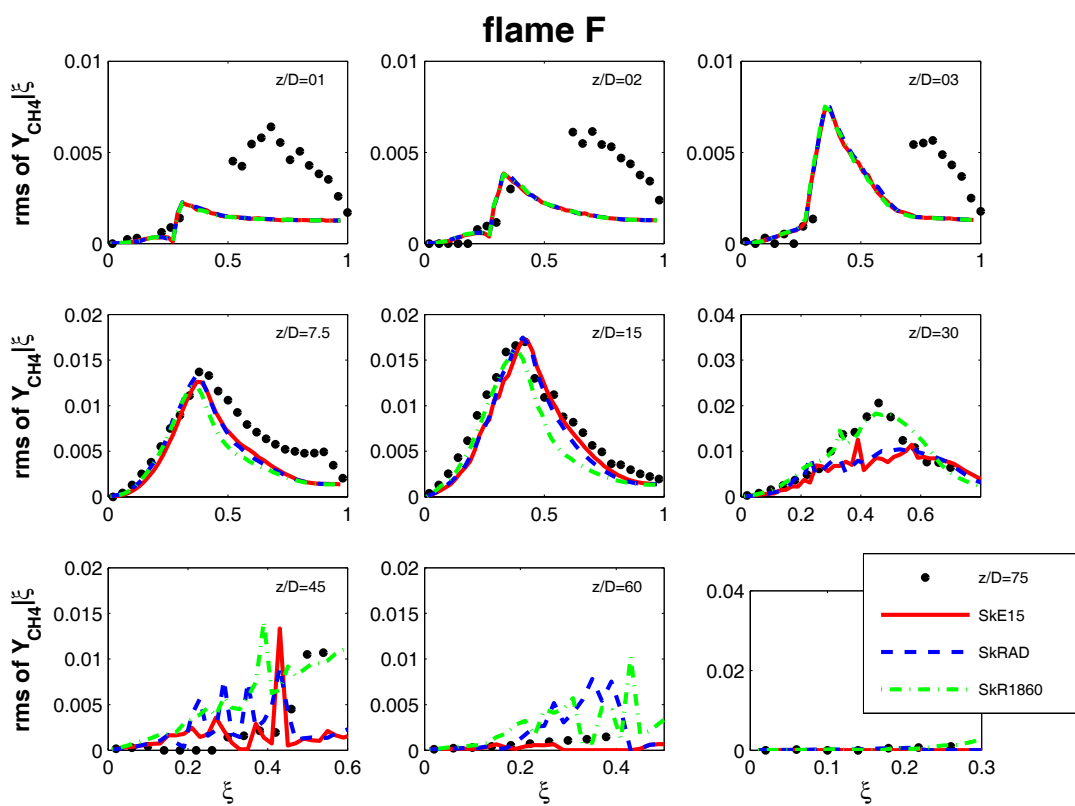
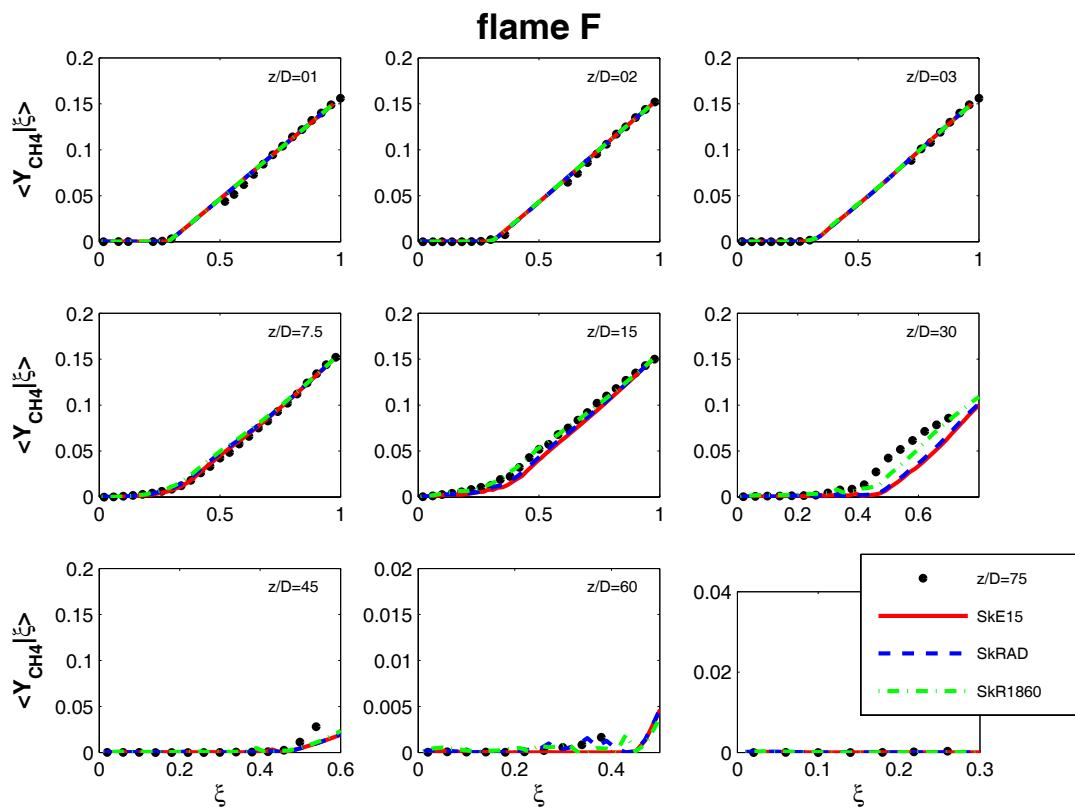


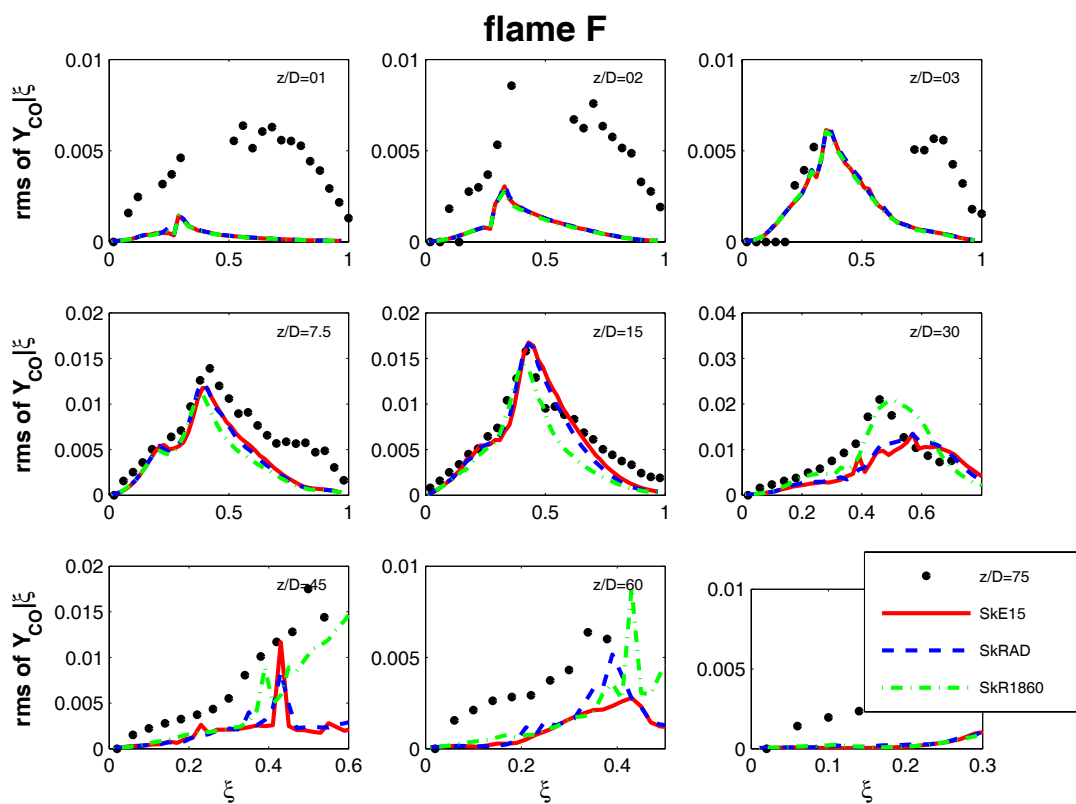
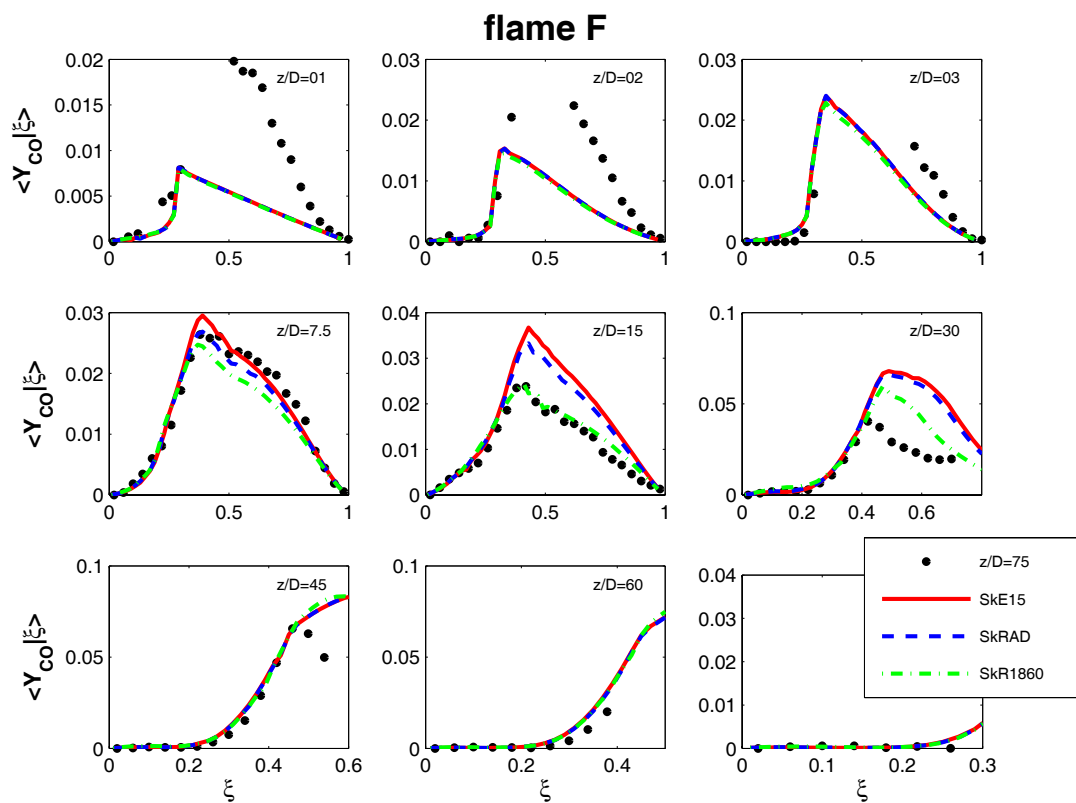


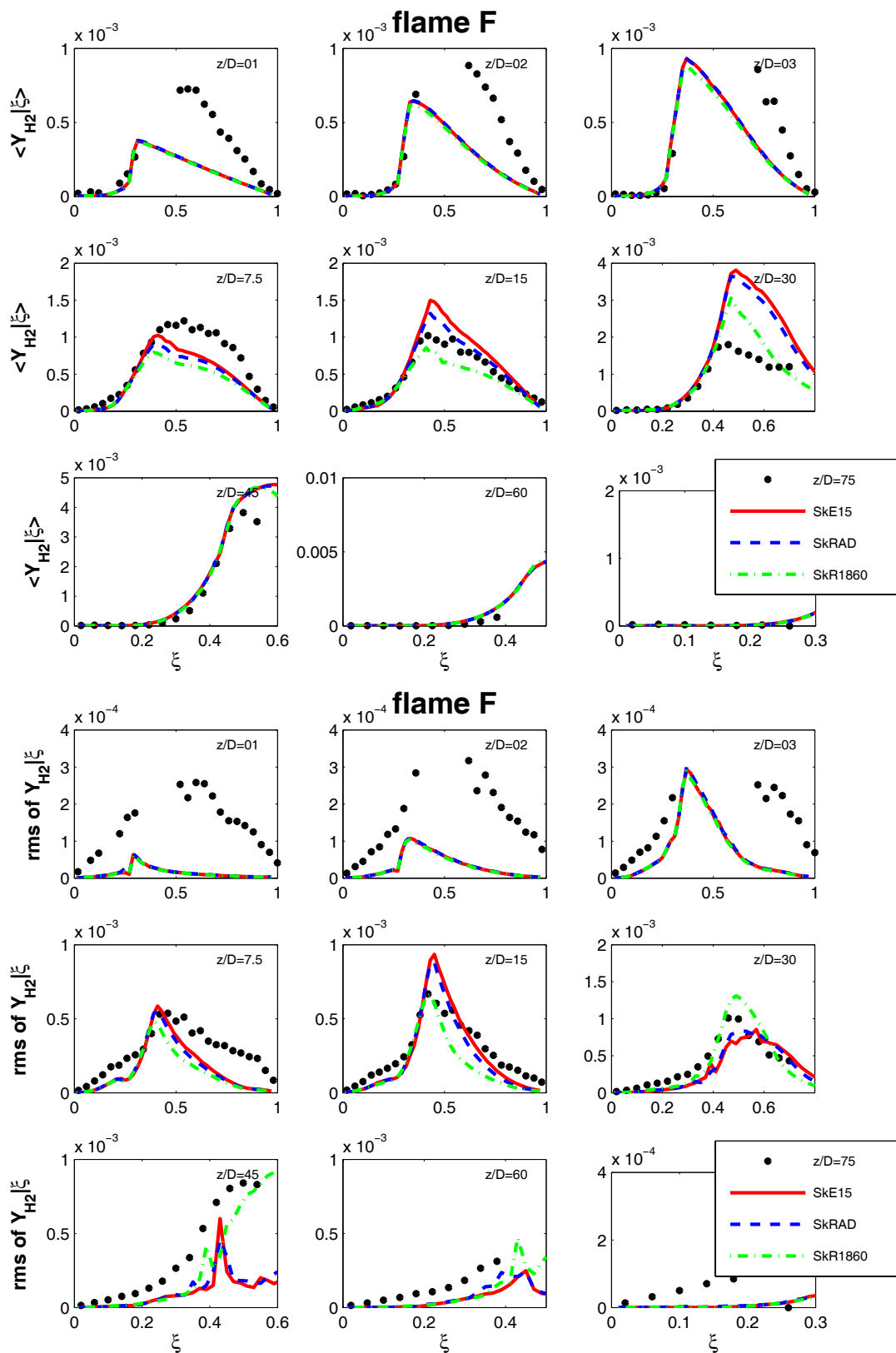


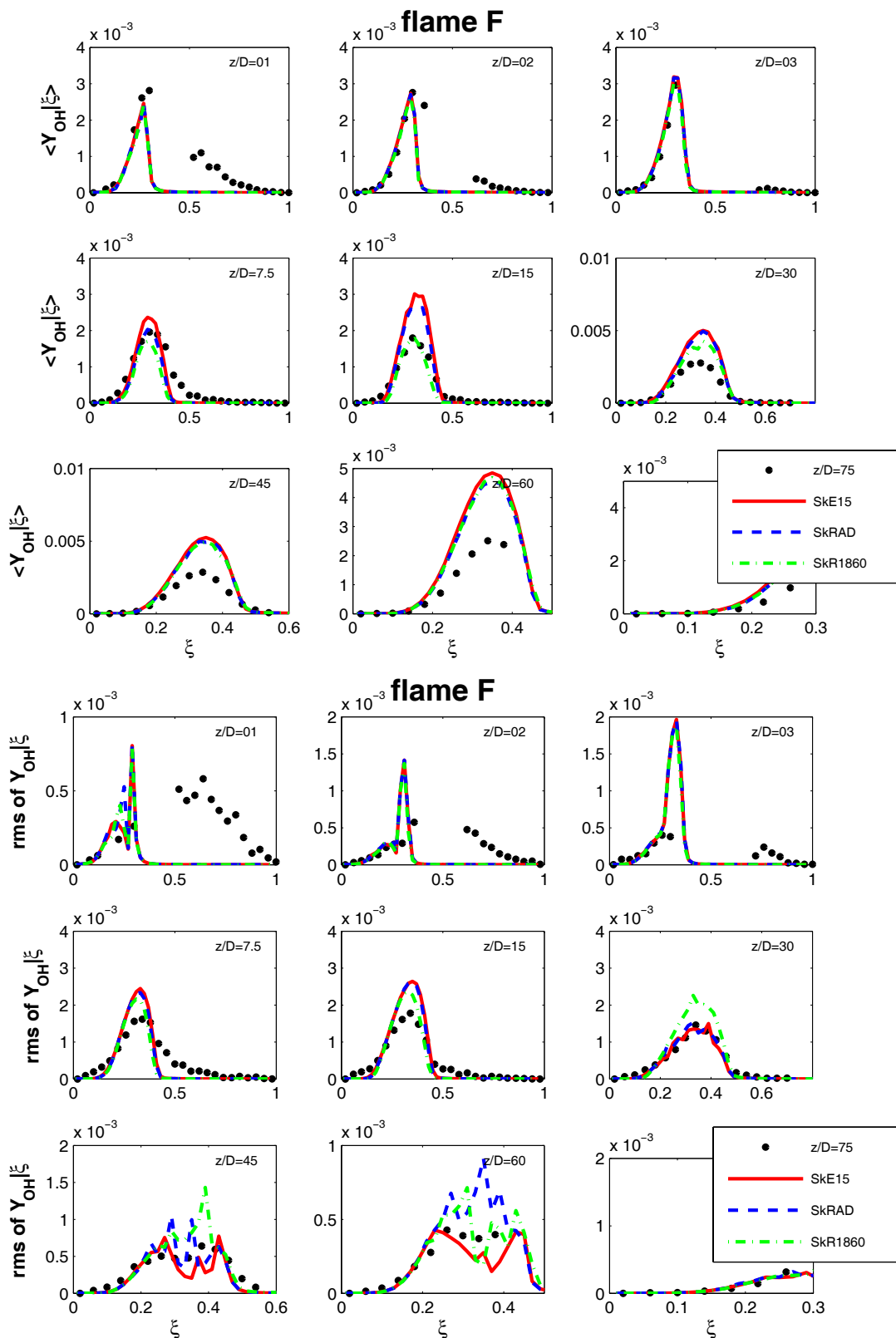




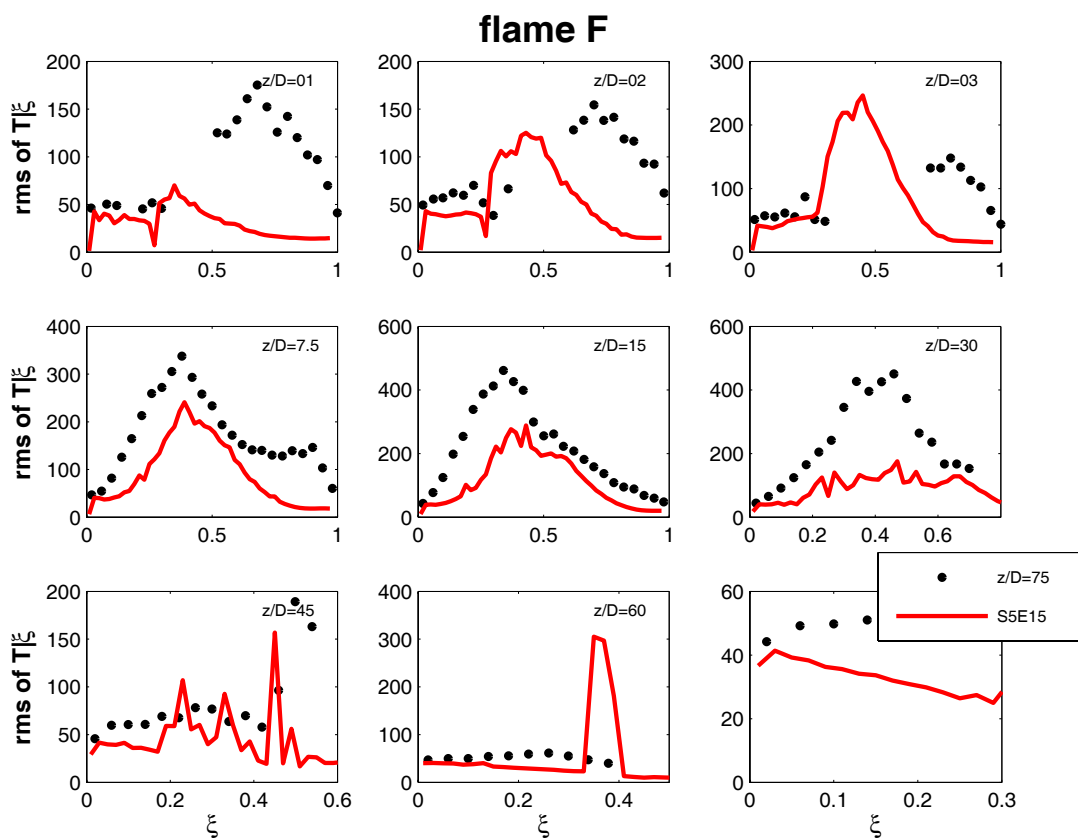
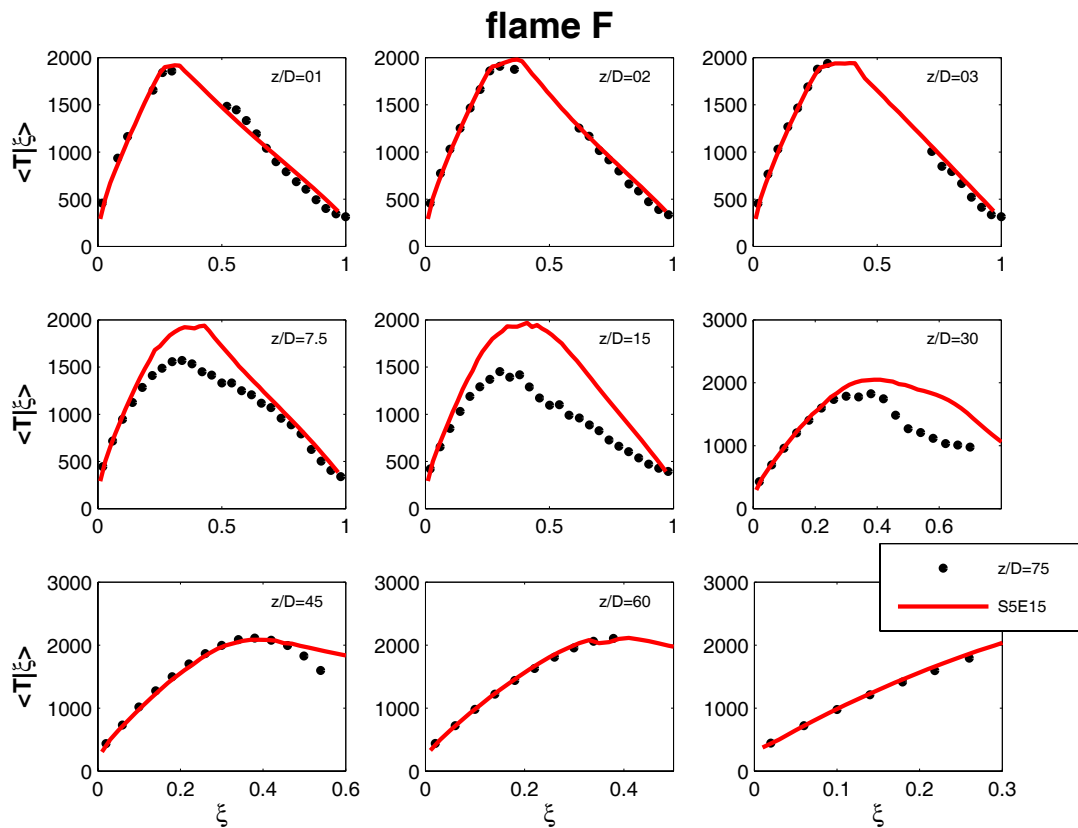


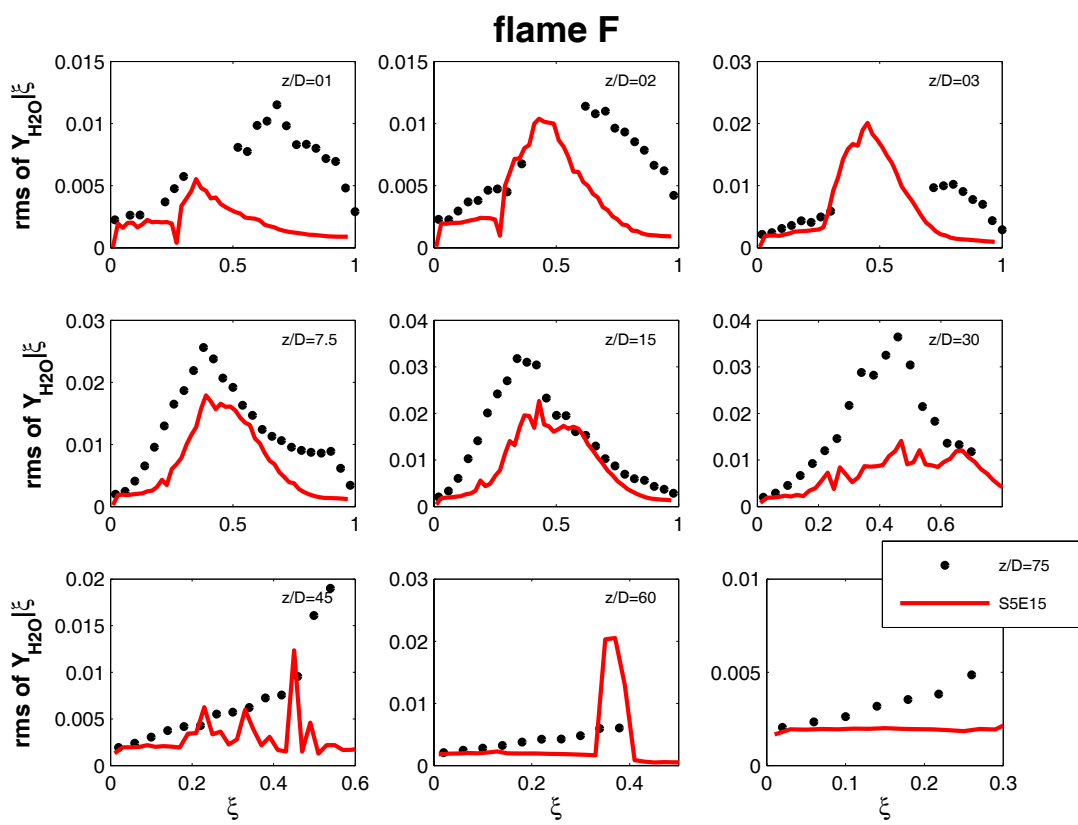
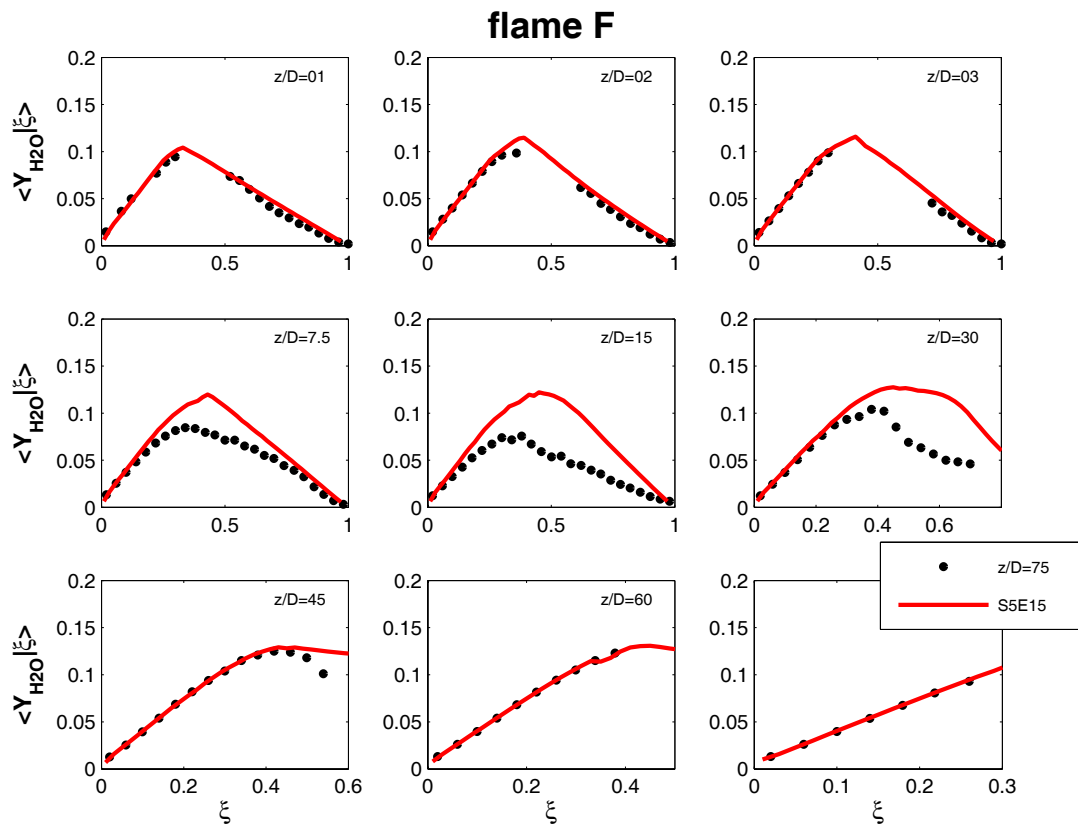


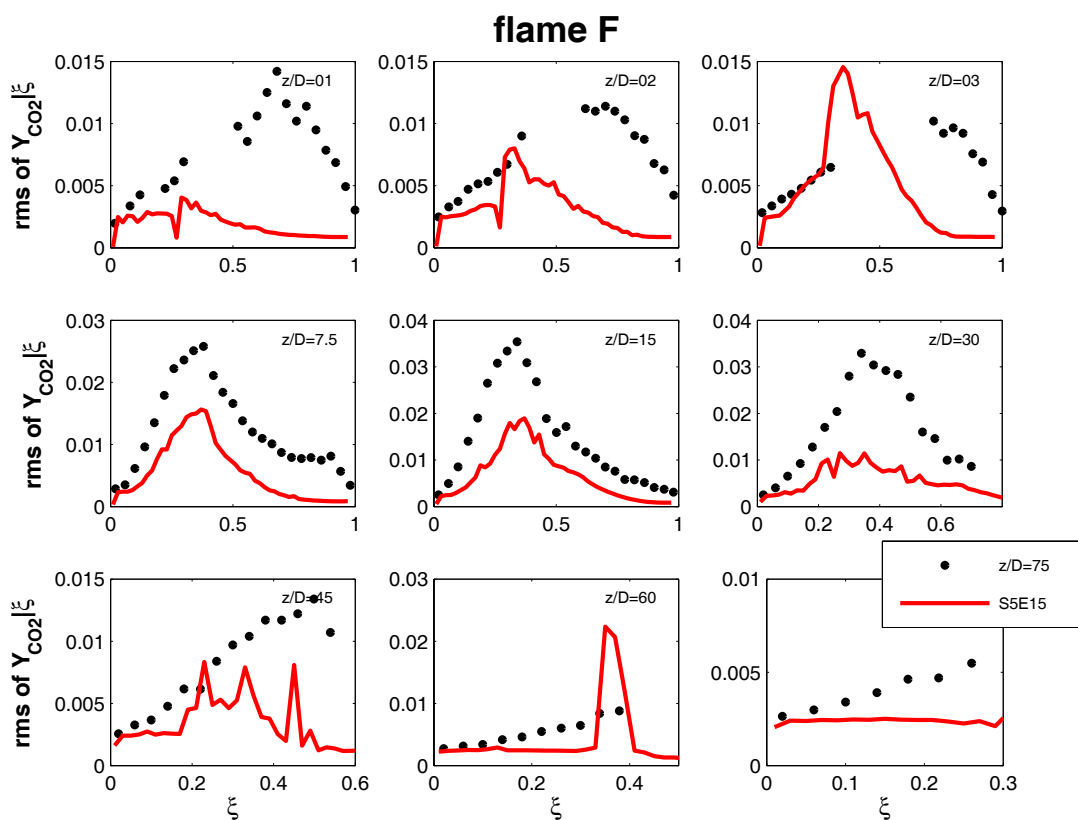
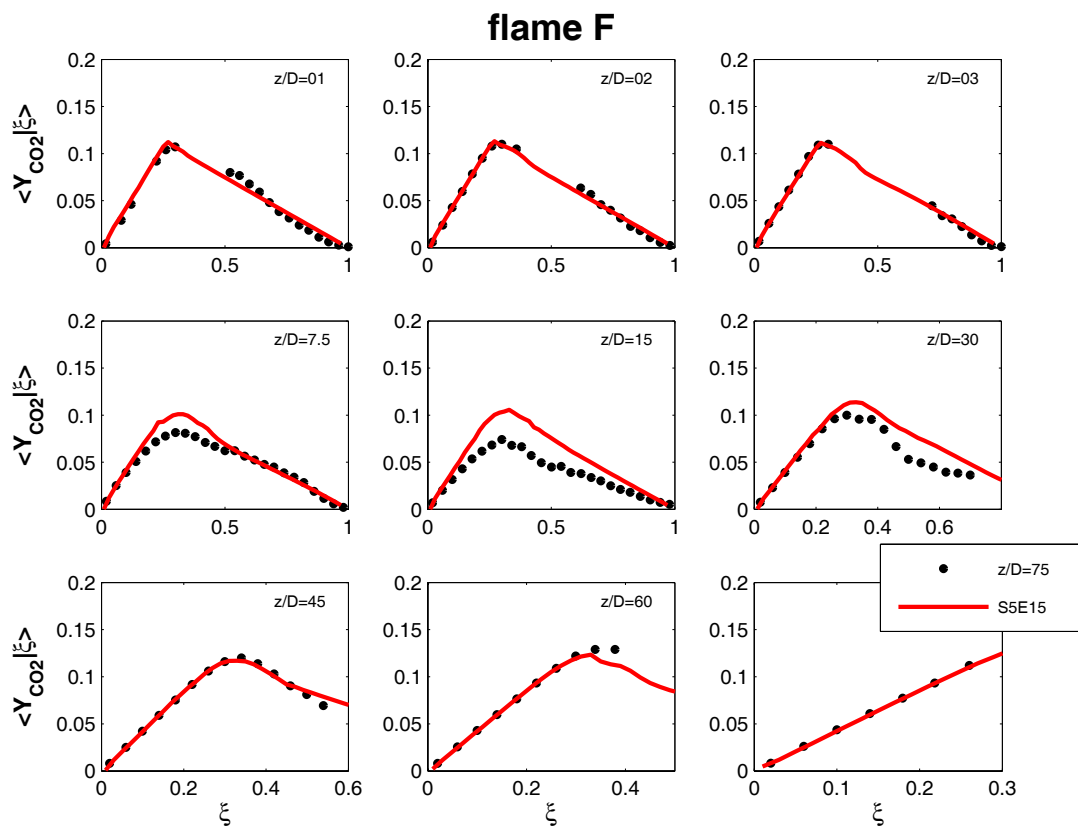


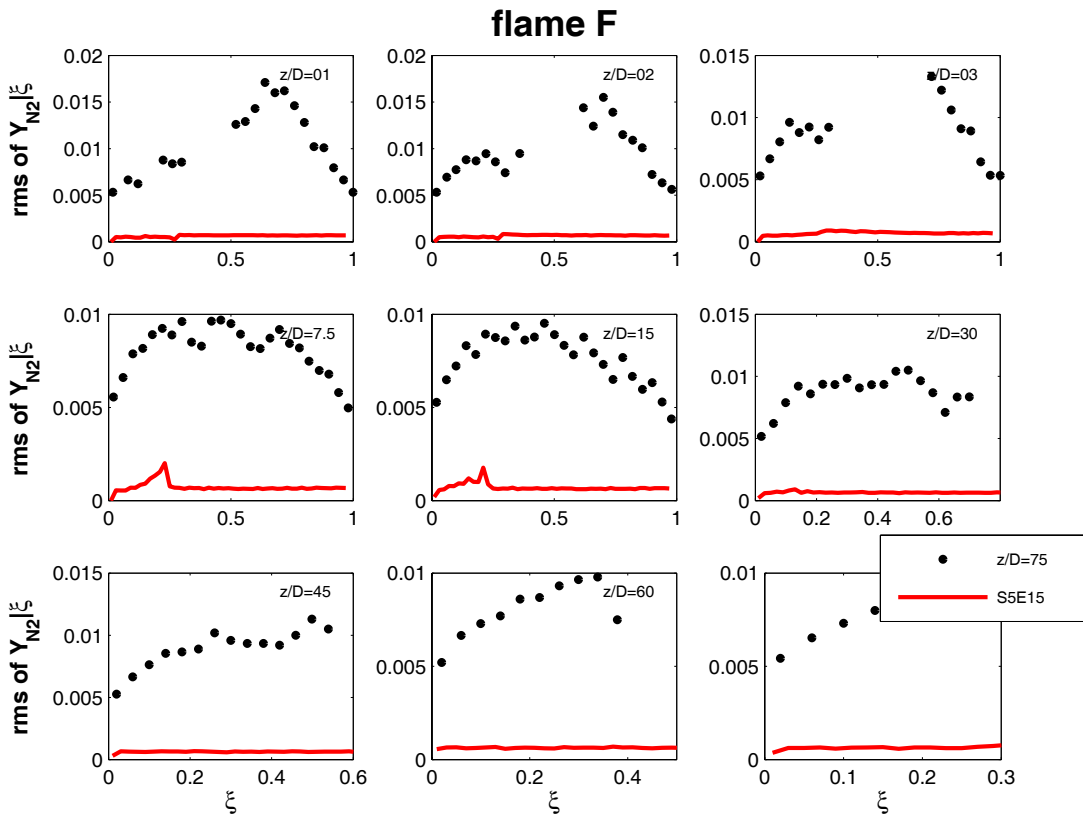
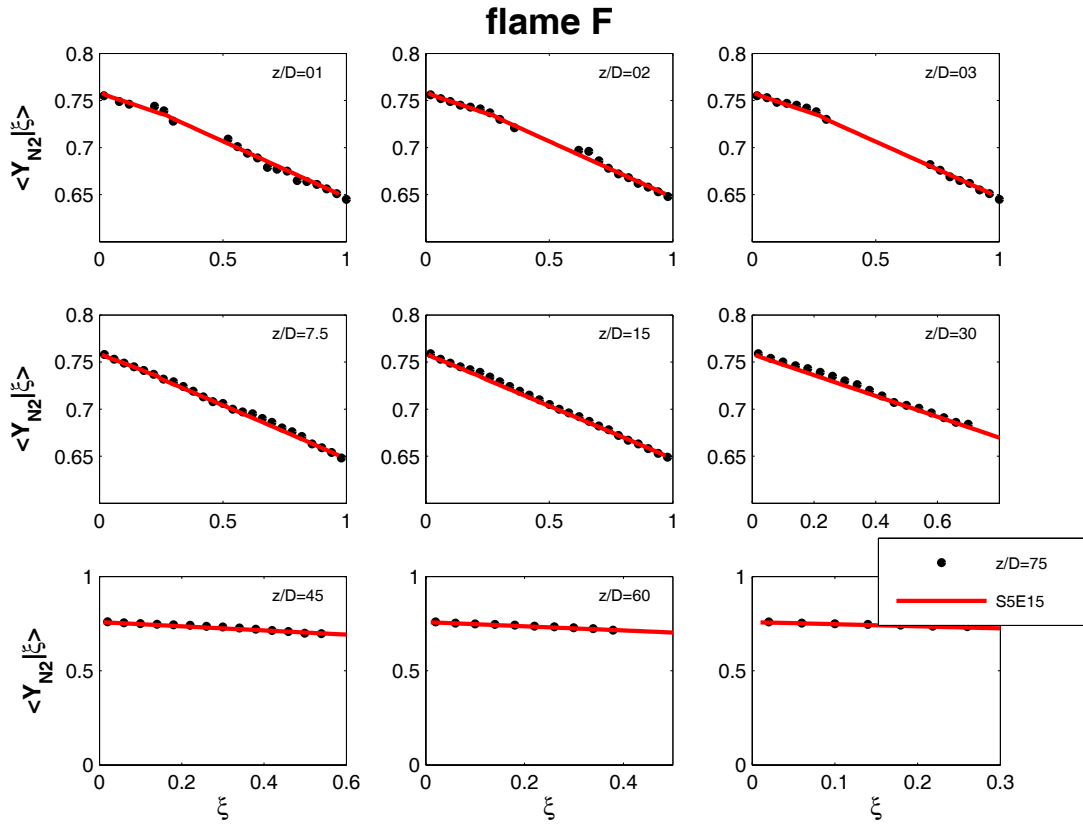


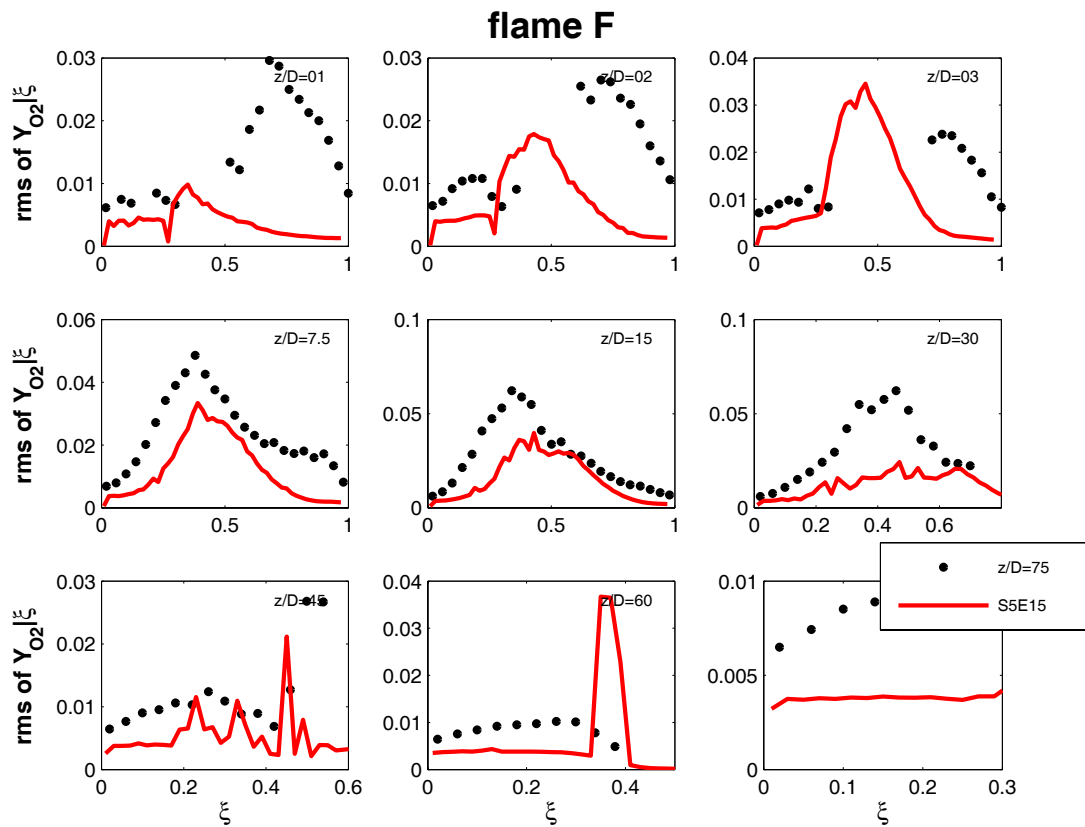
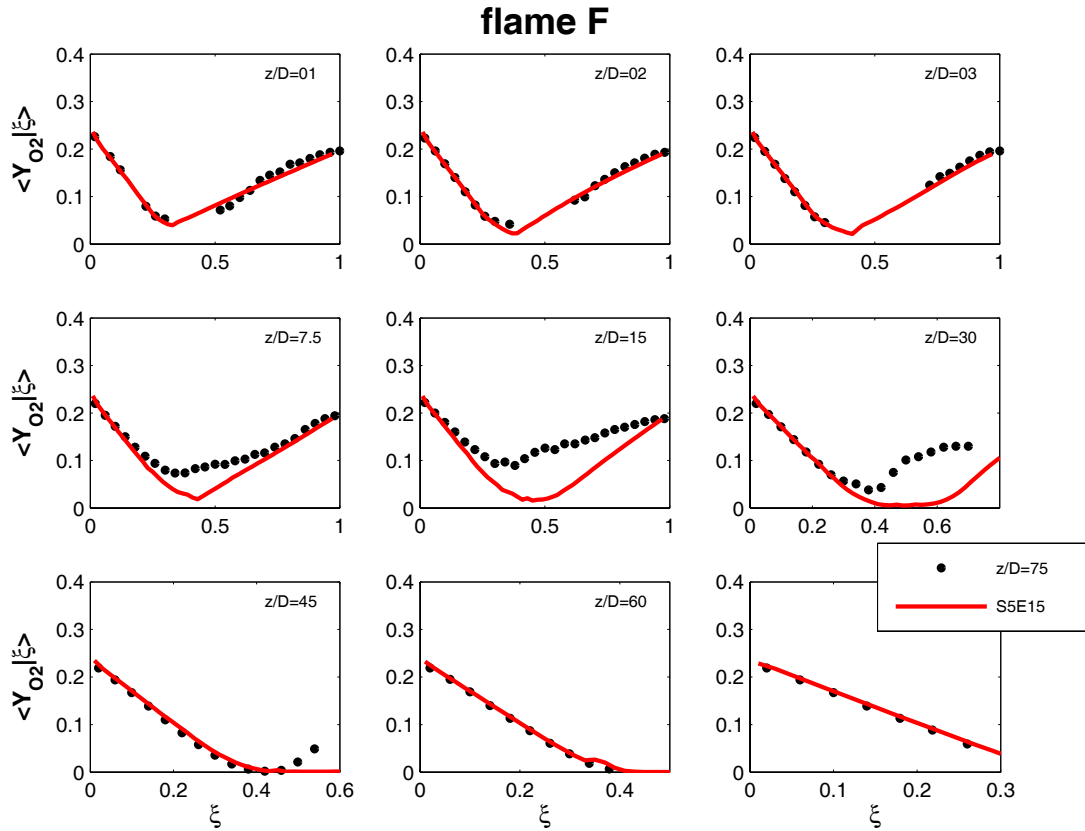
(6) S5E15

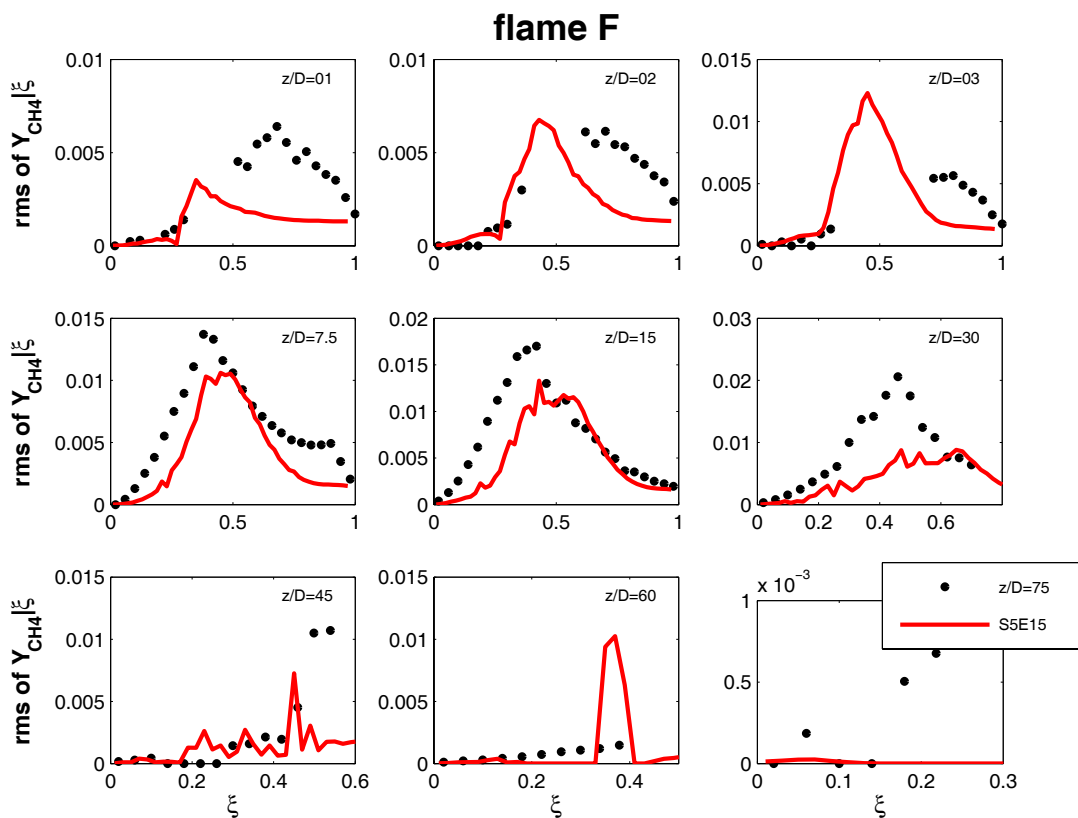
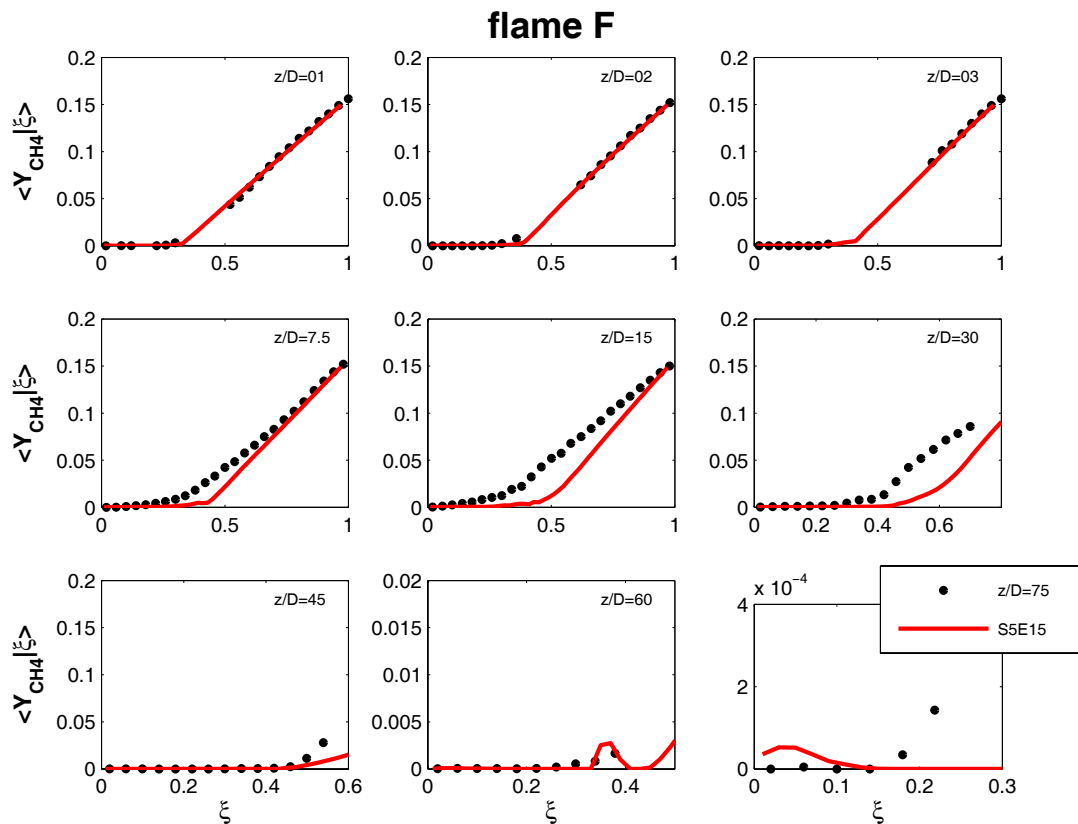


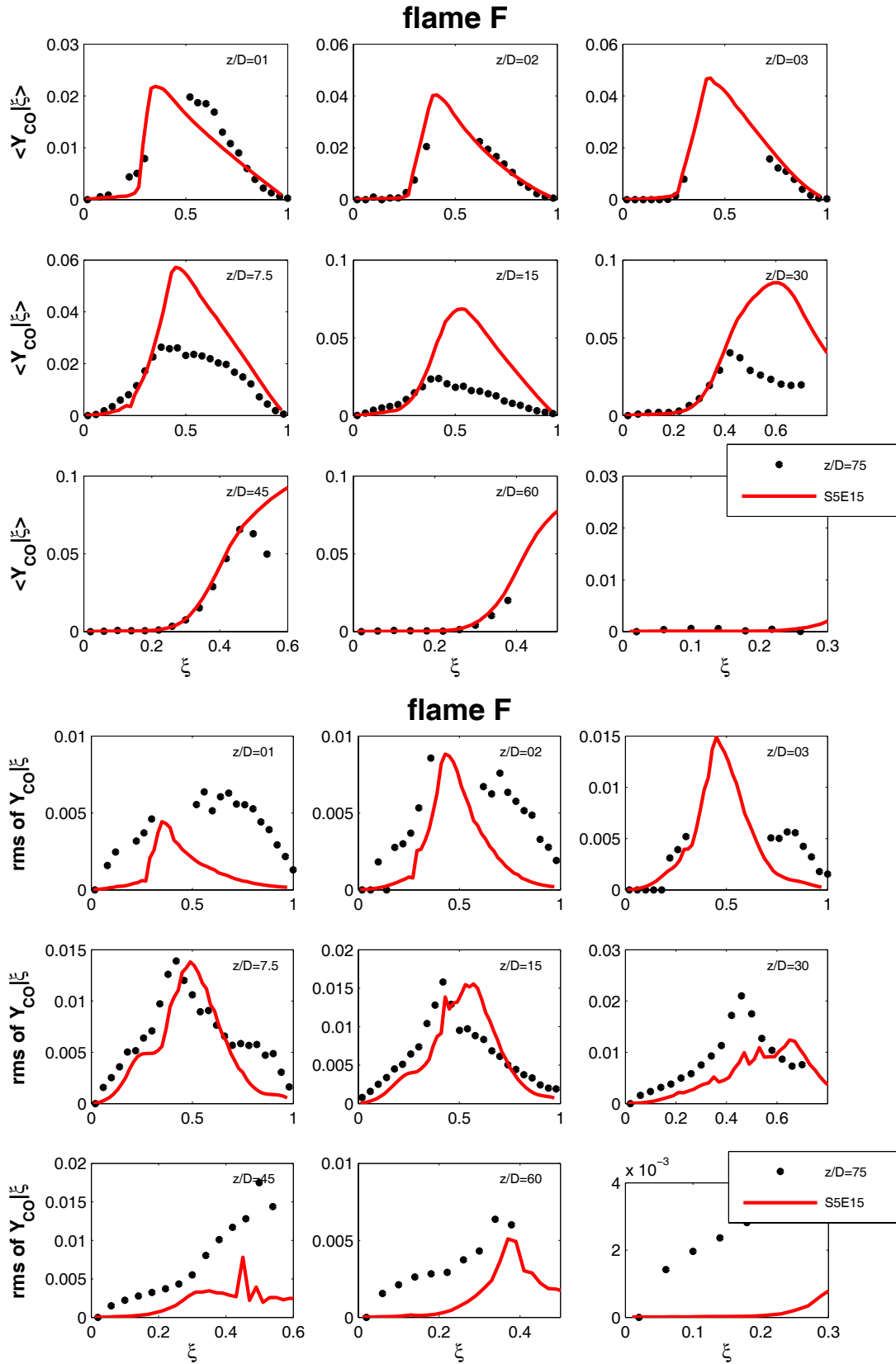


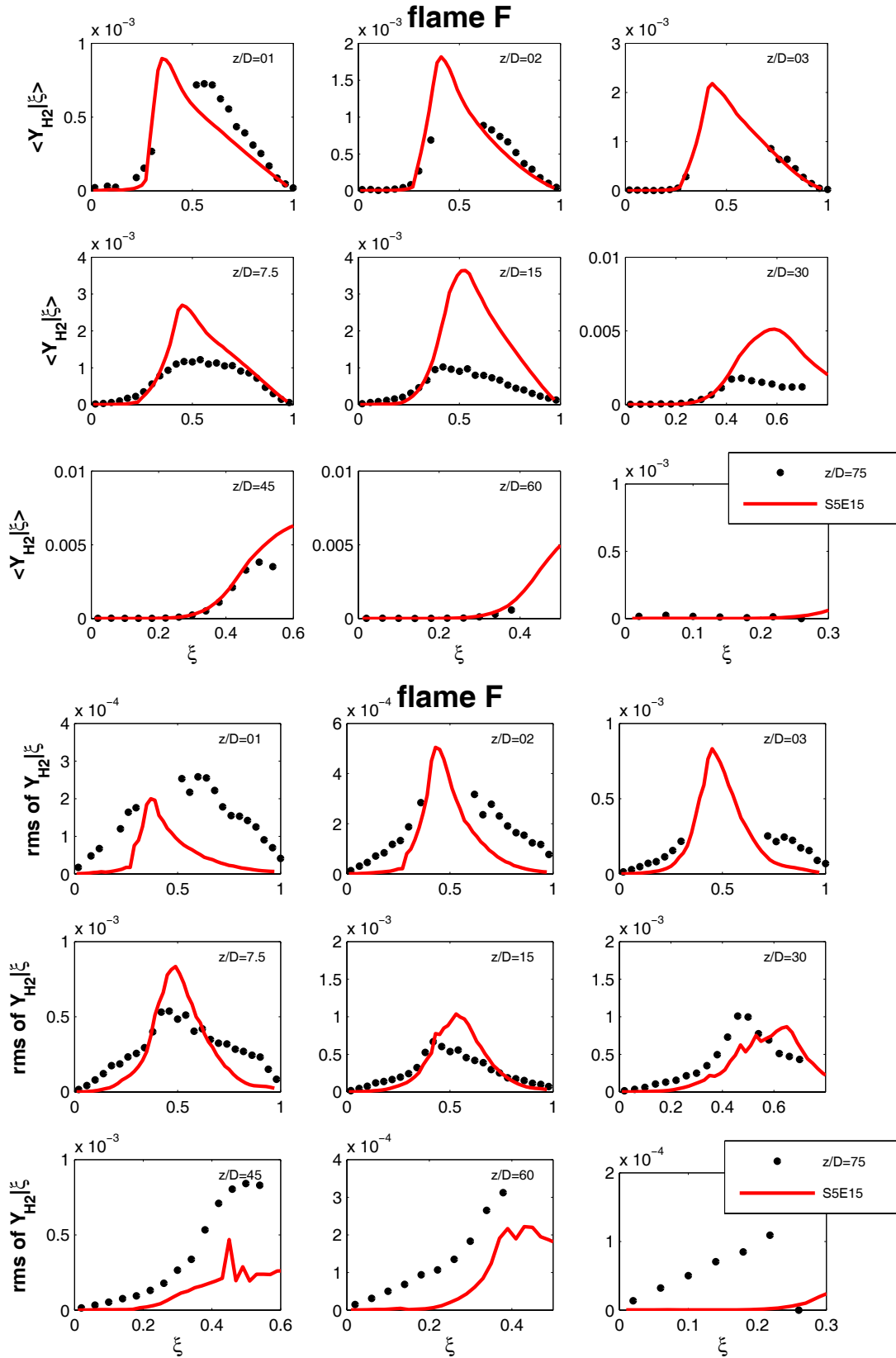


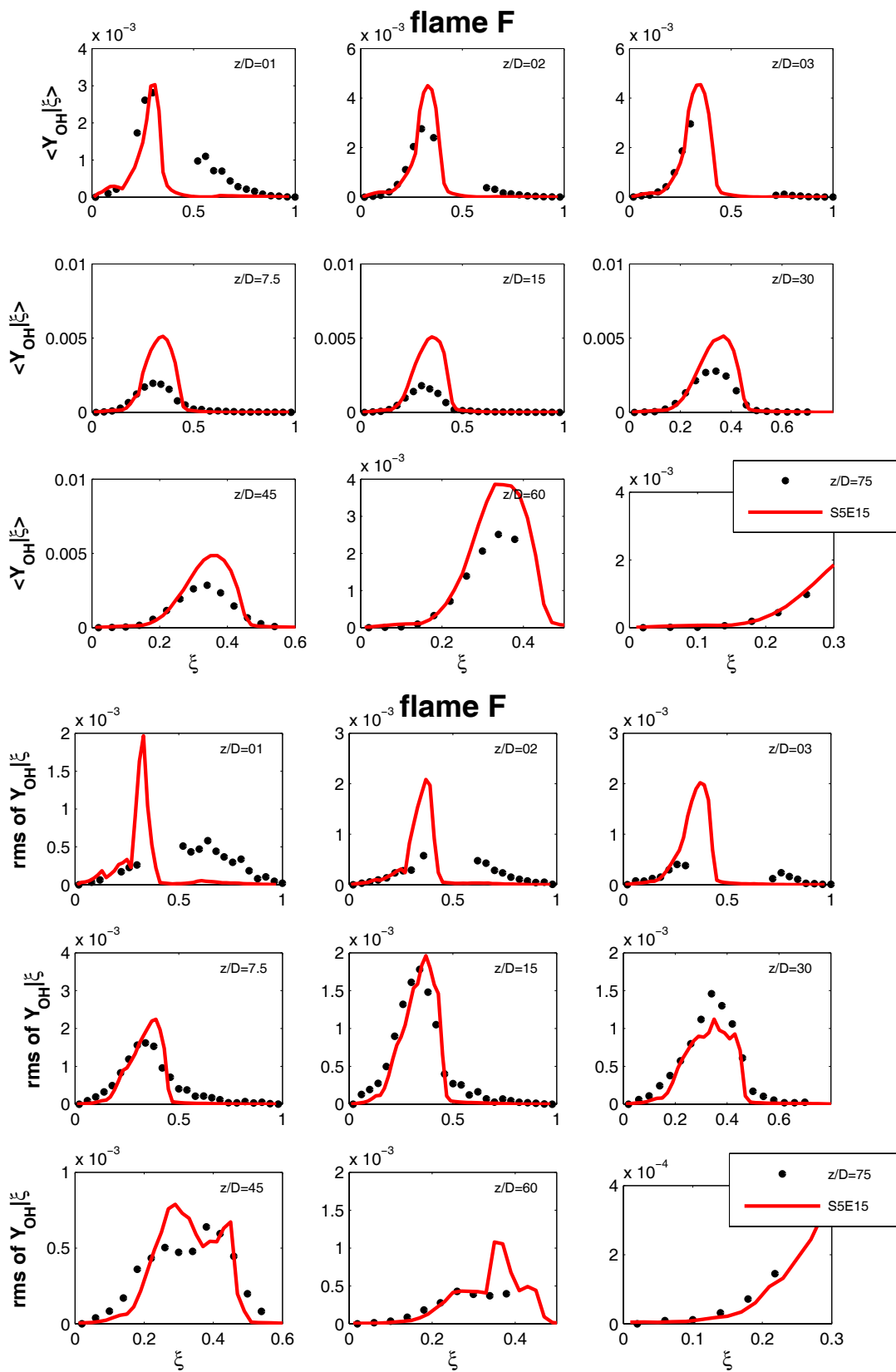


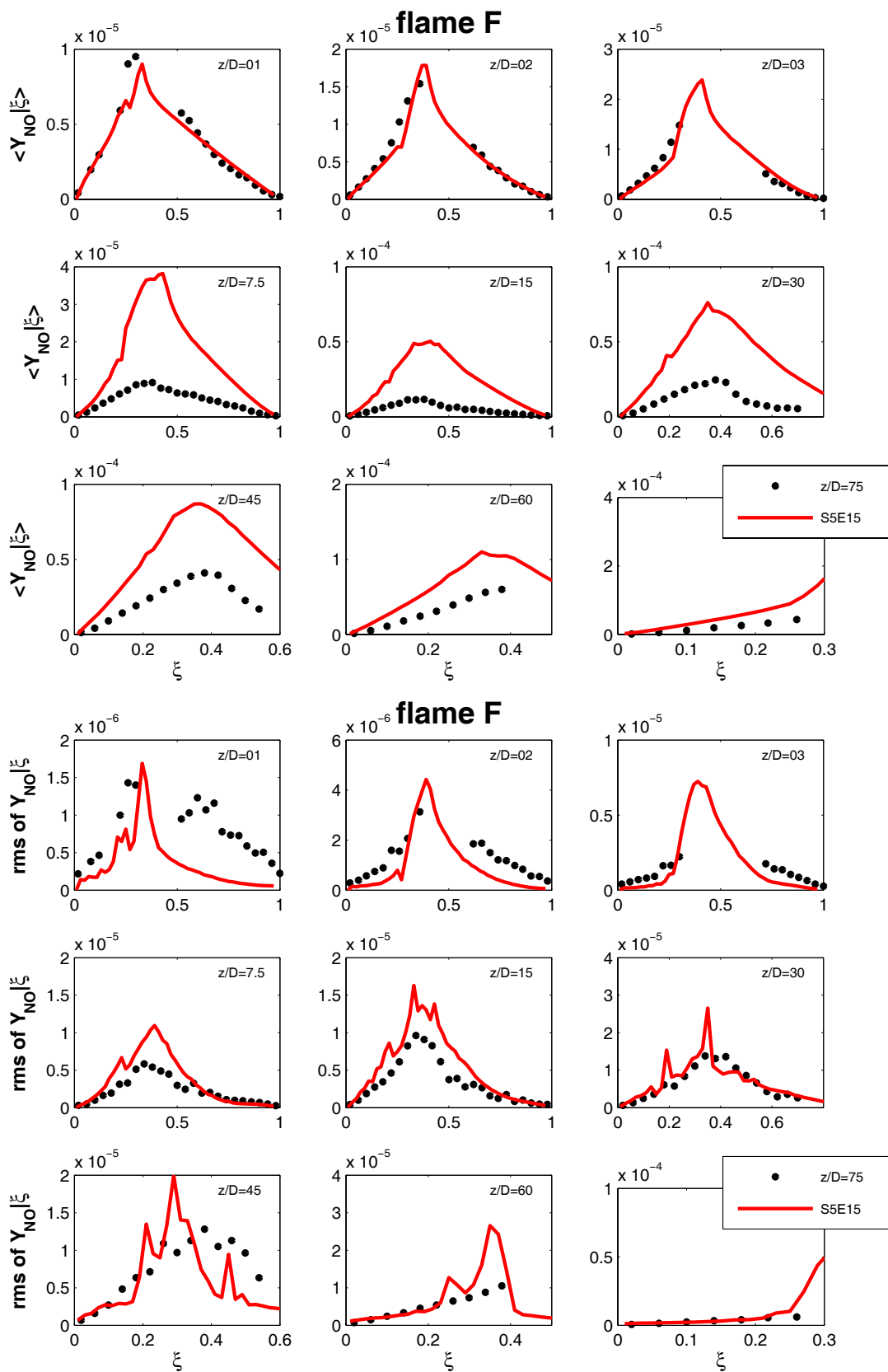








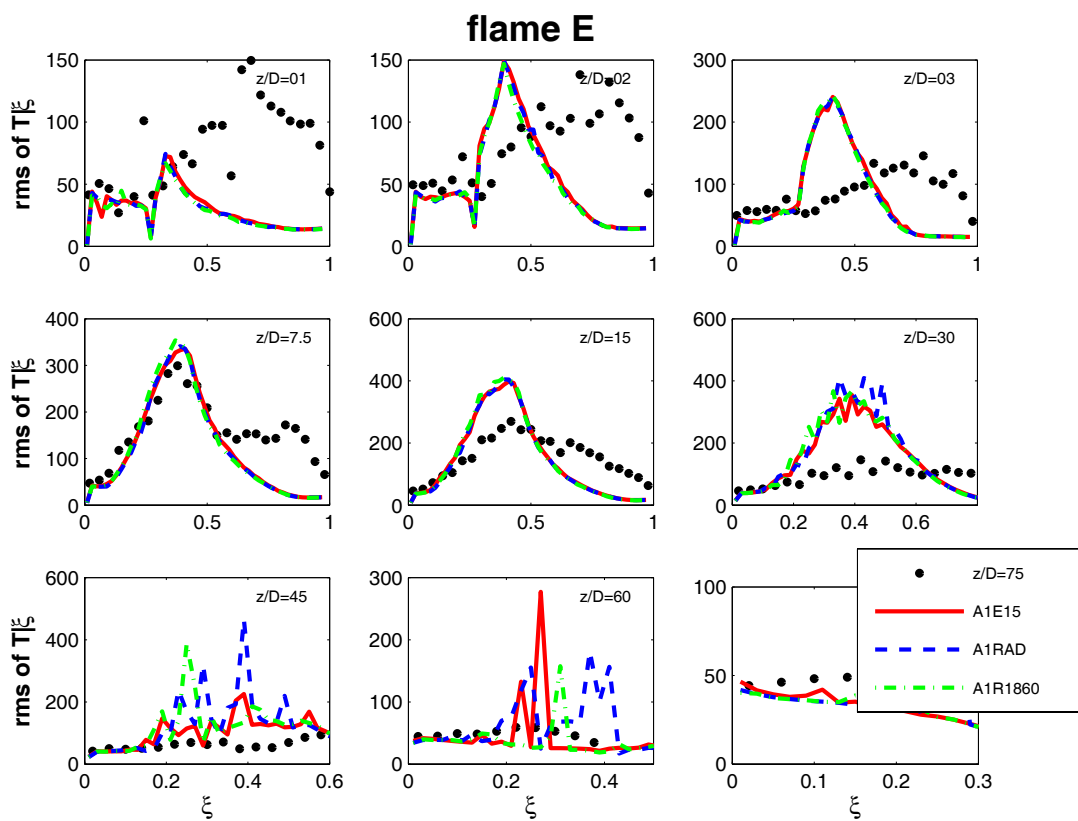
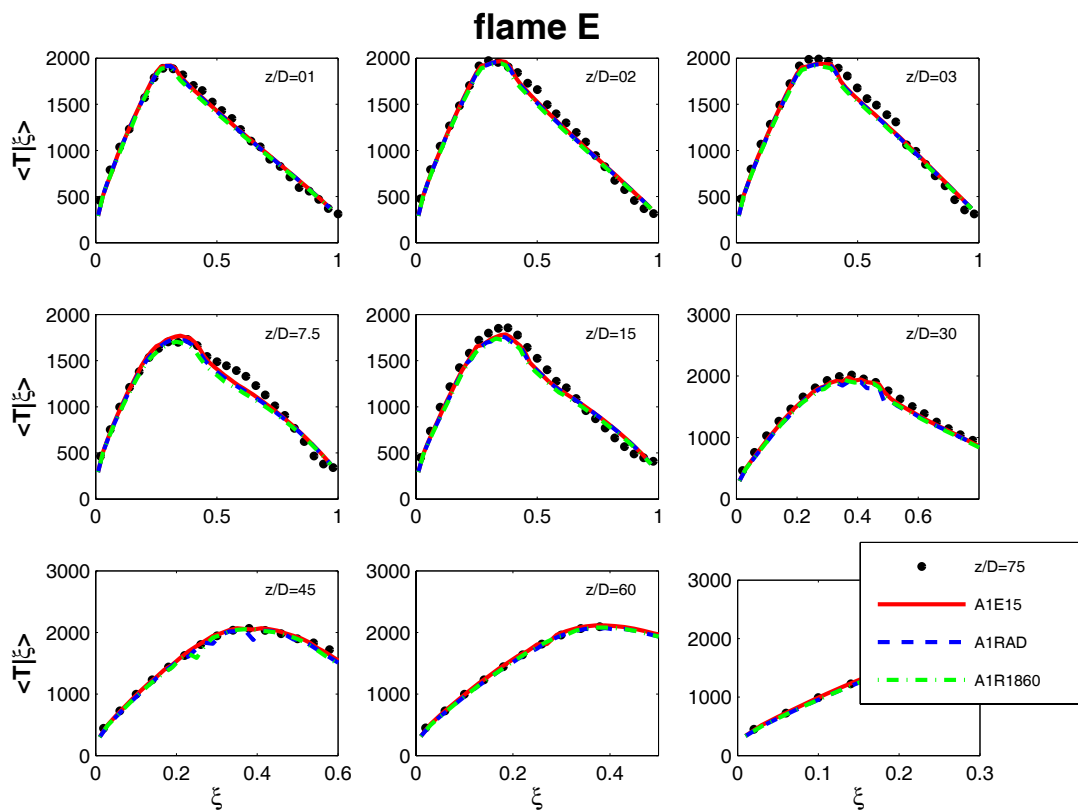


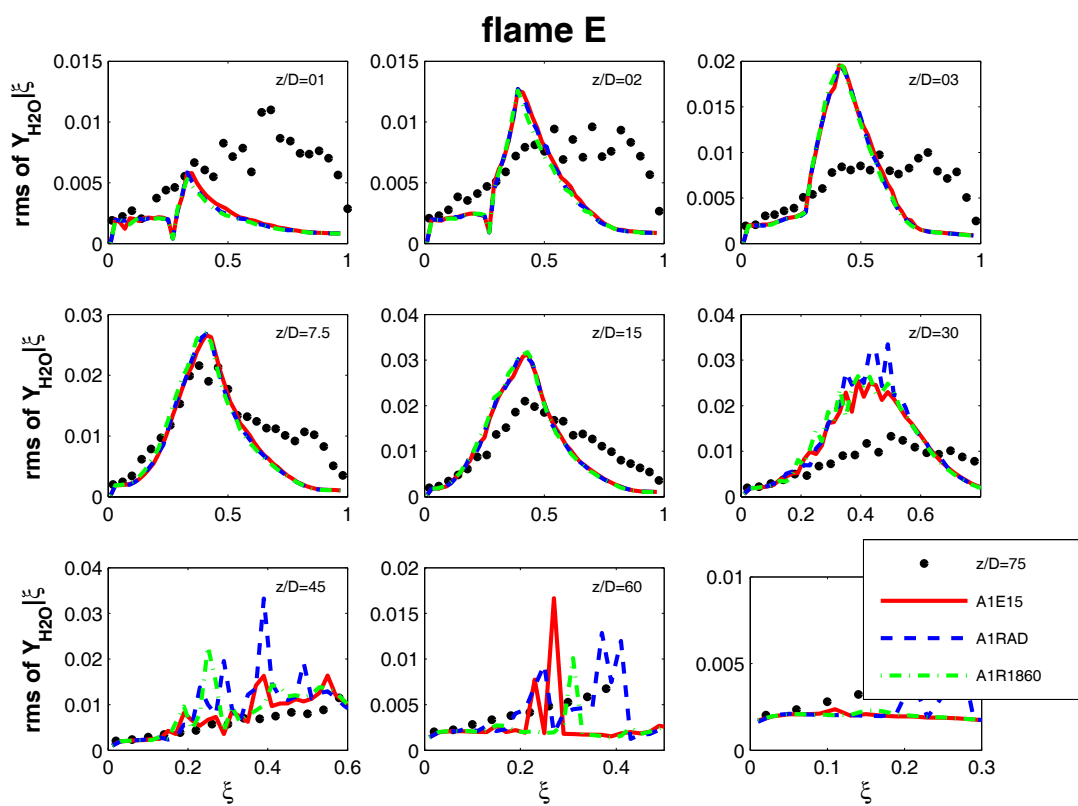
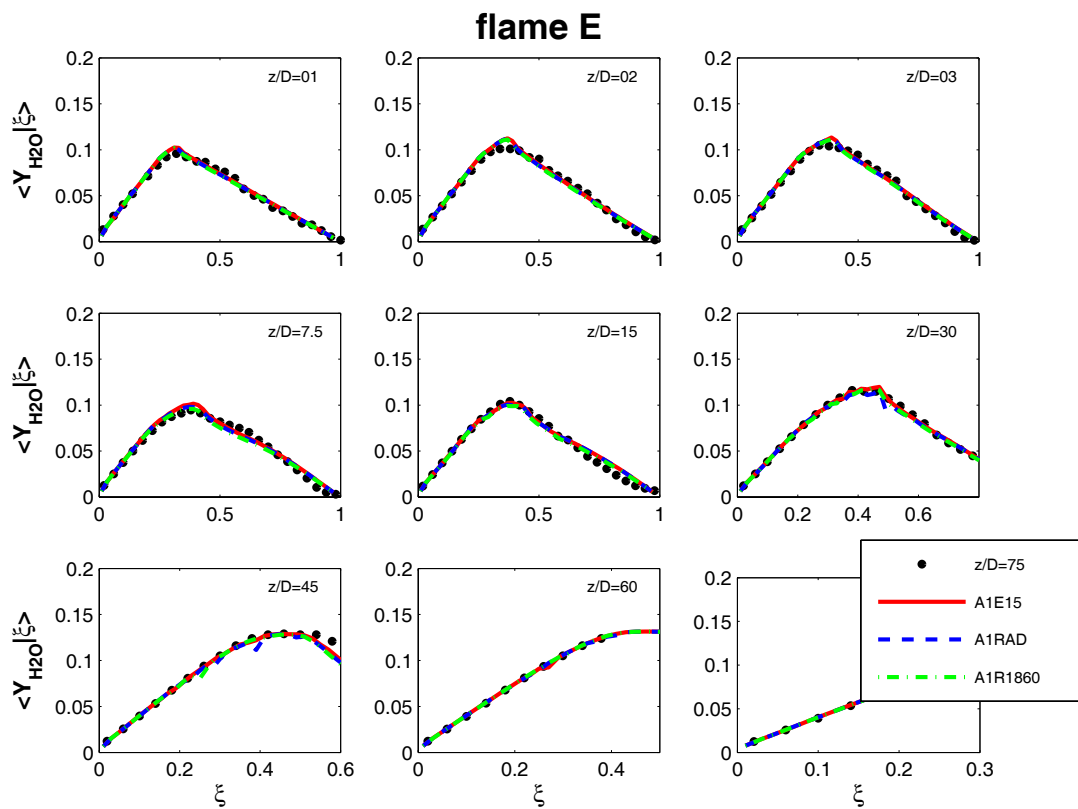


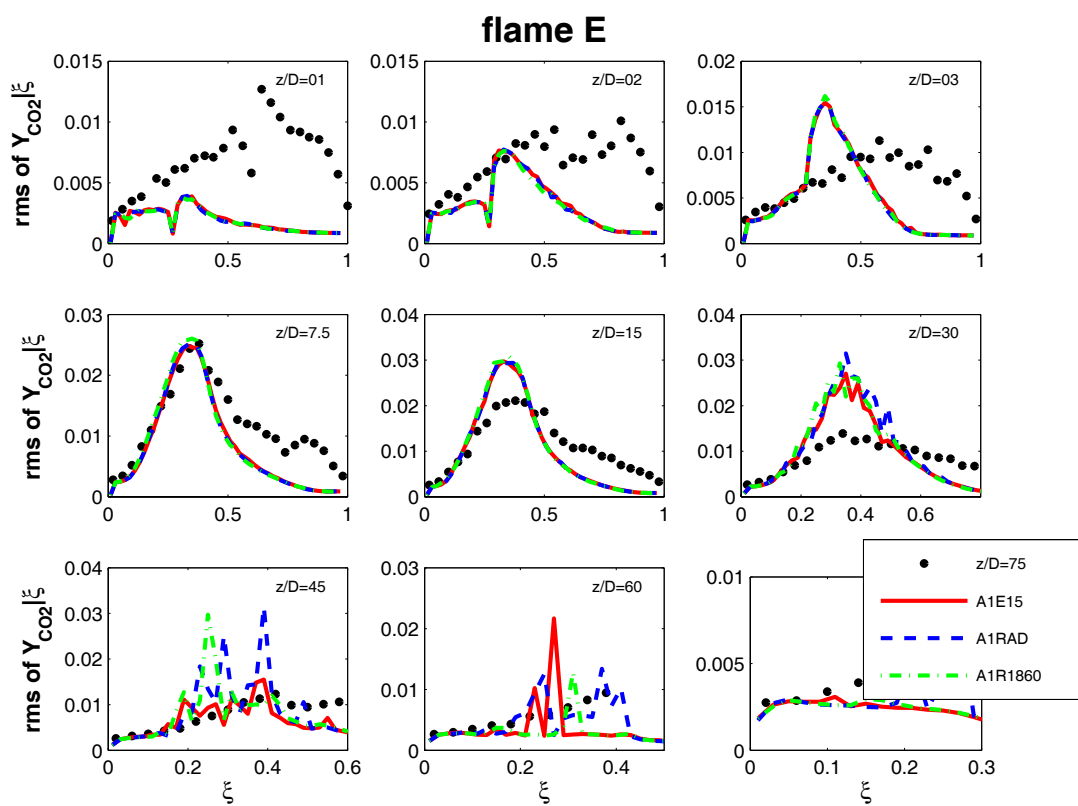
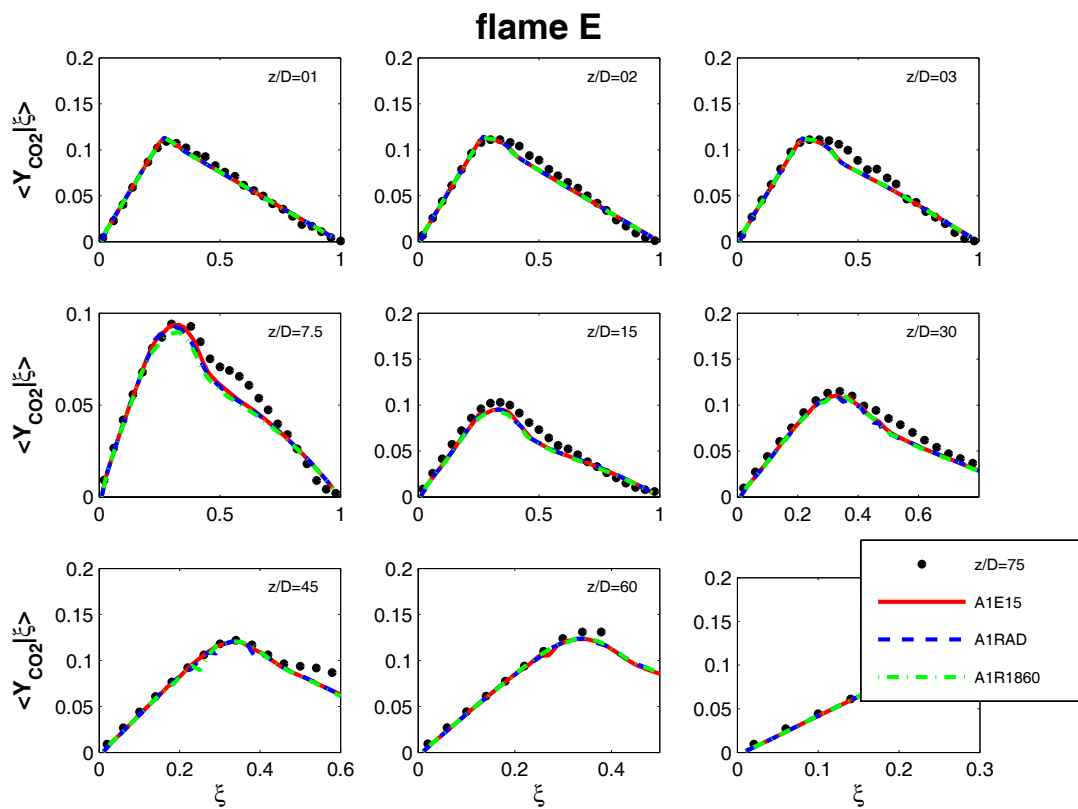
(7) SmE15 and SmRAD: extinguished

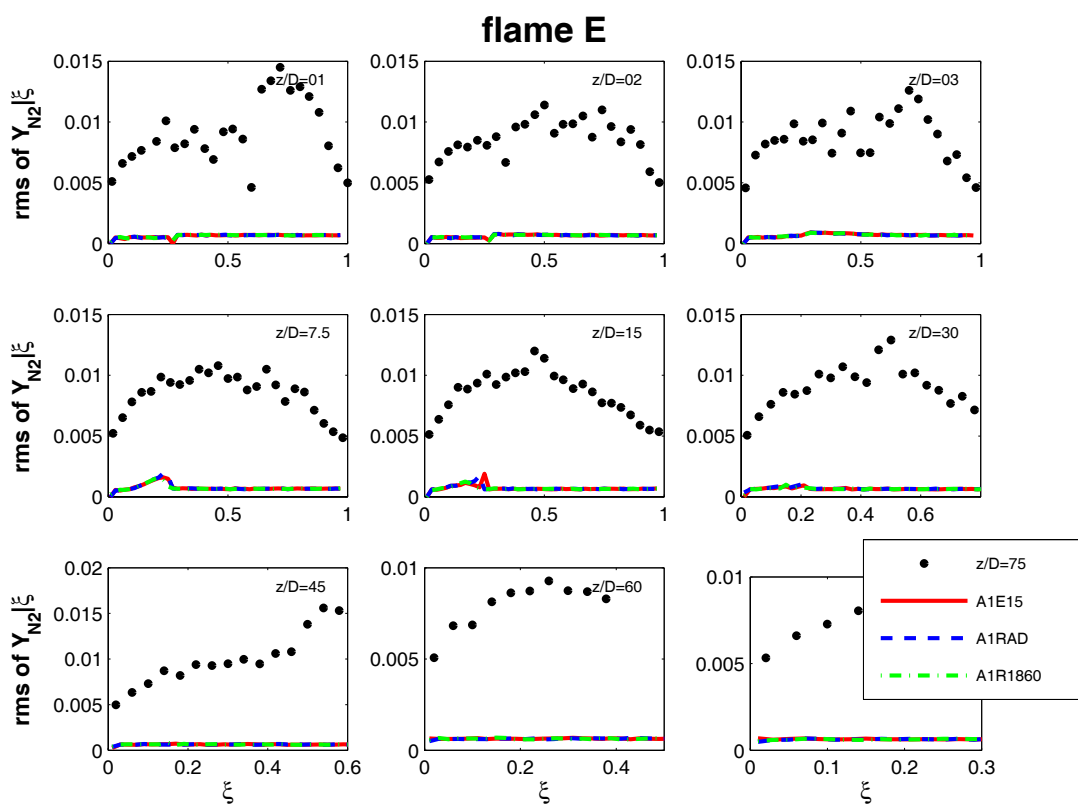
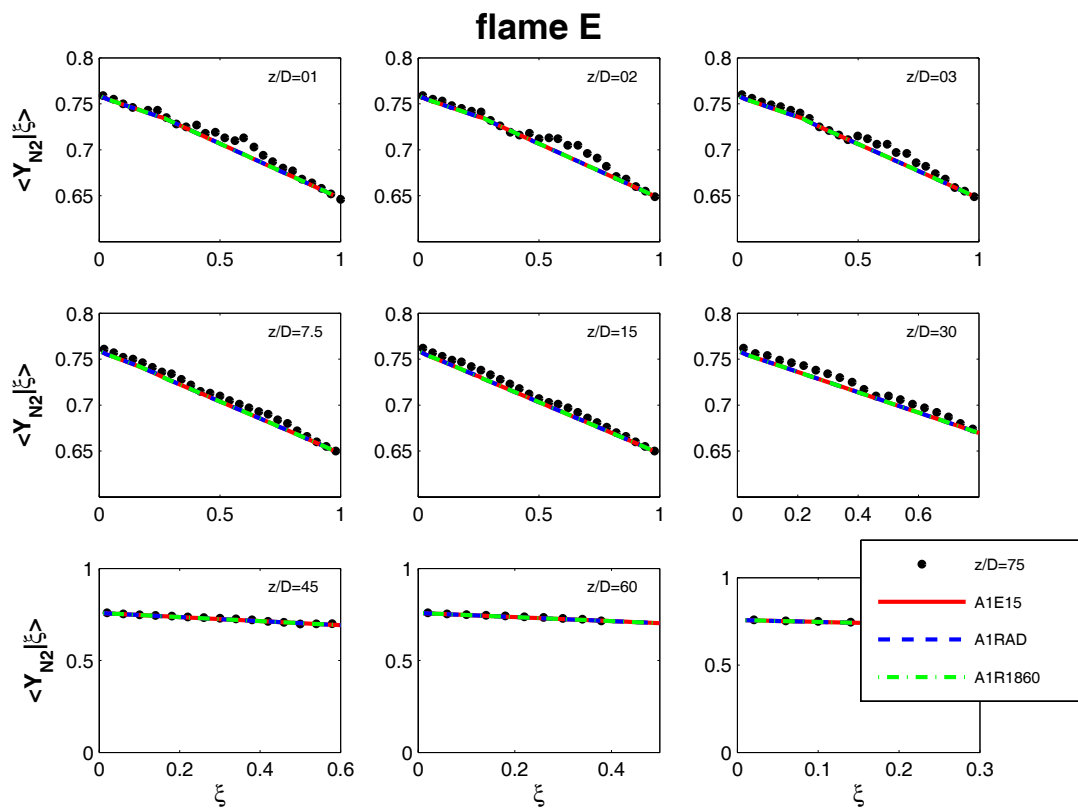
B-3 Flame E calculations

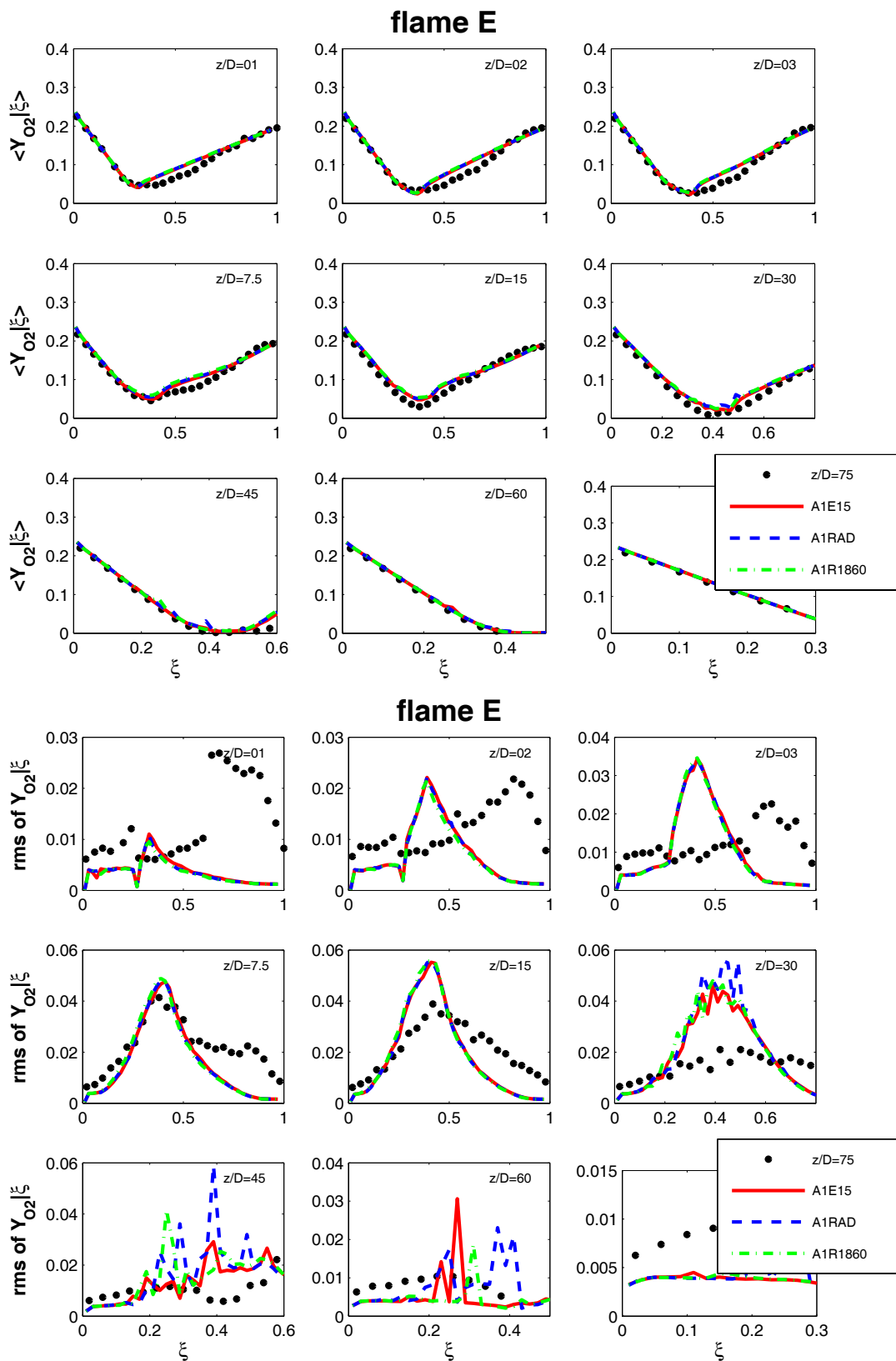
(1) A1E15, A1RAD and A1R1860

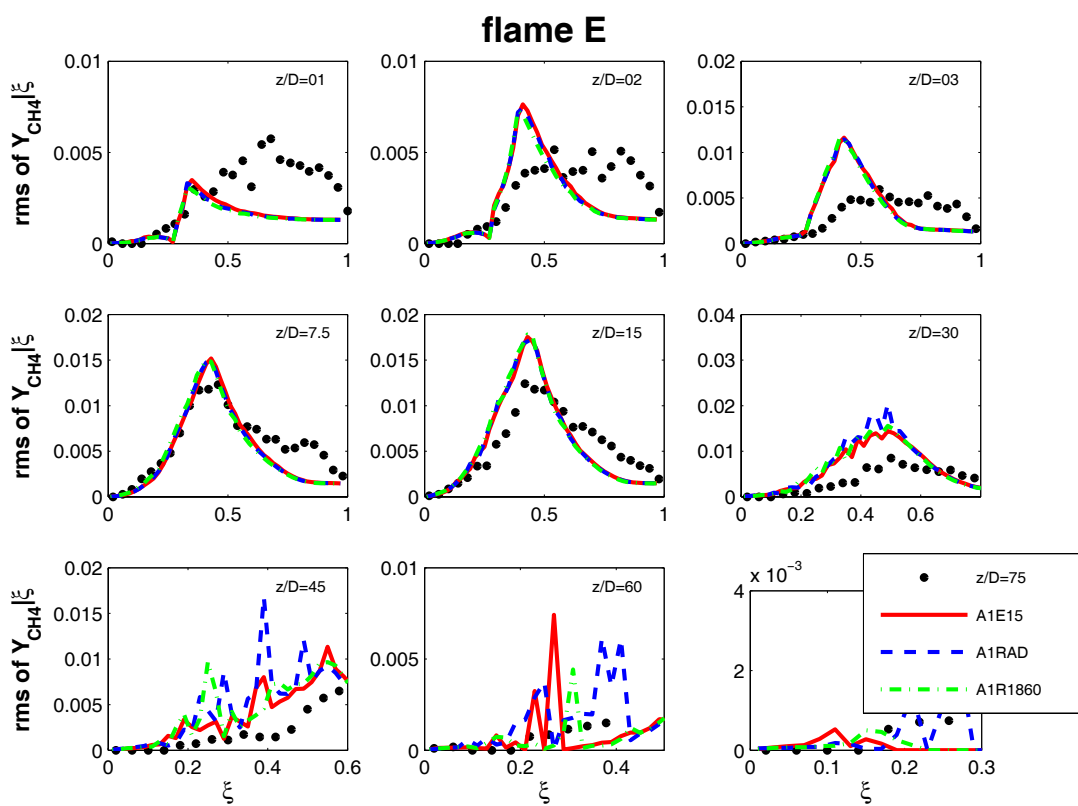
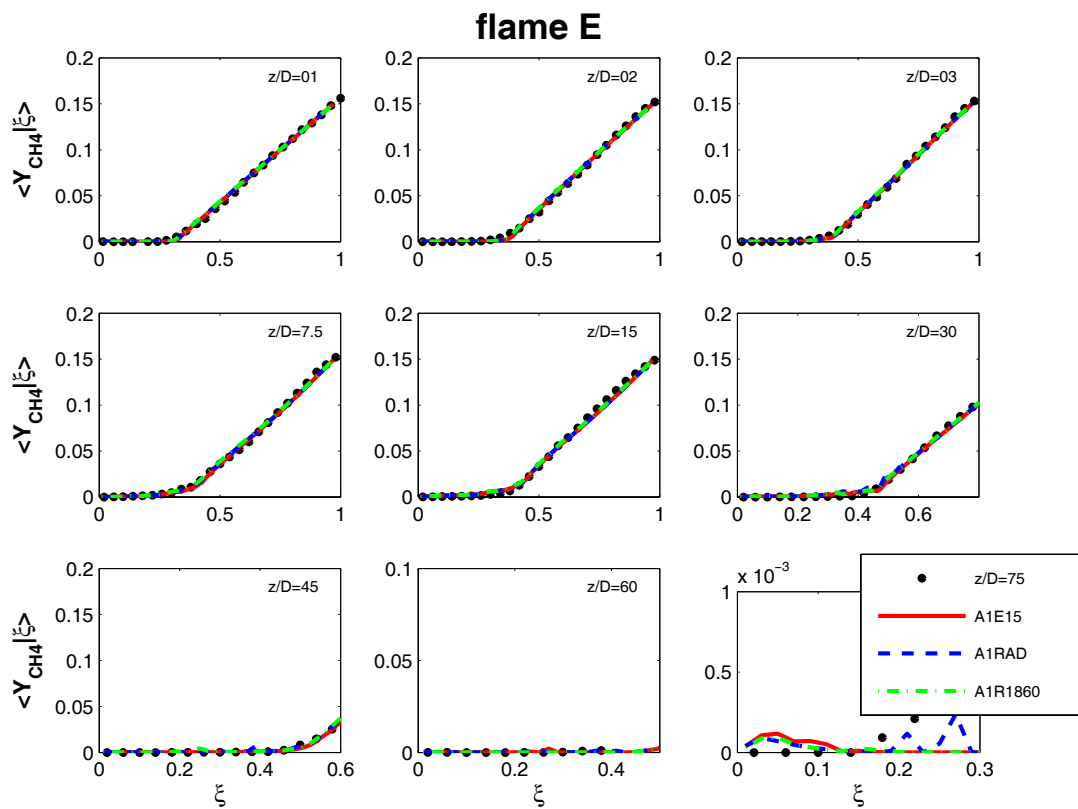


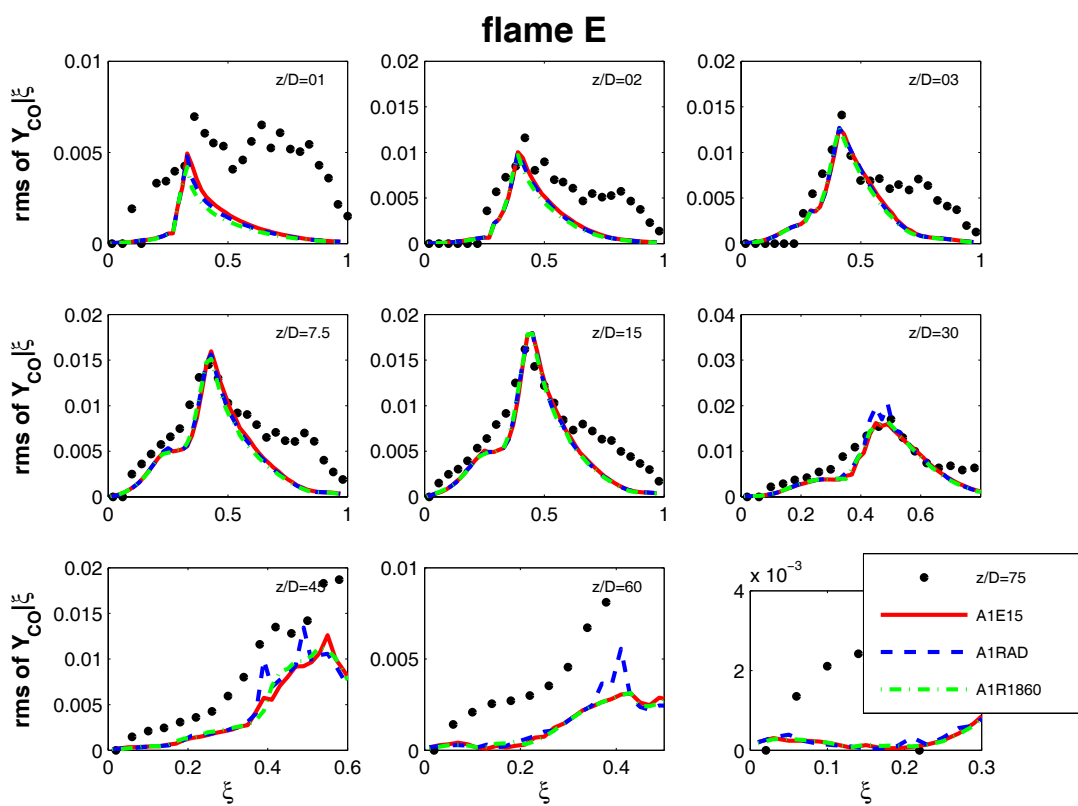
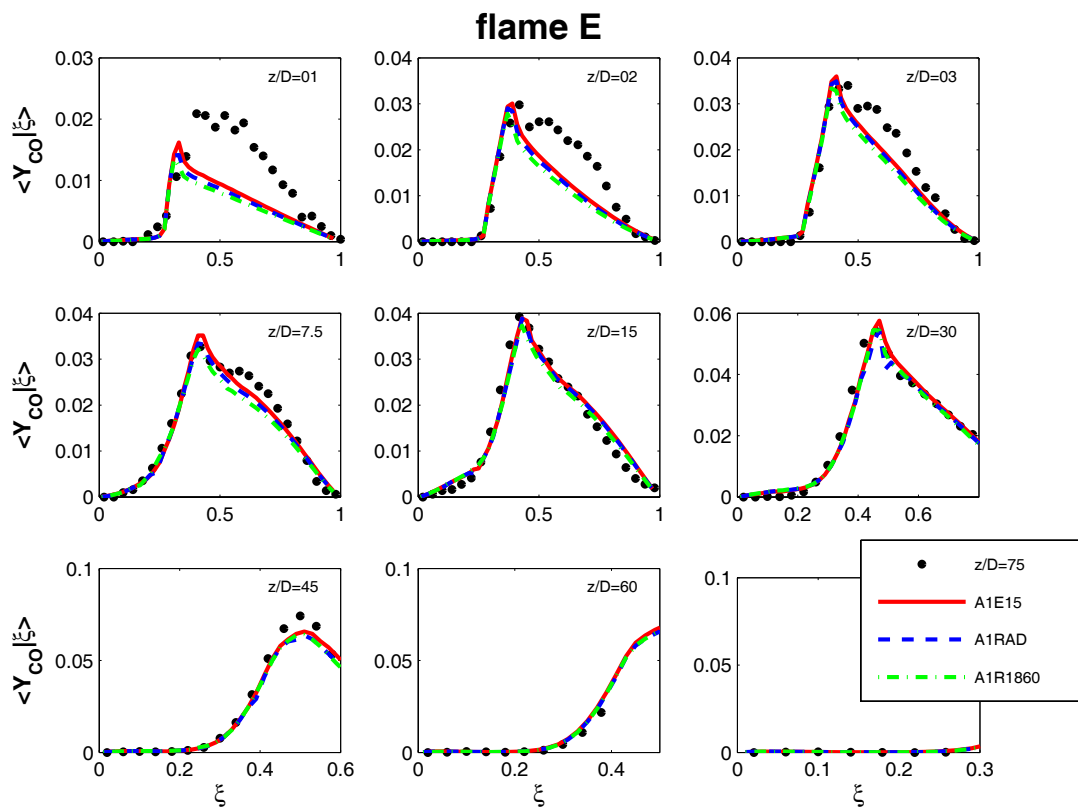


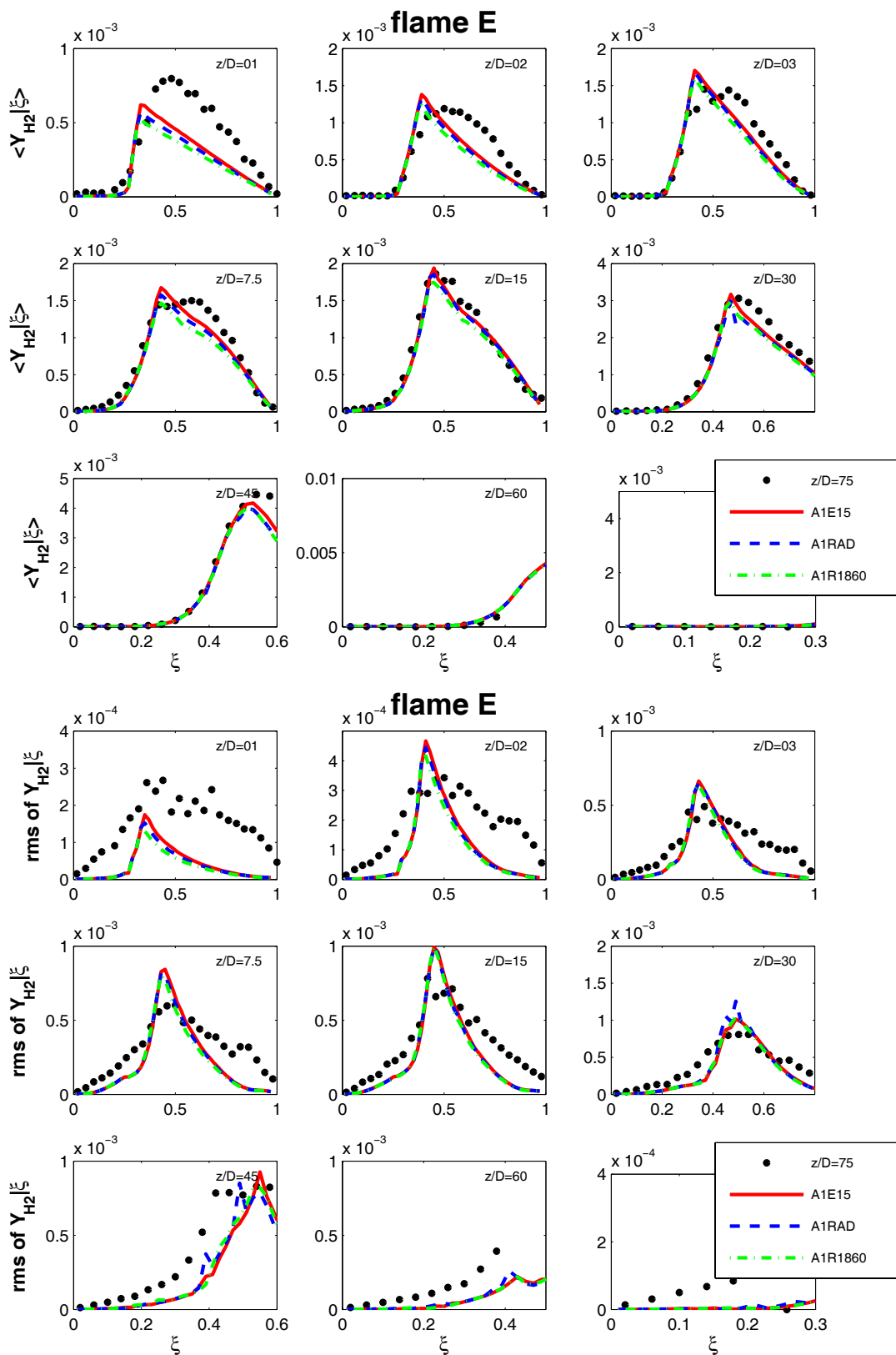


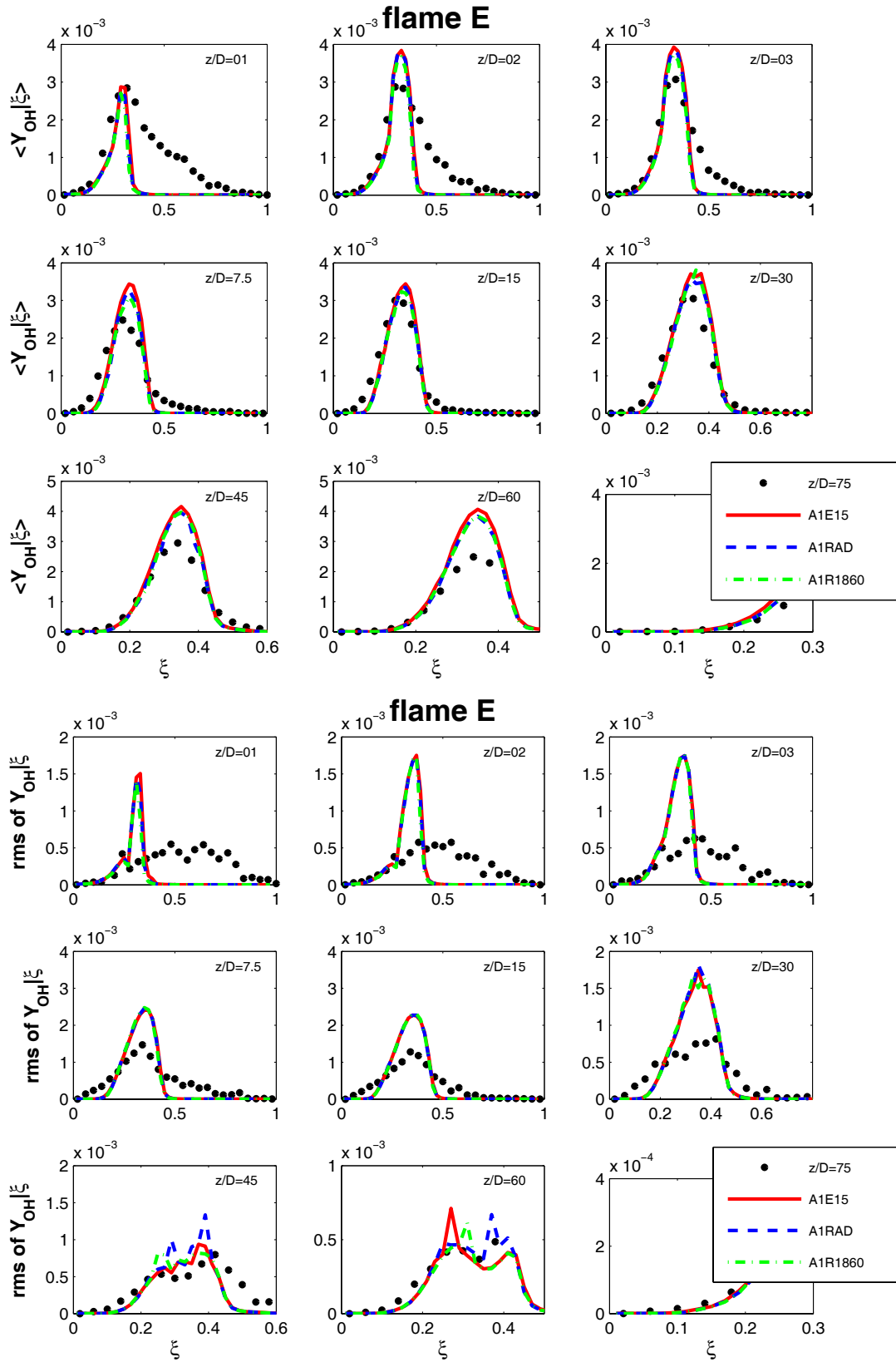




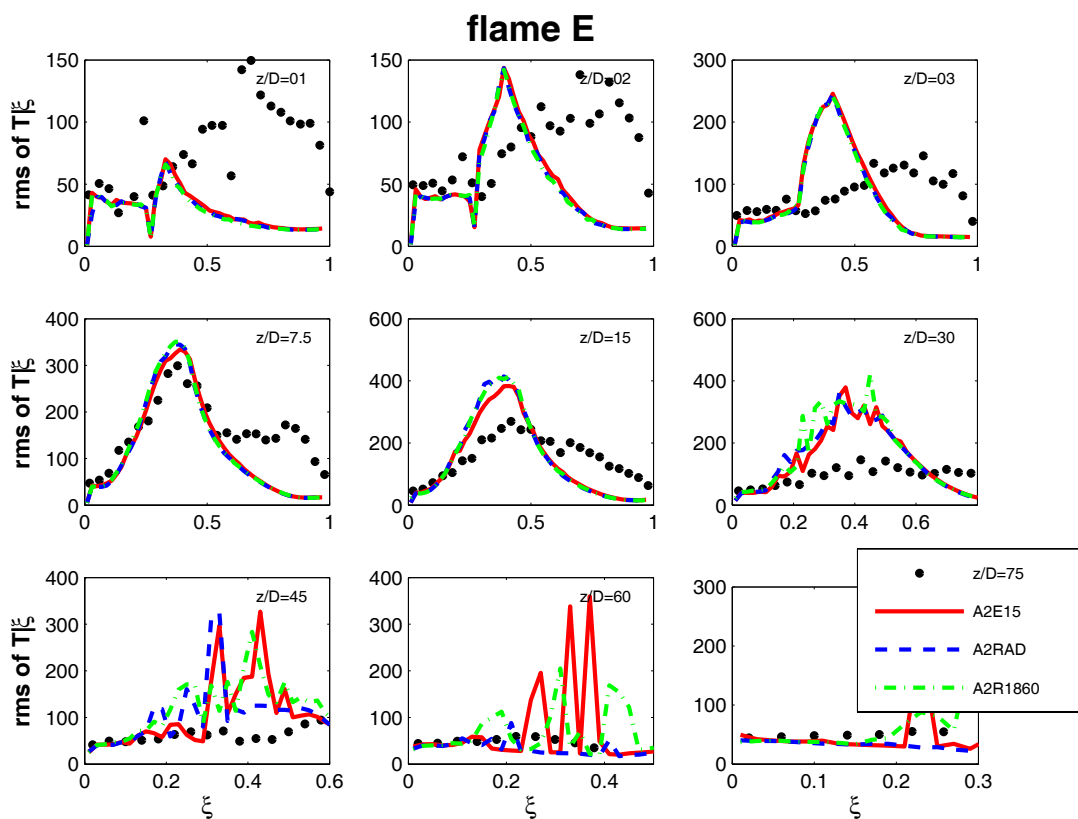
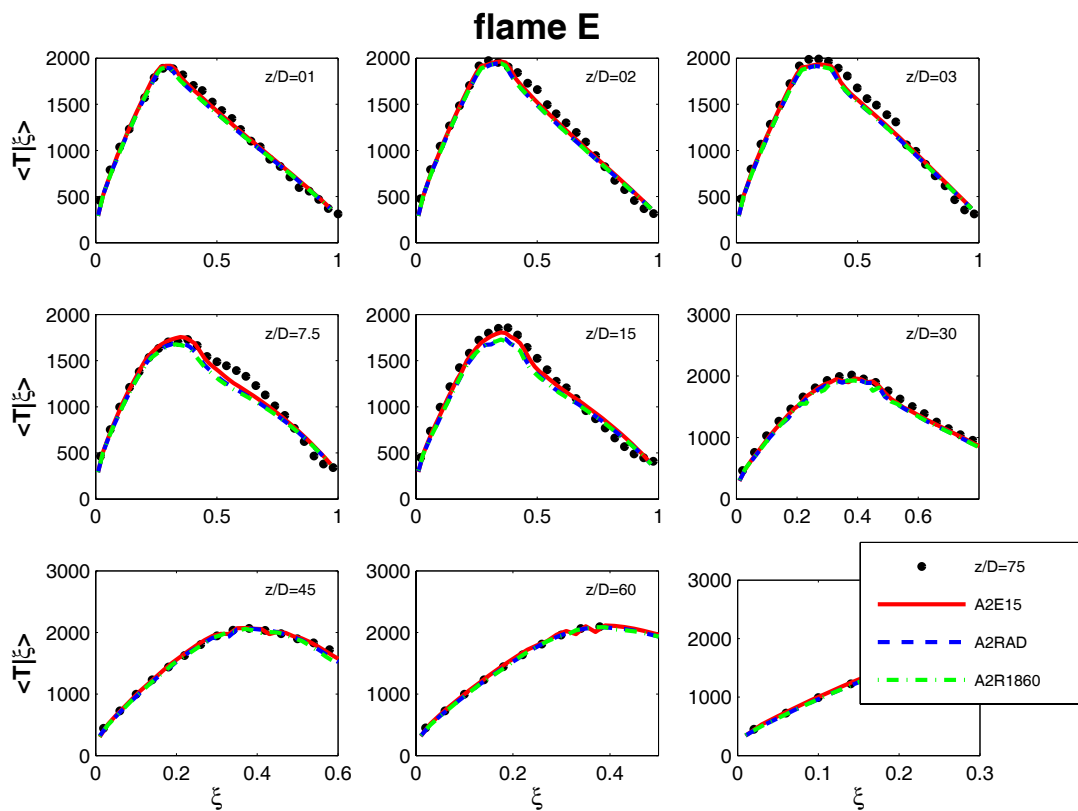


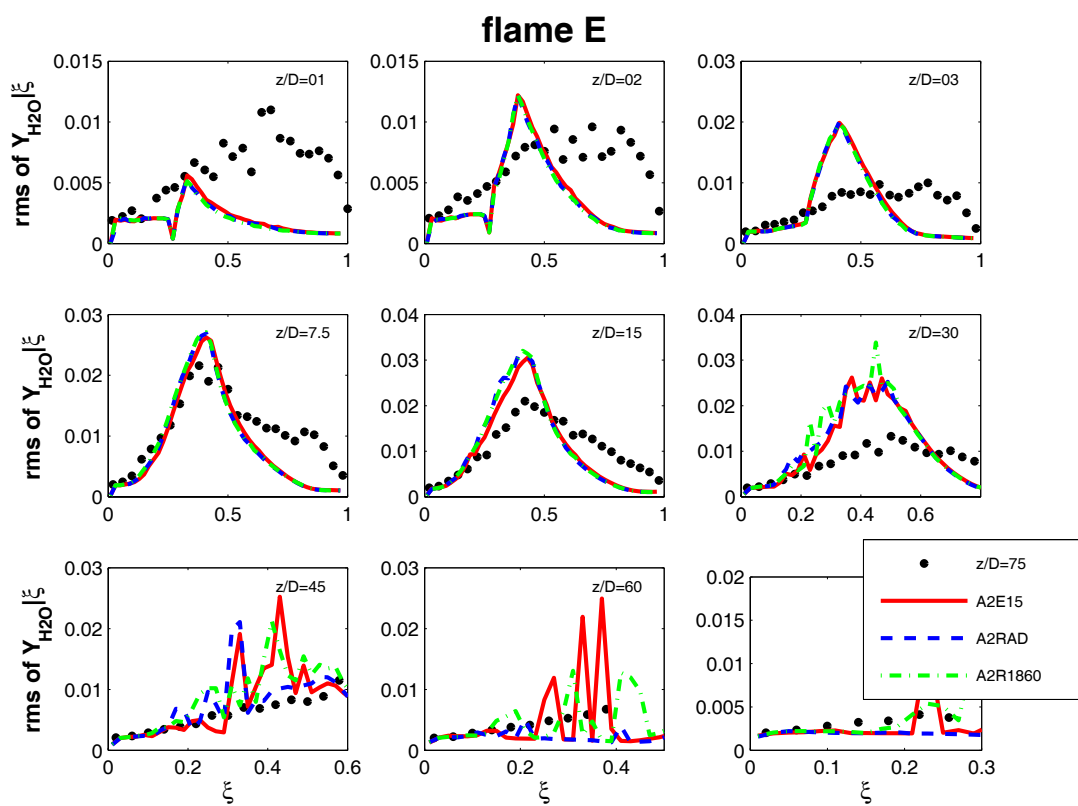
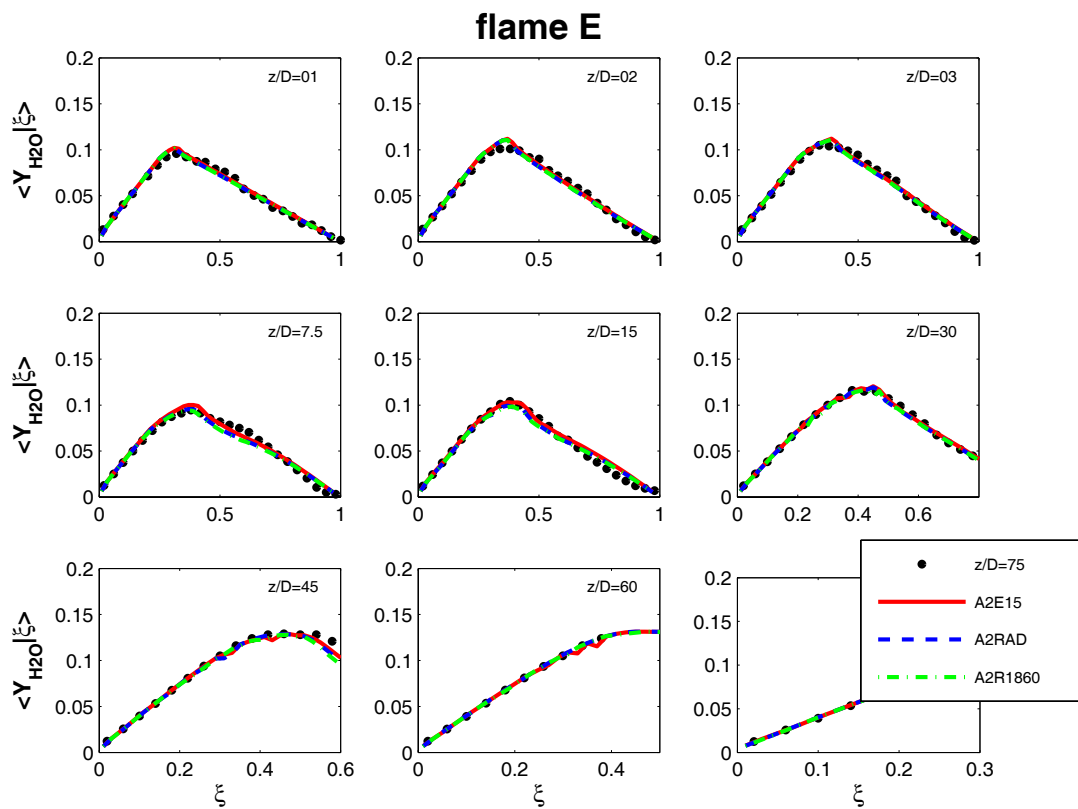


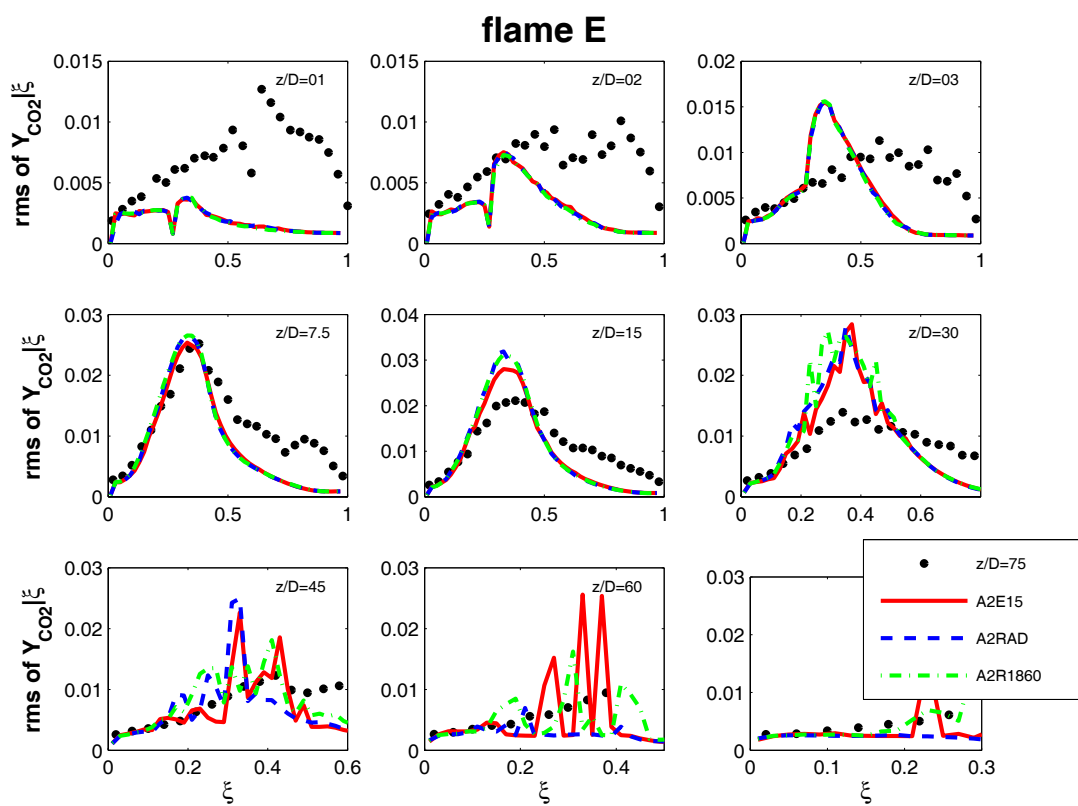
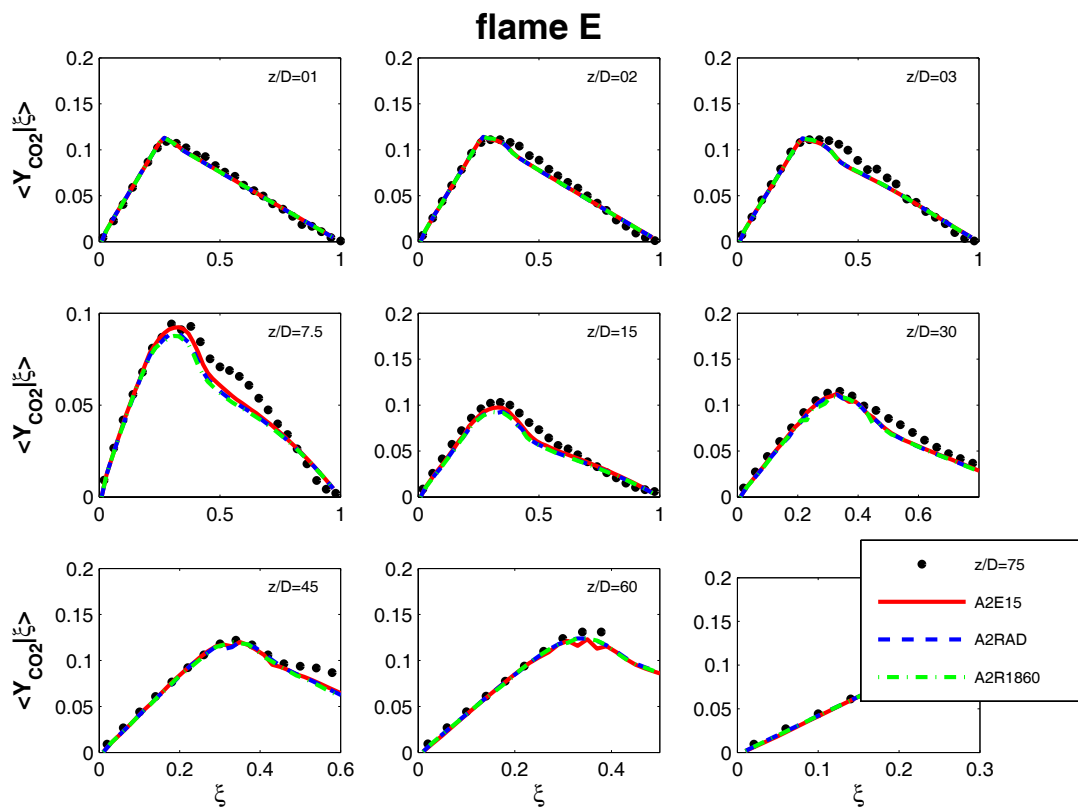


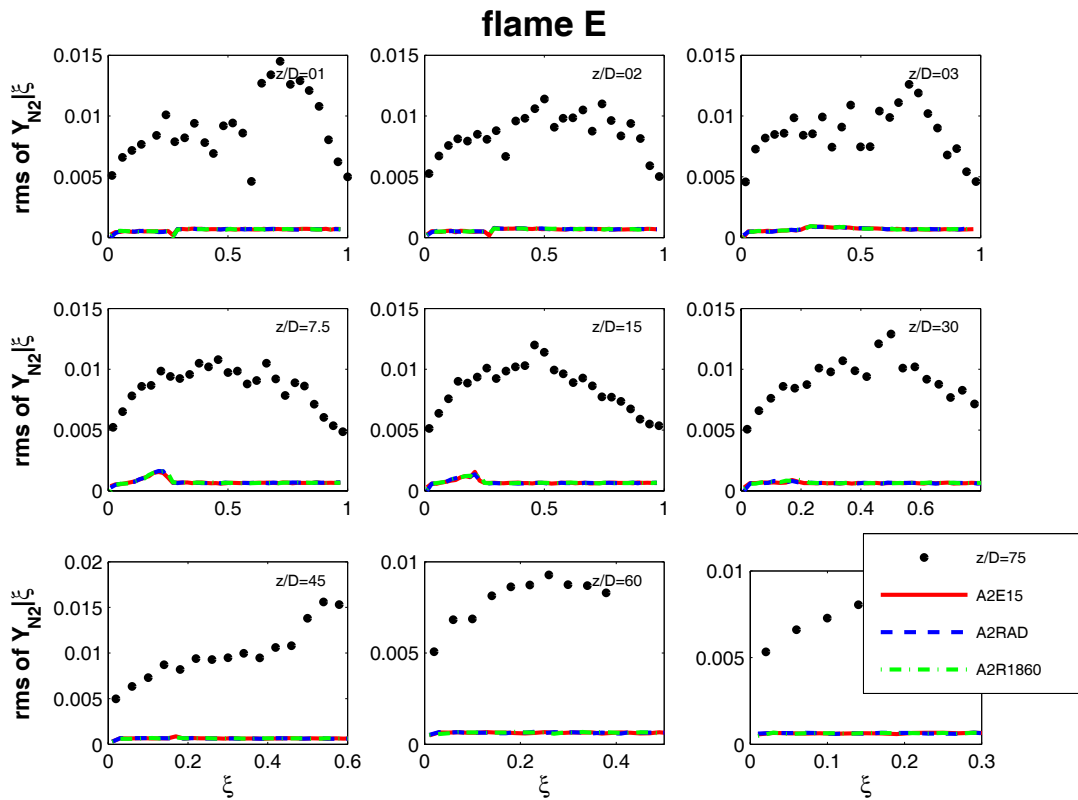
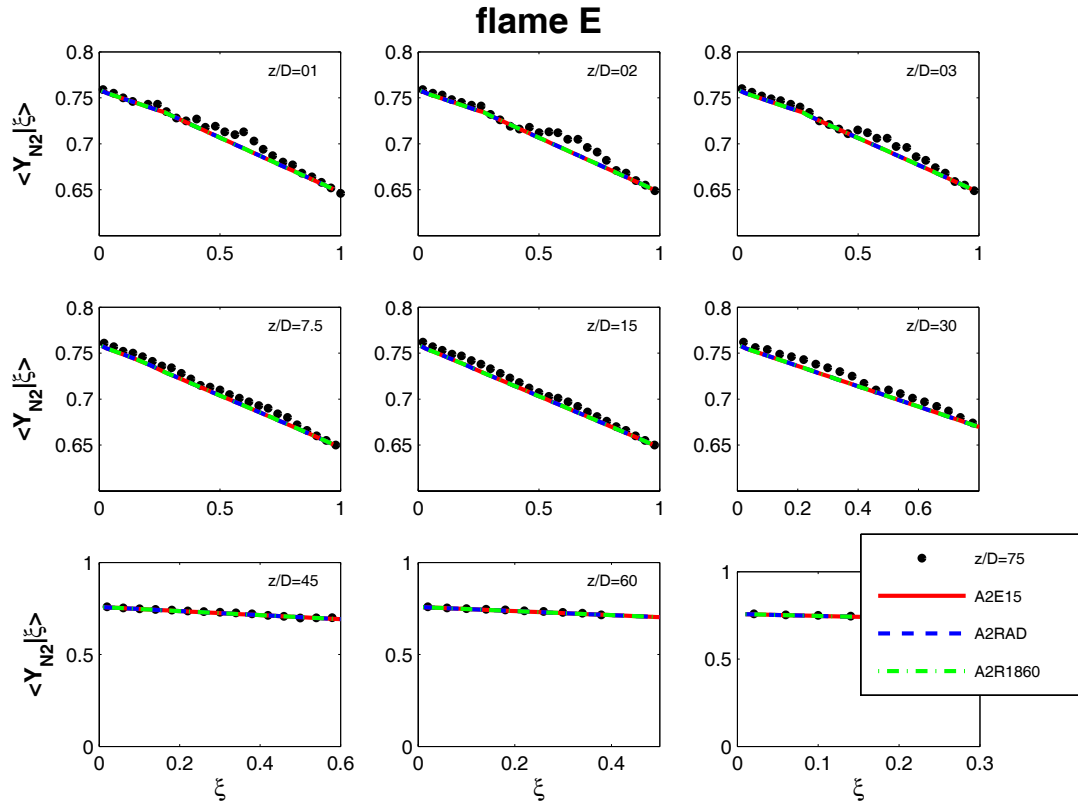


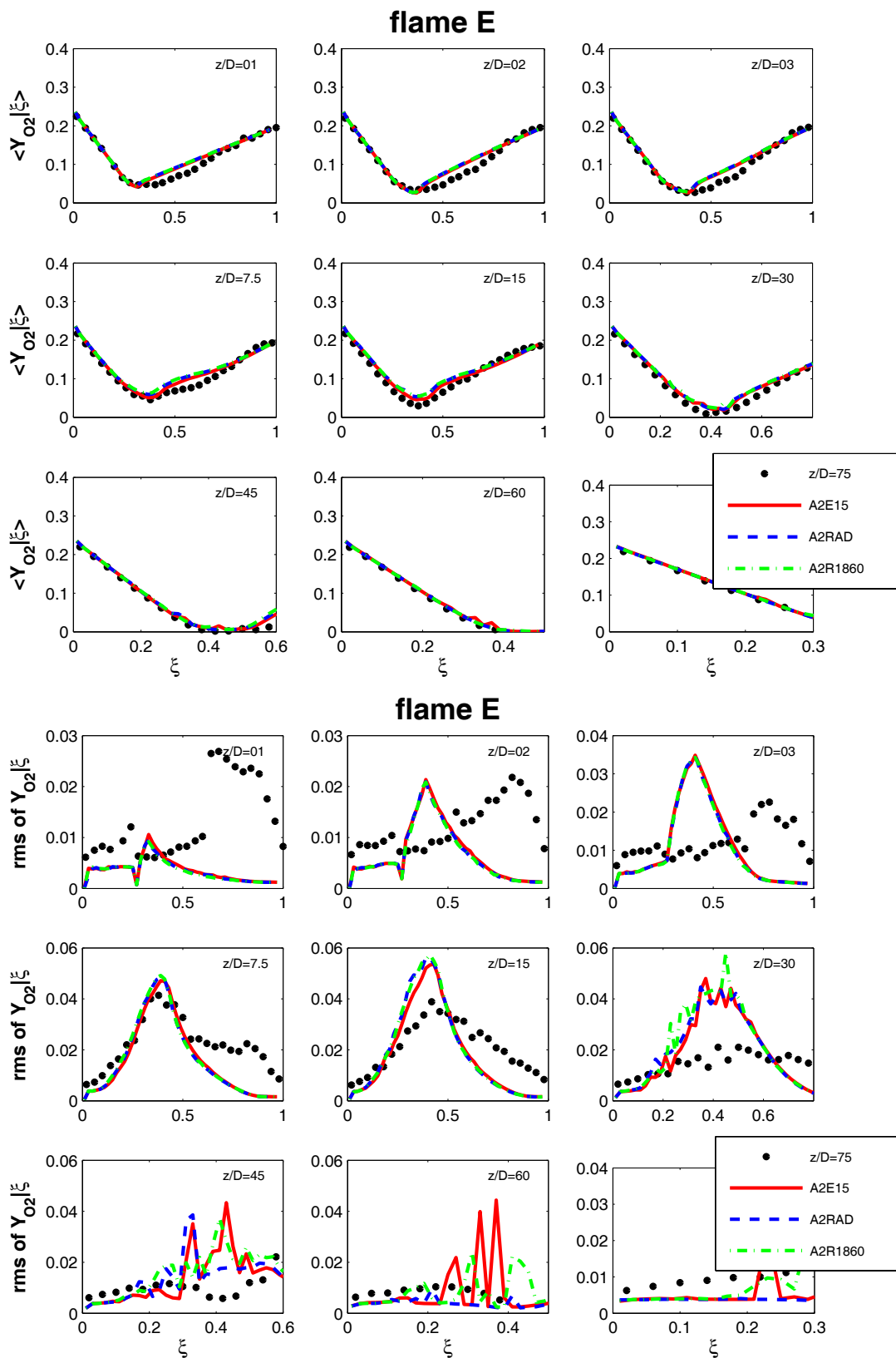
(2) A2E15, A2RAD, and A2R1860

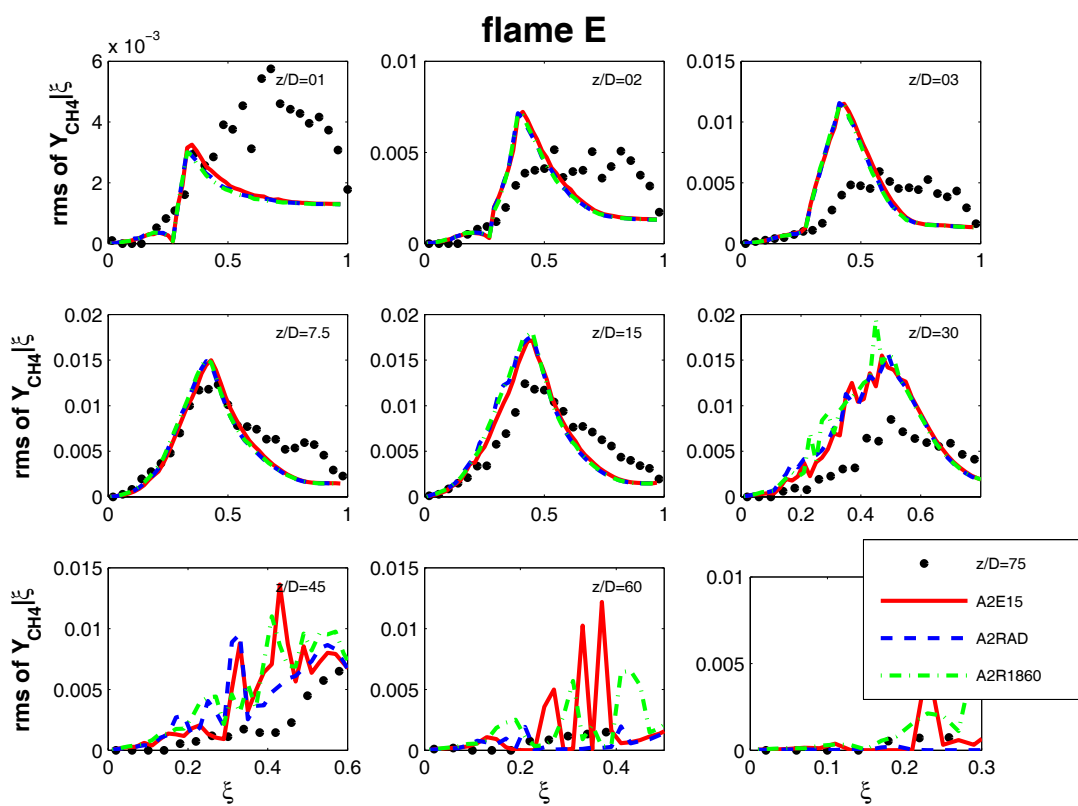
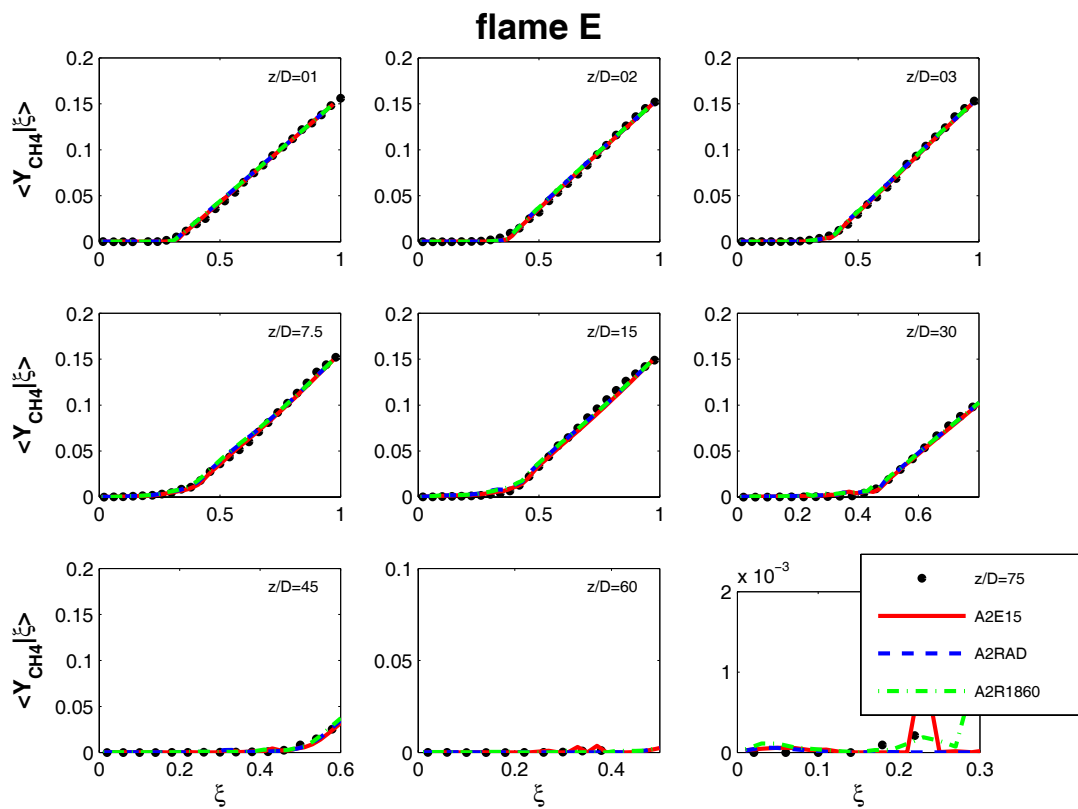


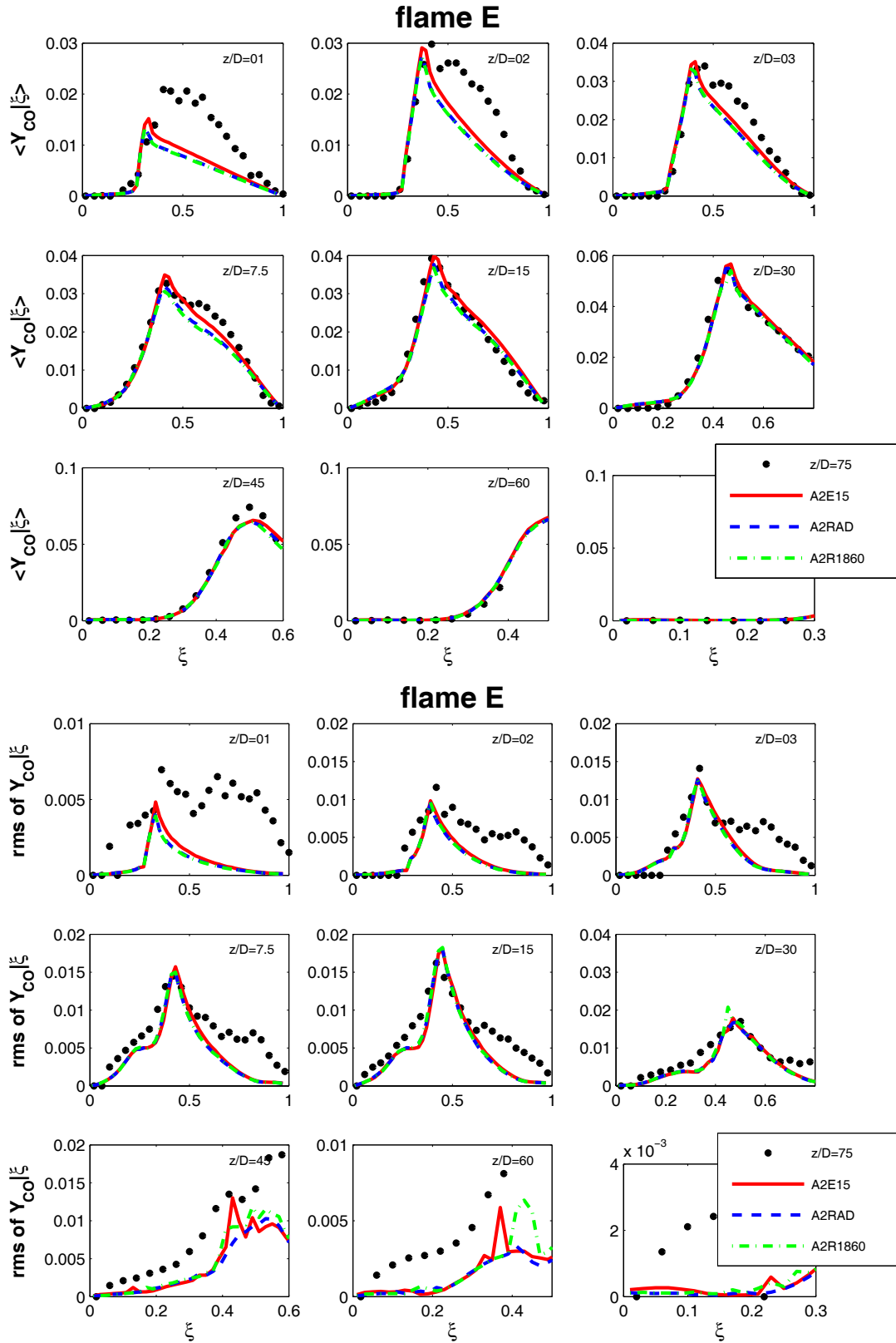


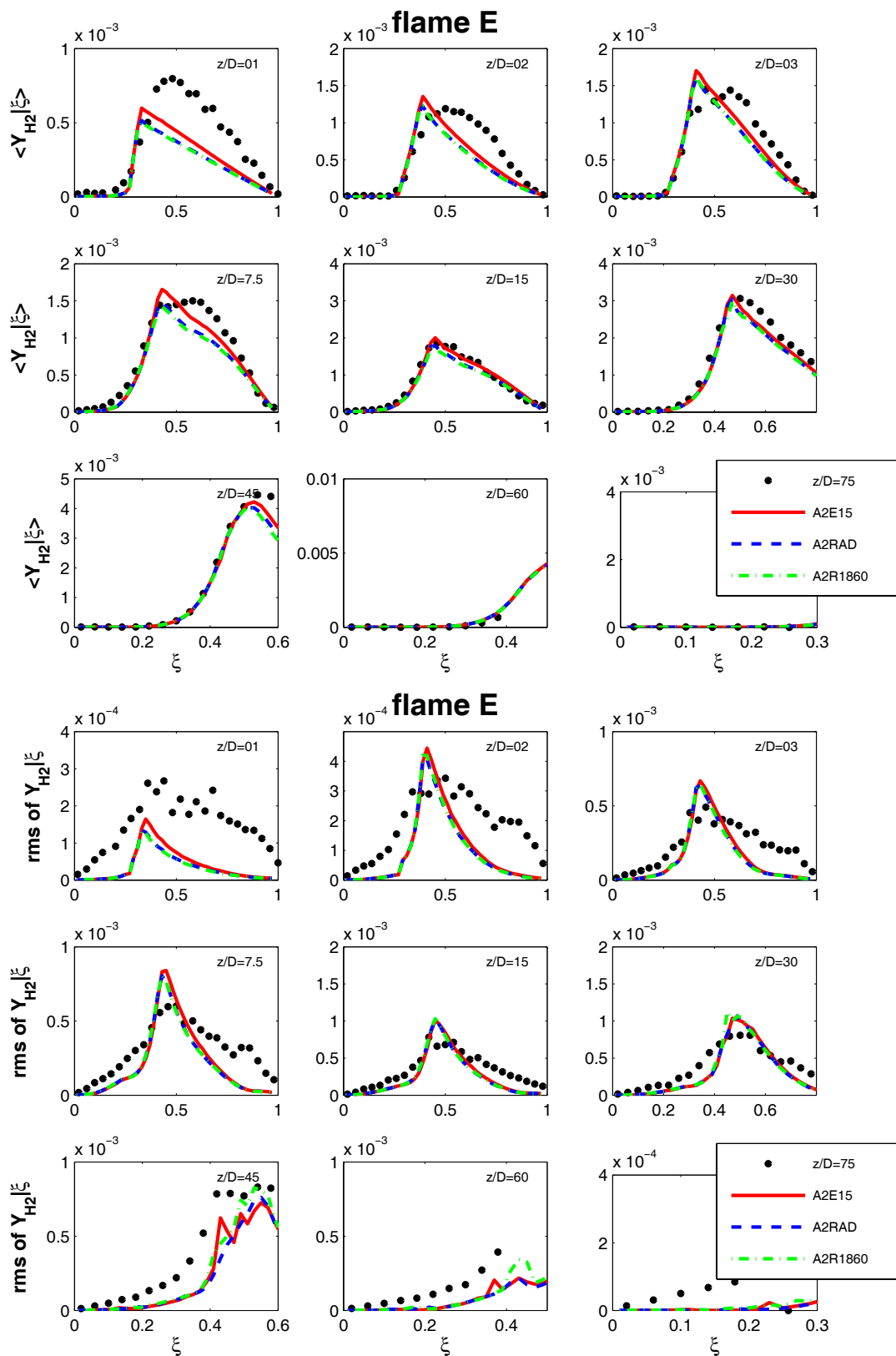


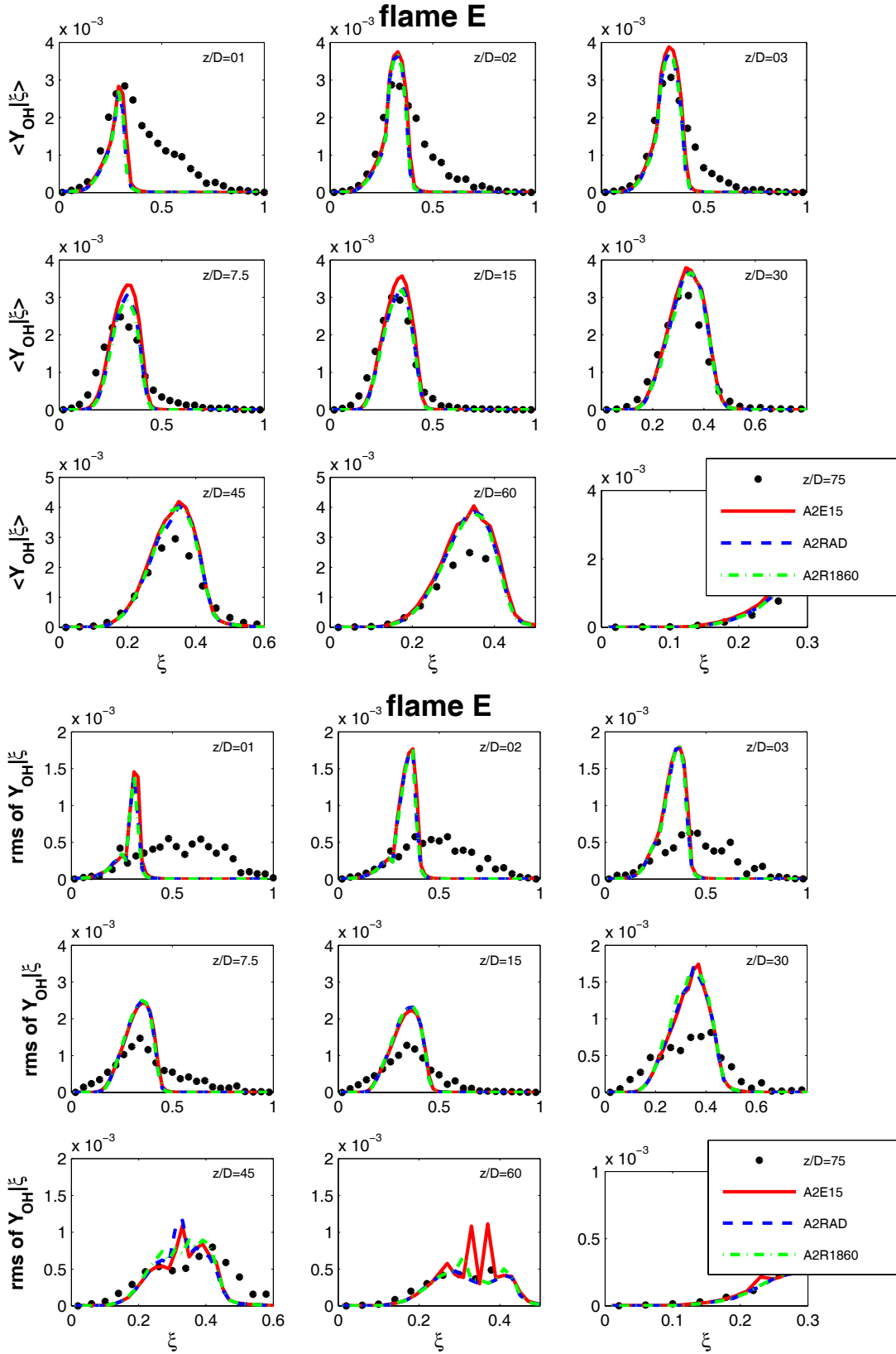


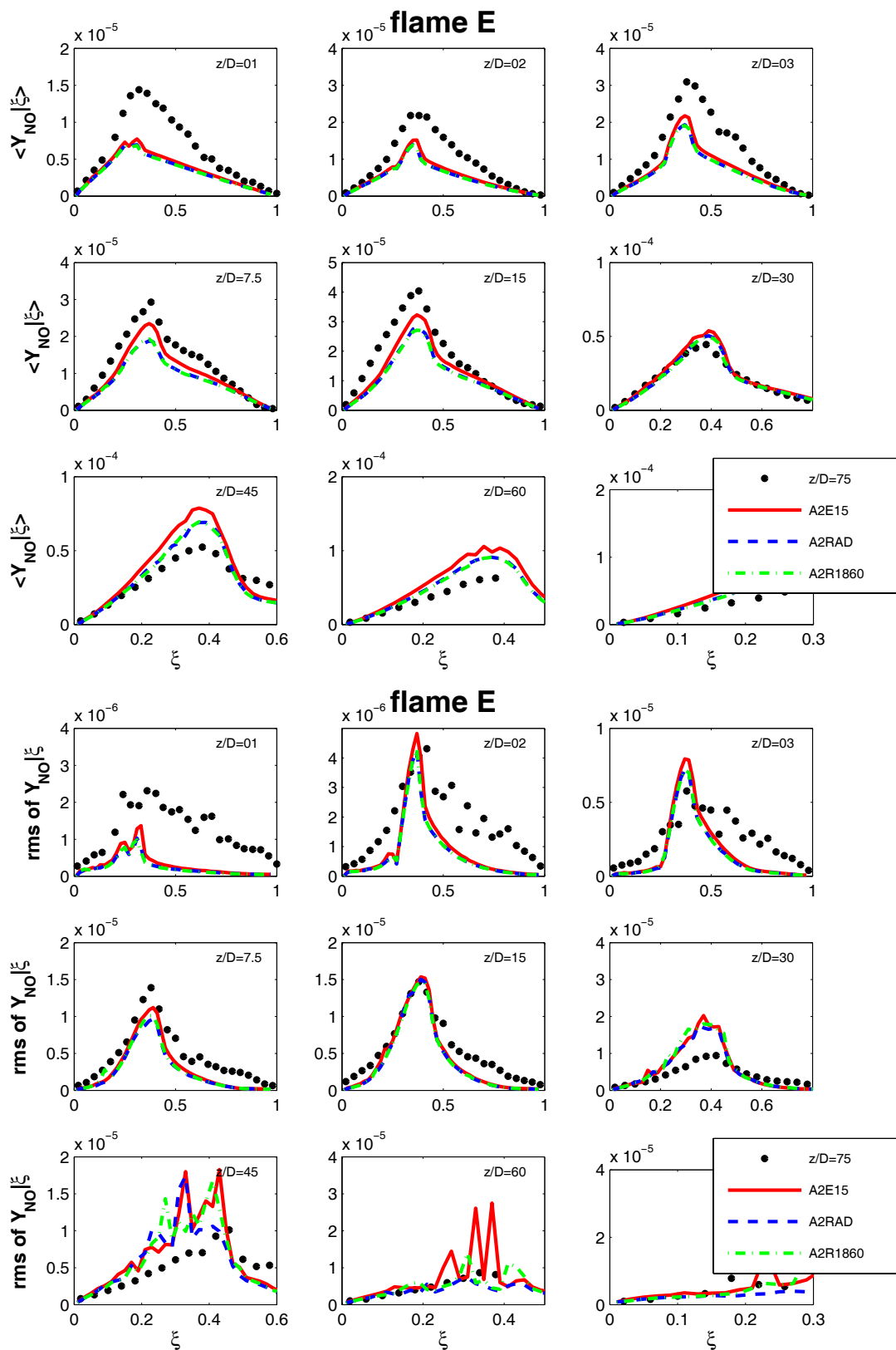




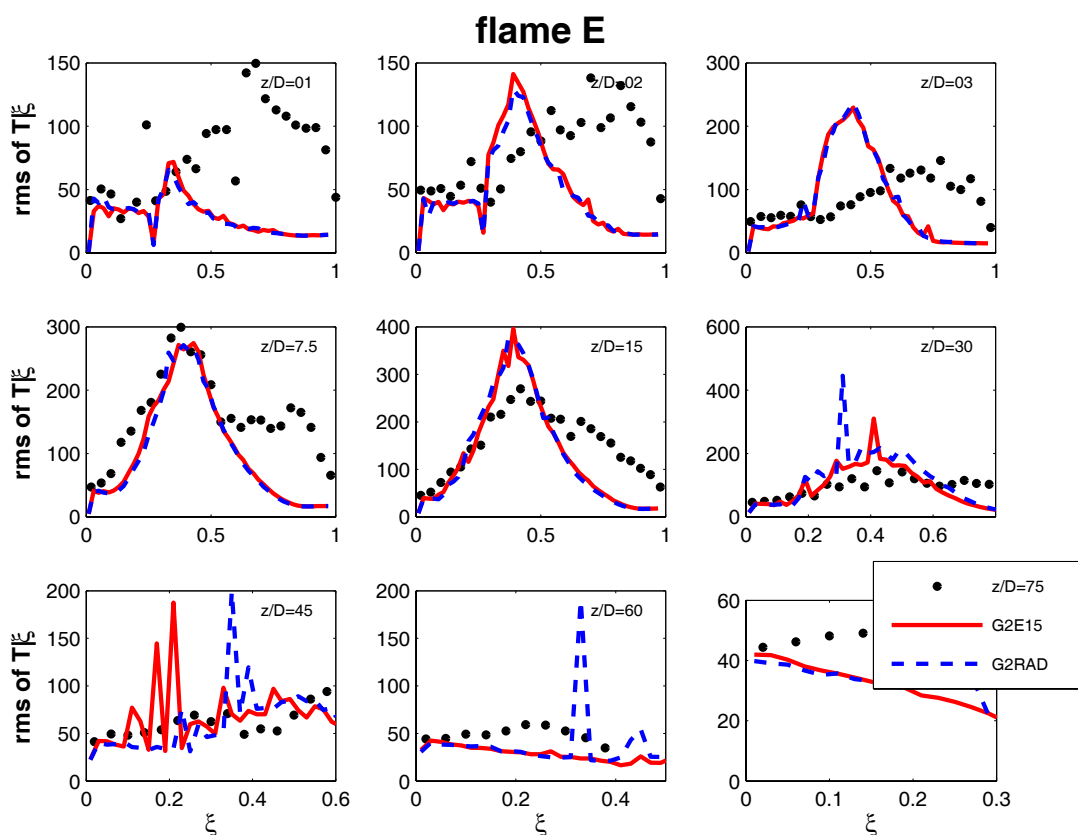
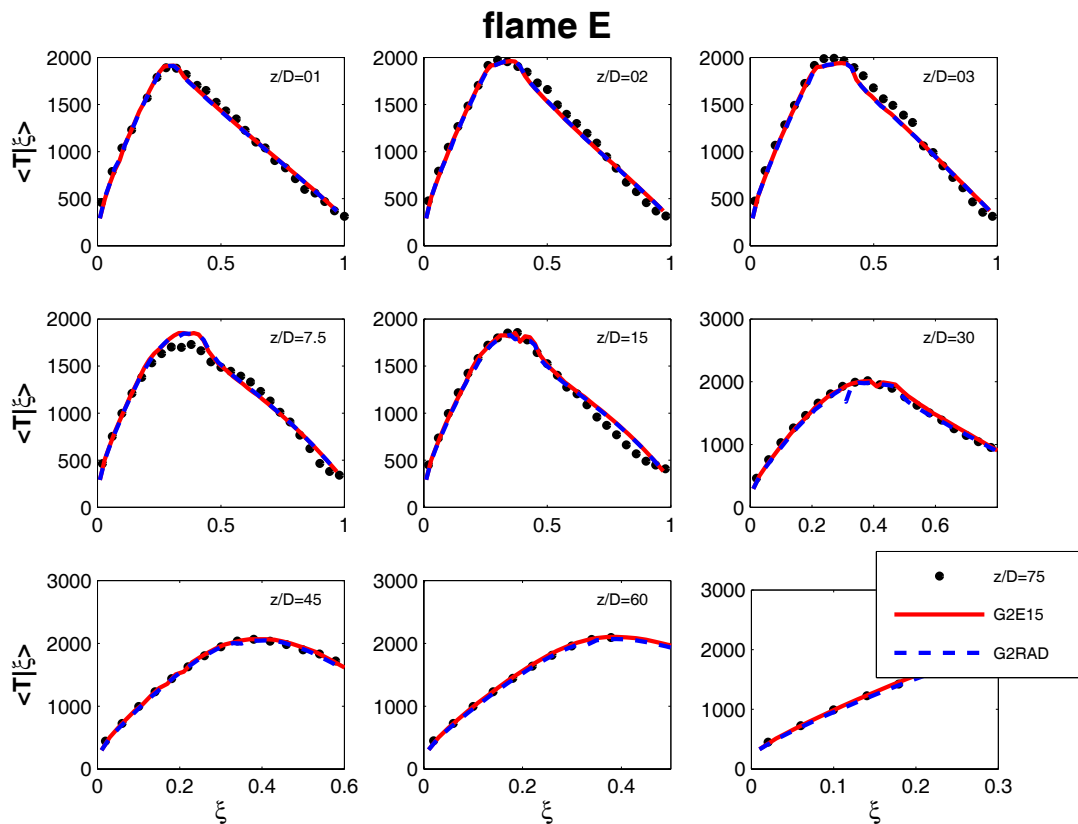


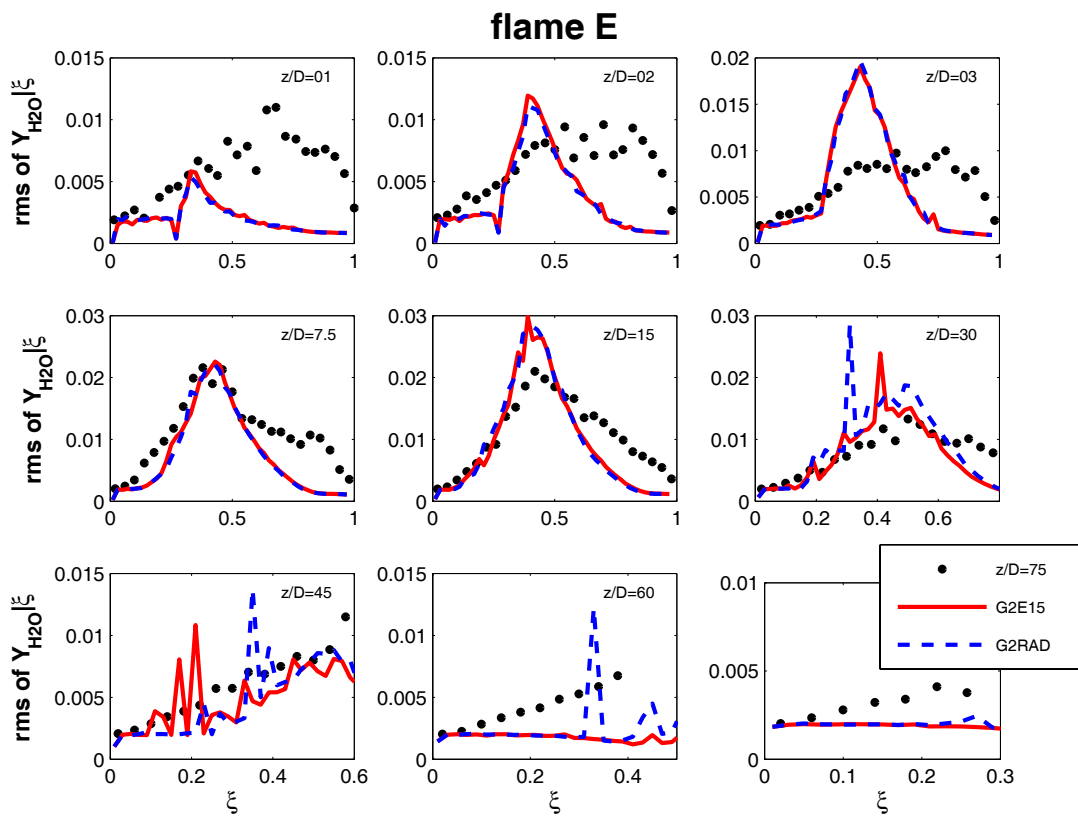
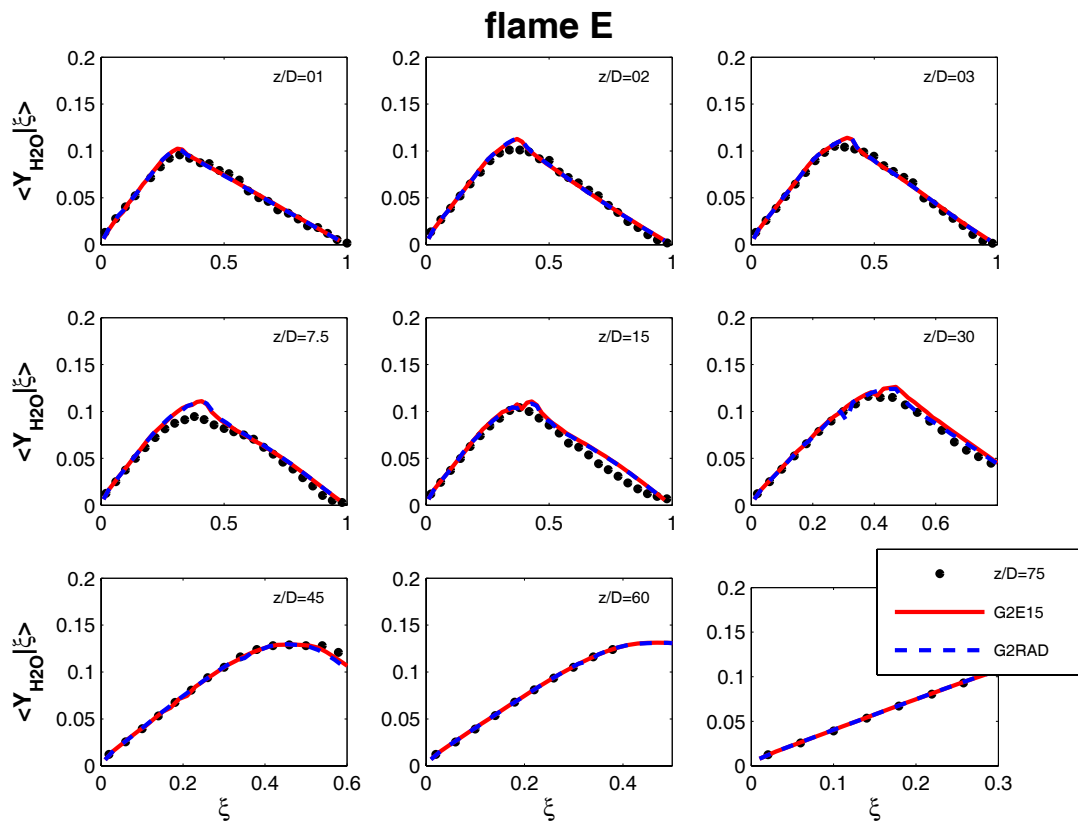


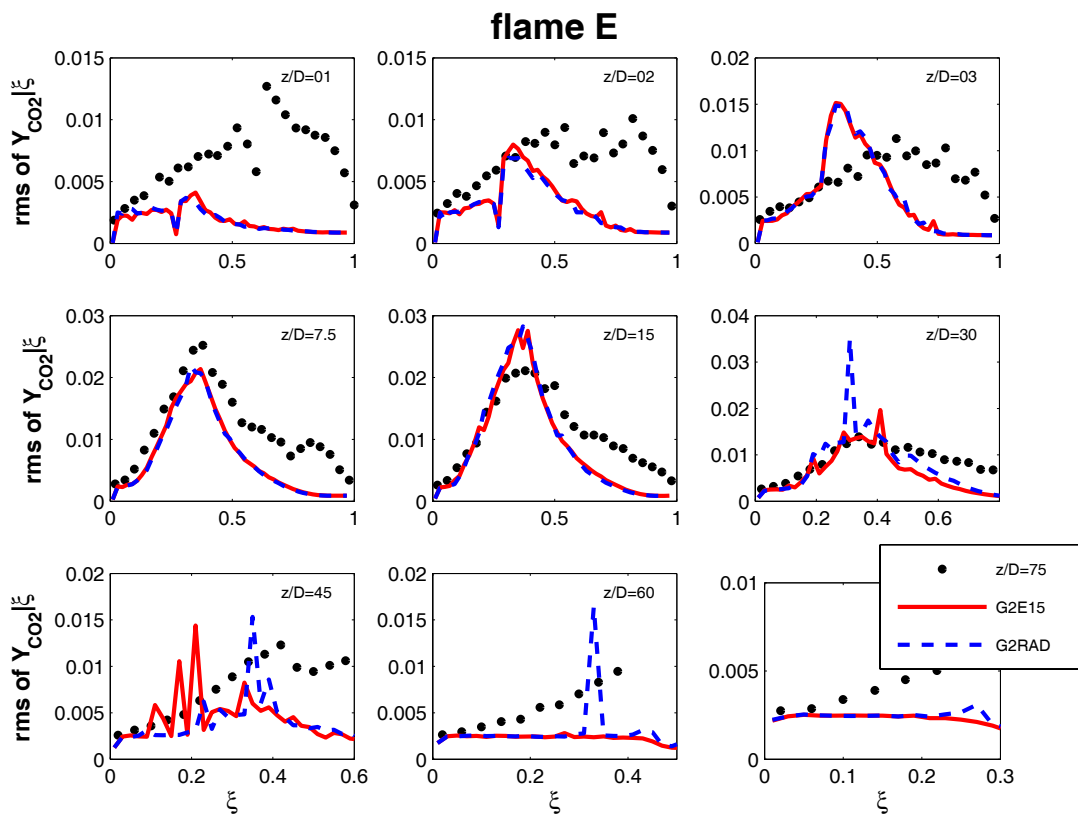
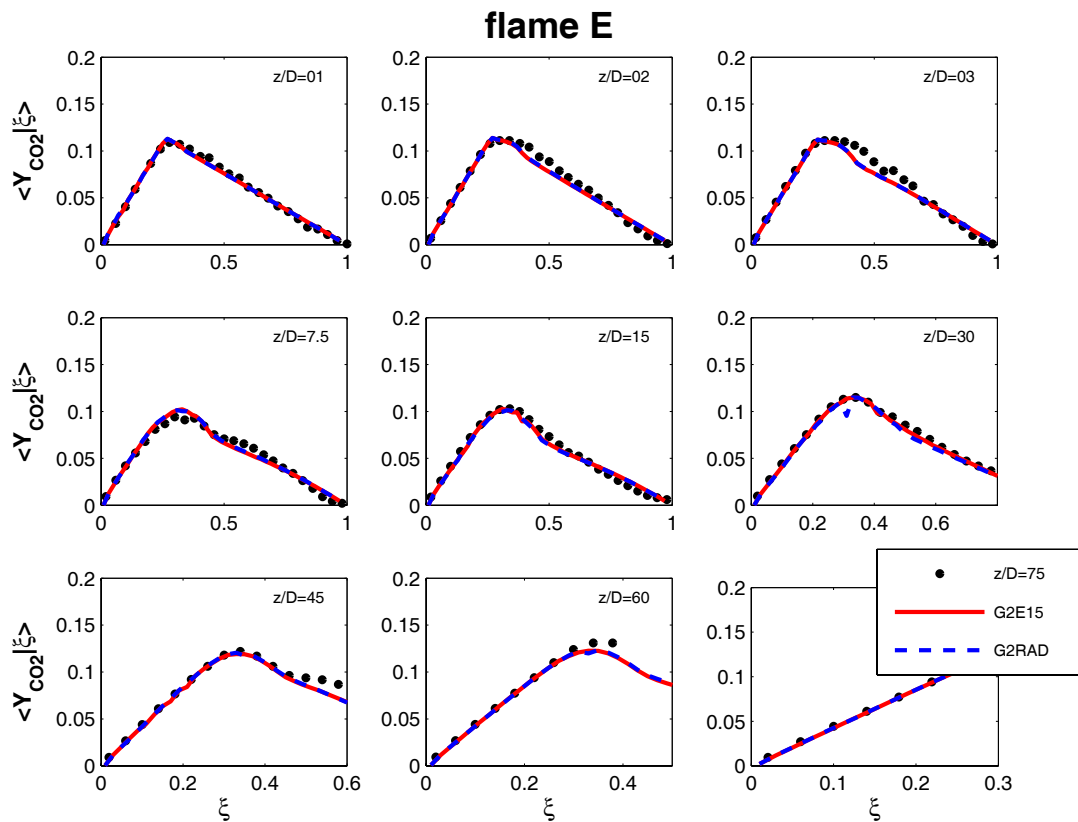


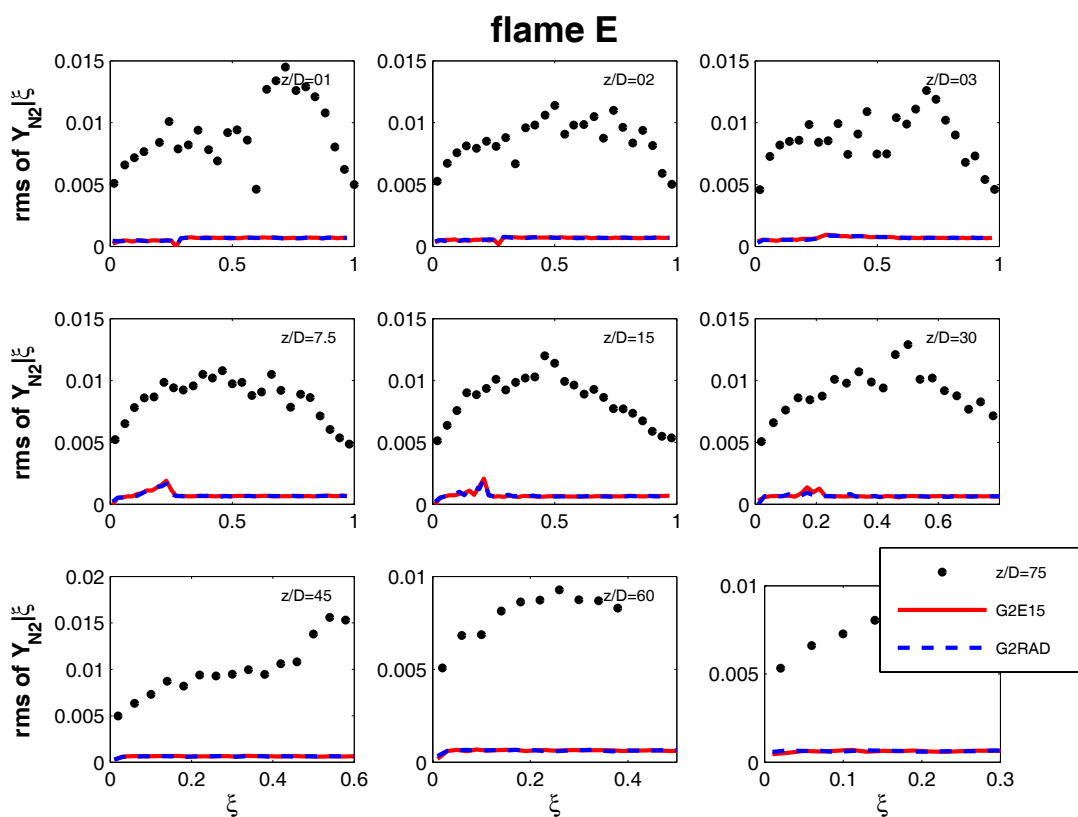
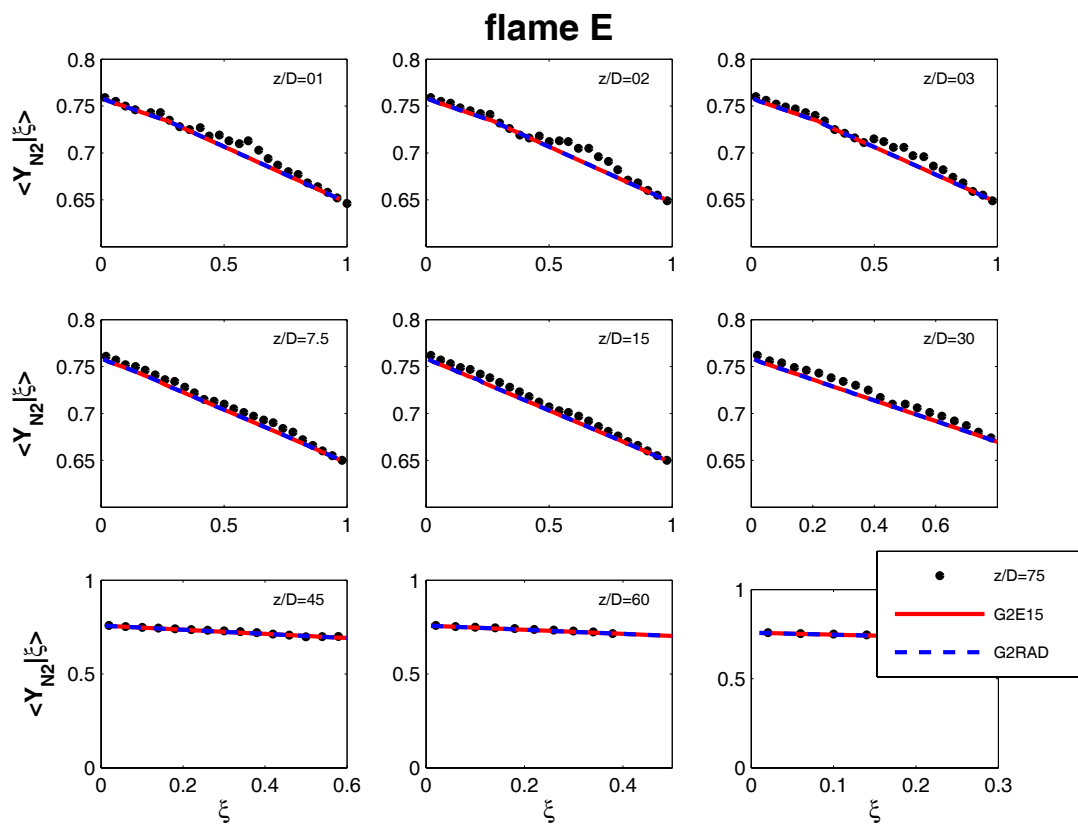


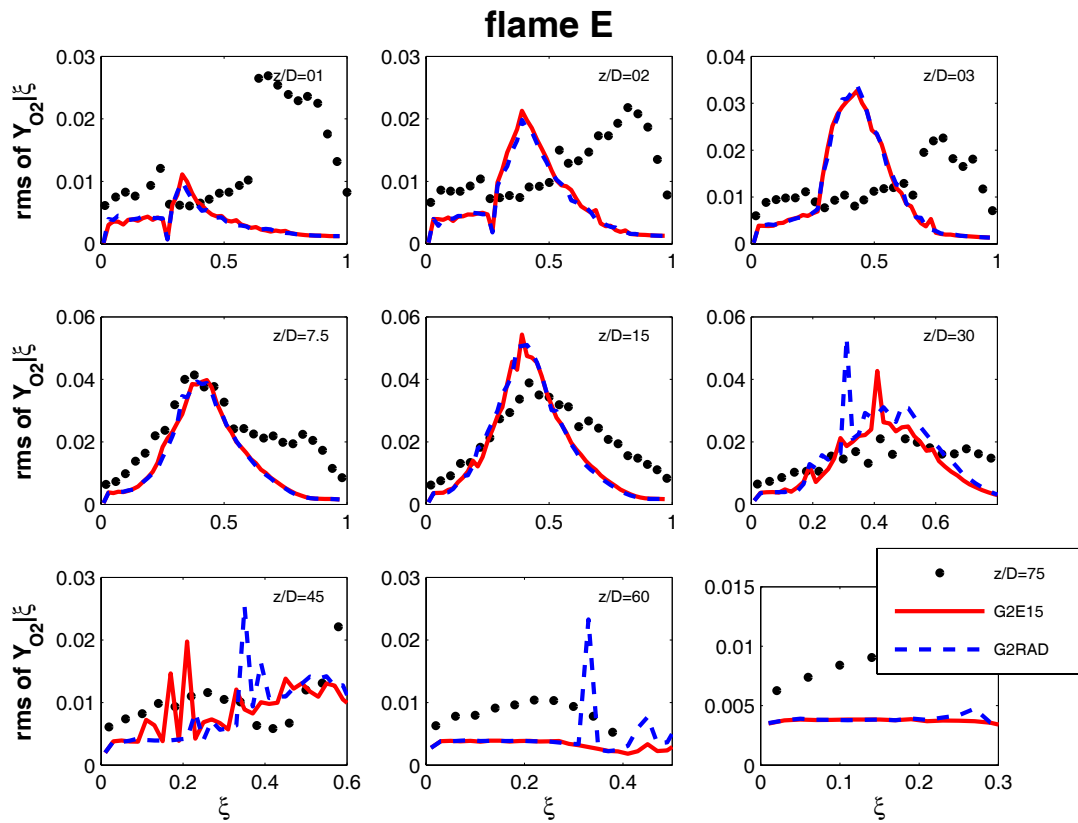
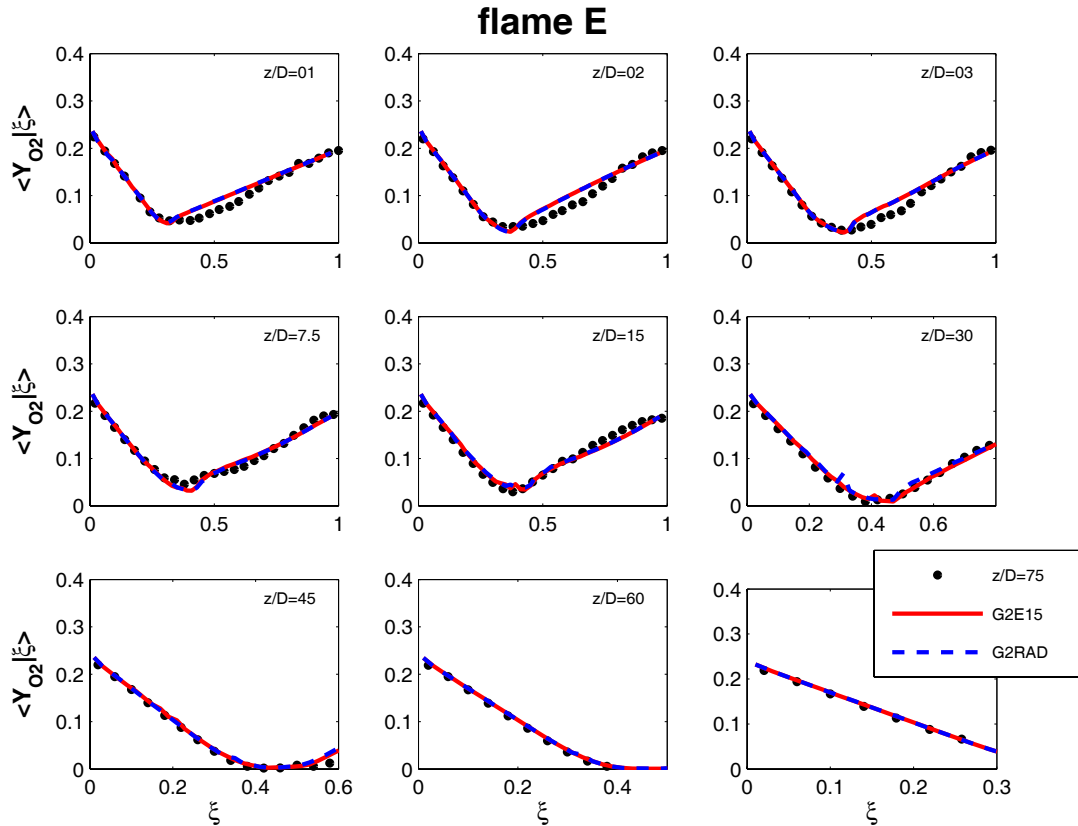
(3) G2E15 and G2RAD

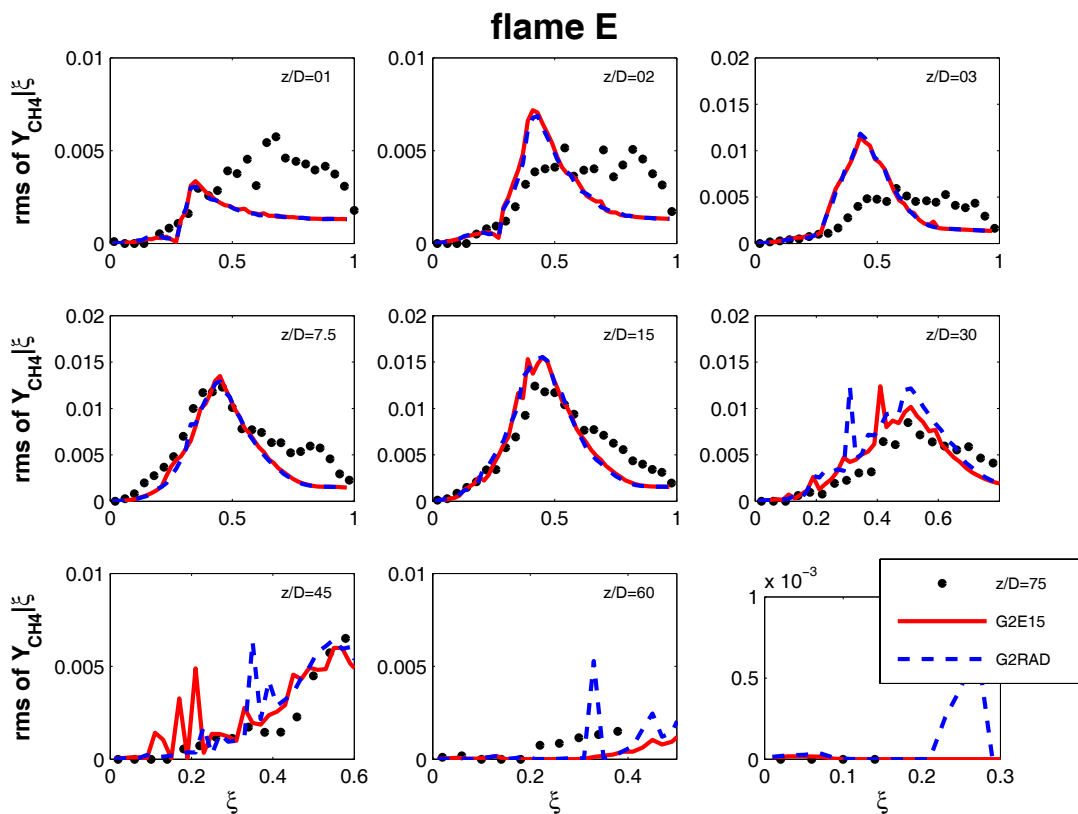
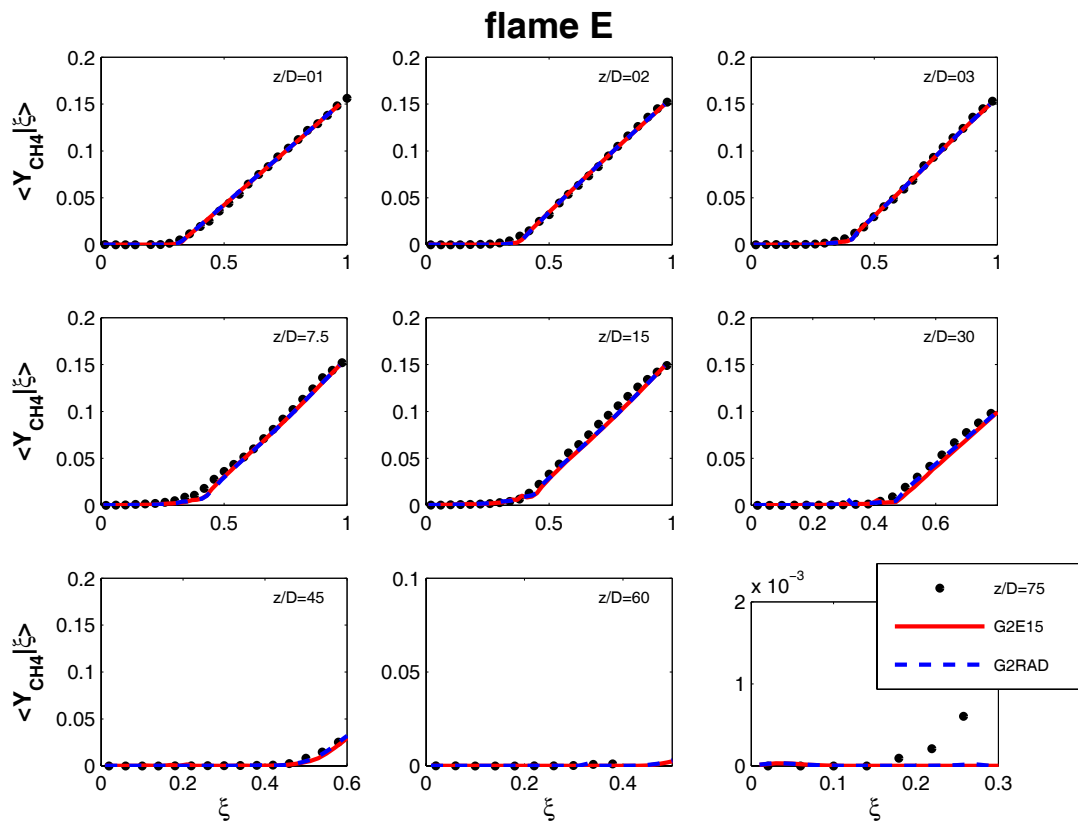


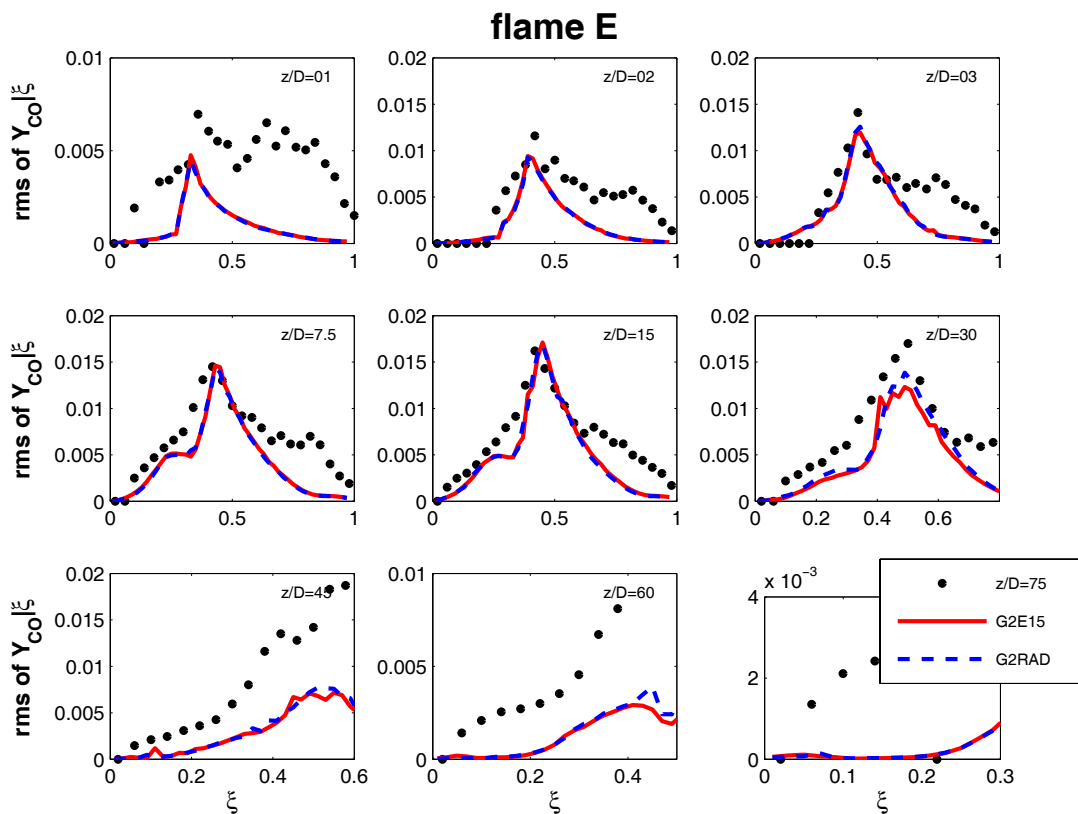
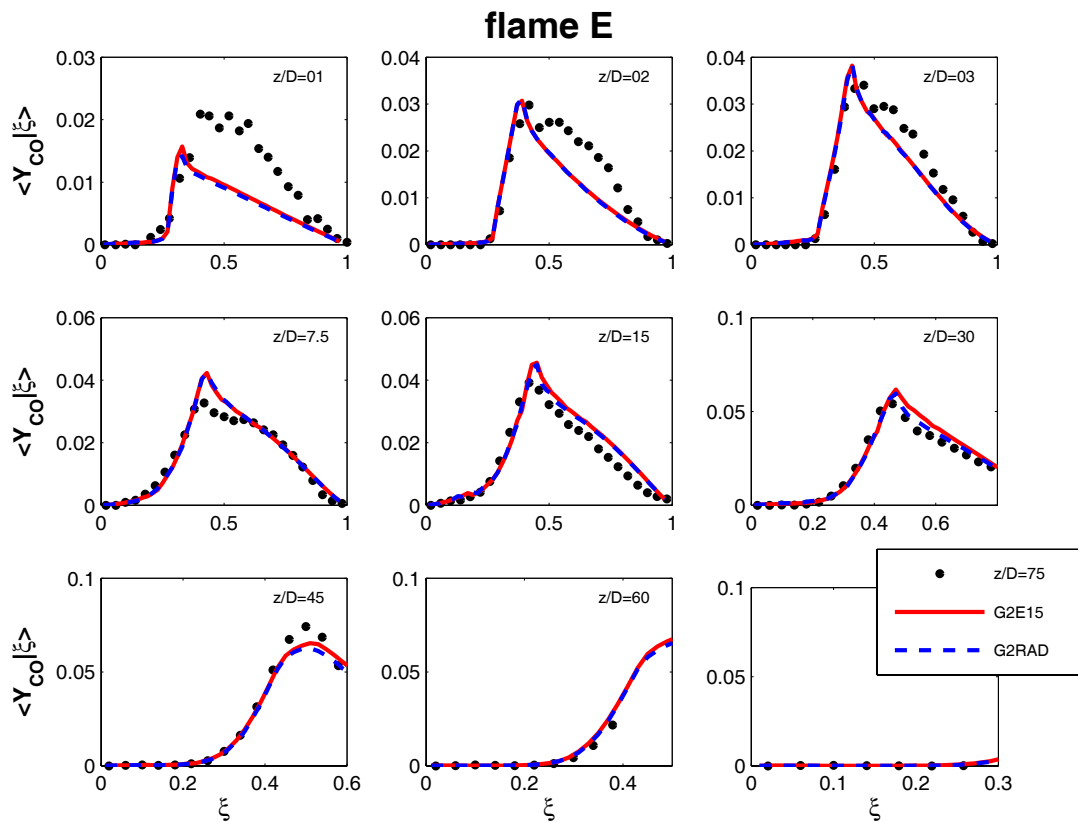


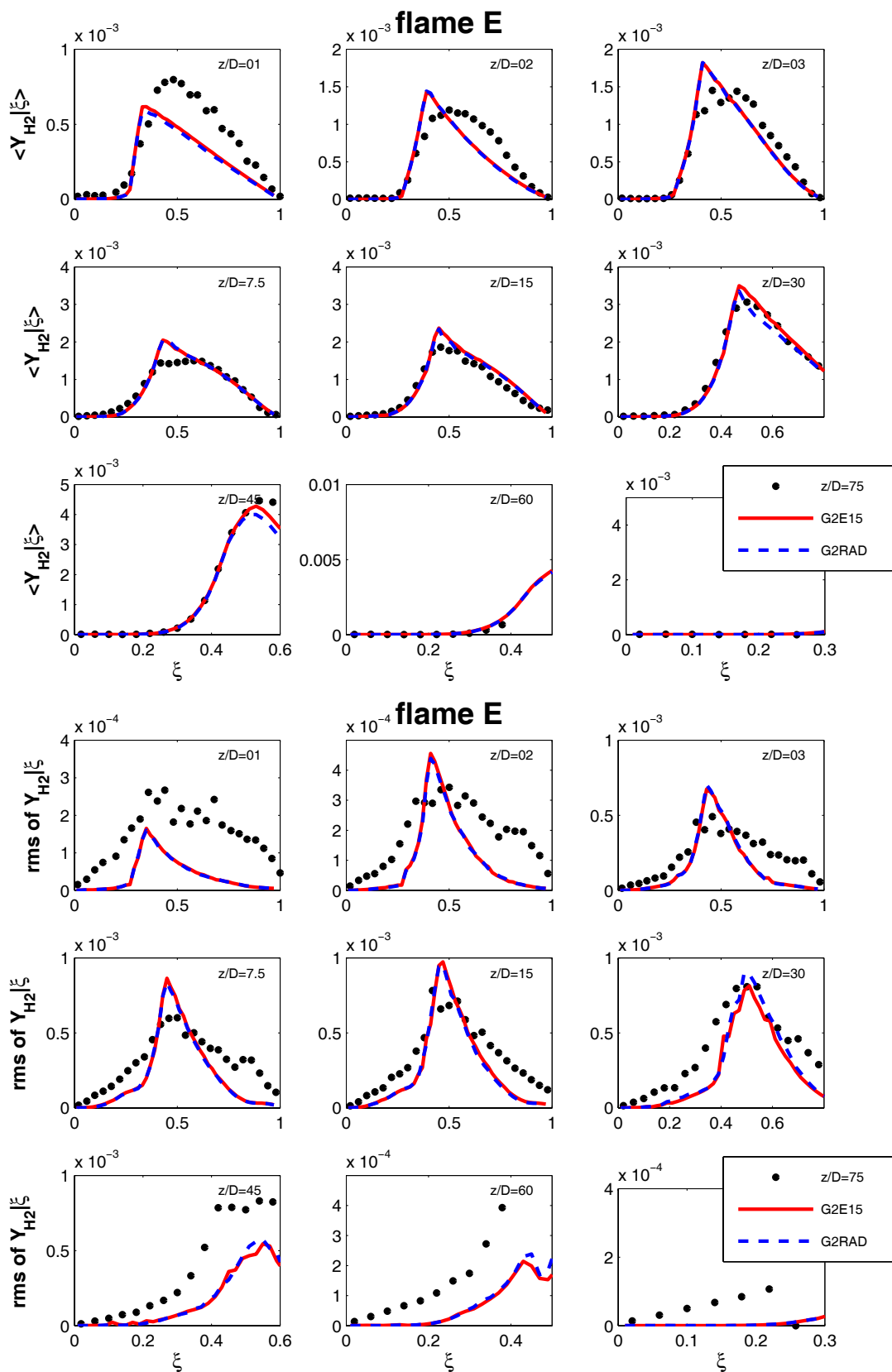


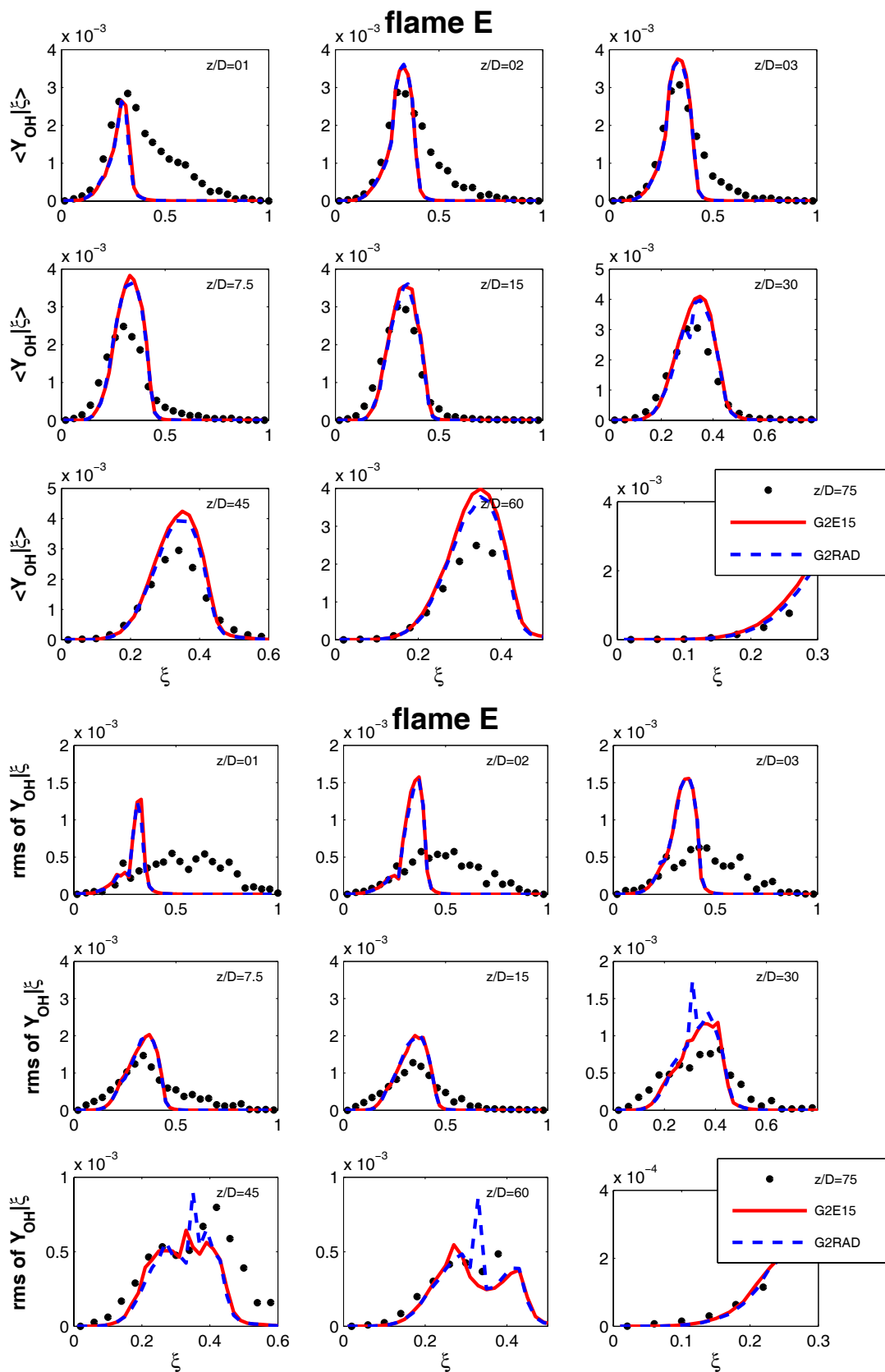


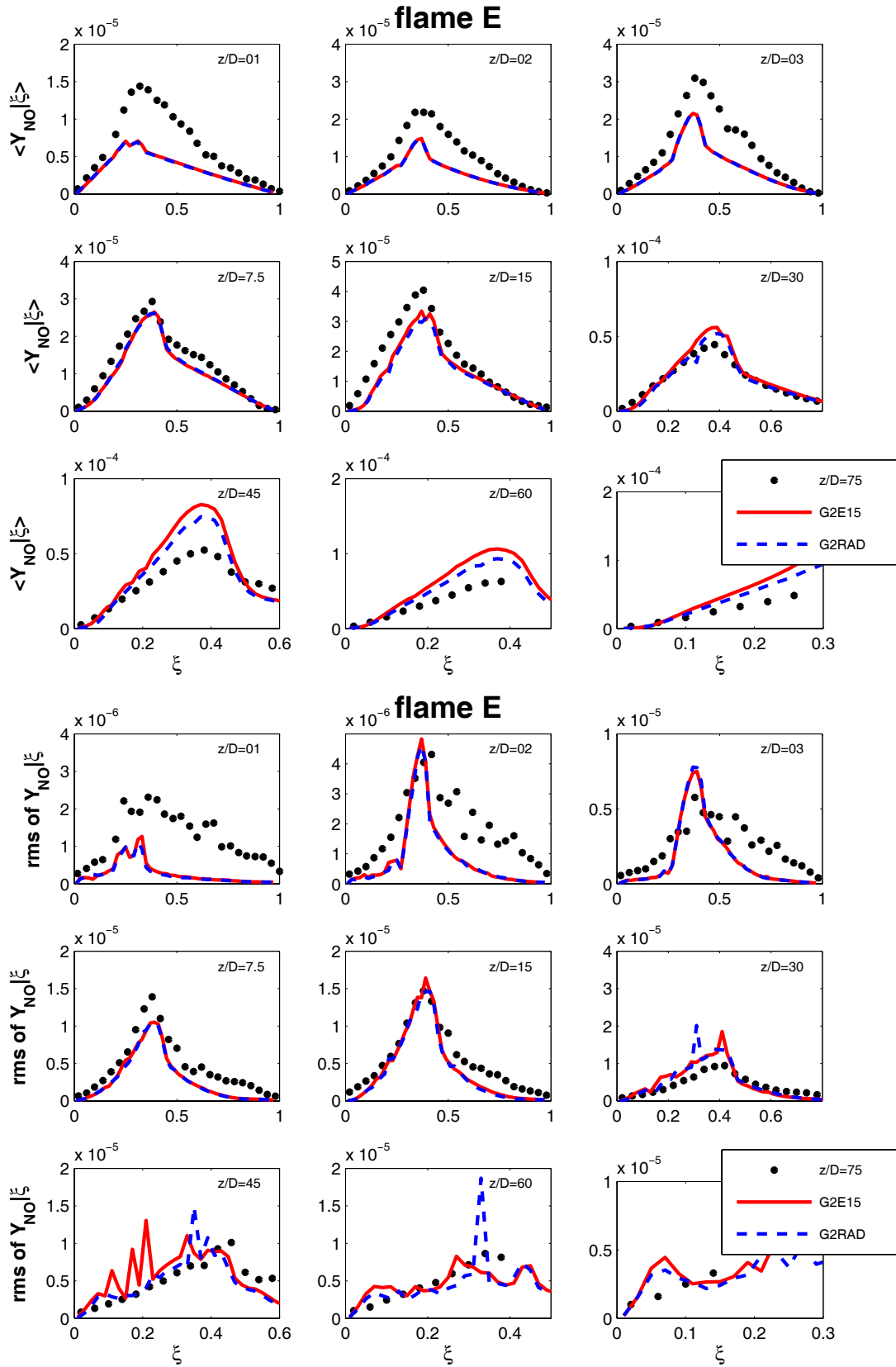




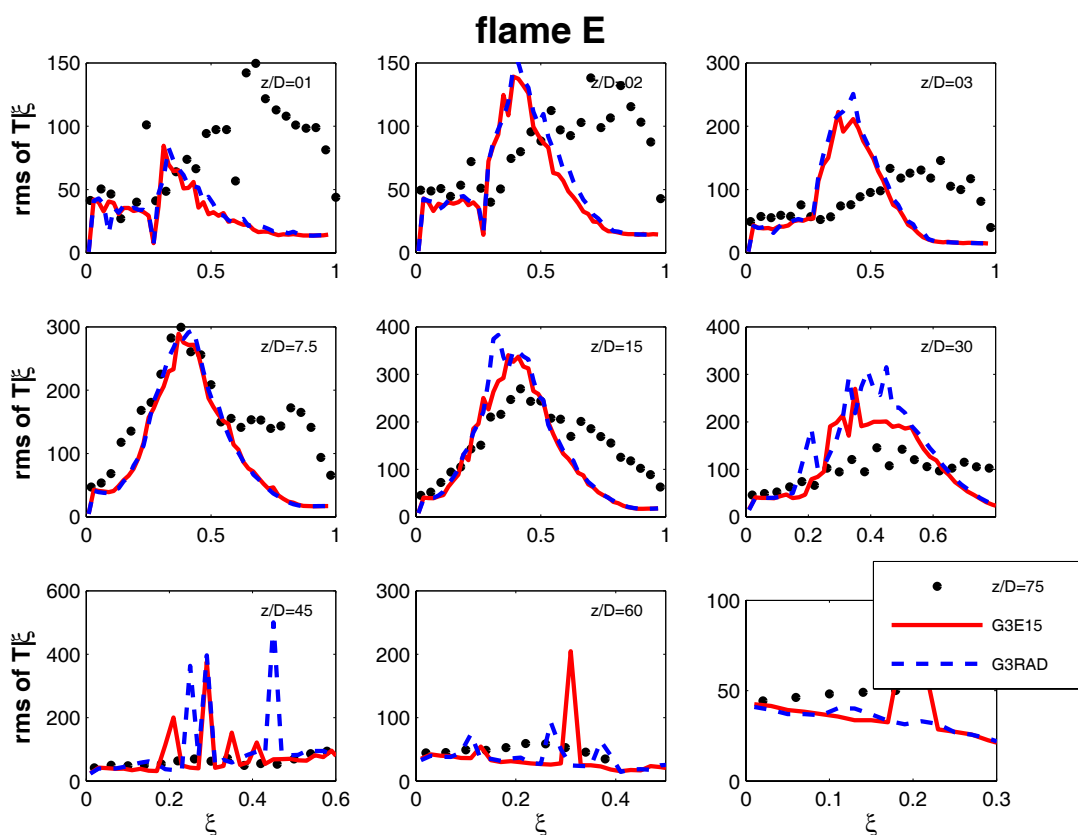
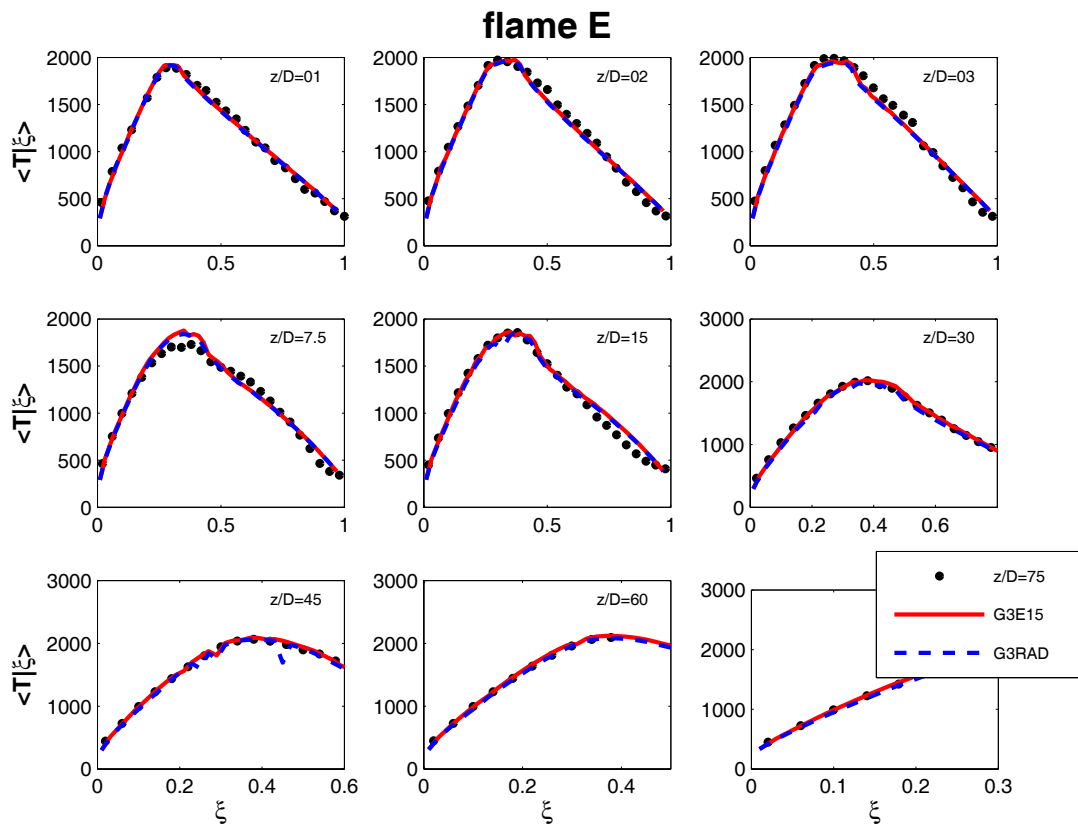


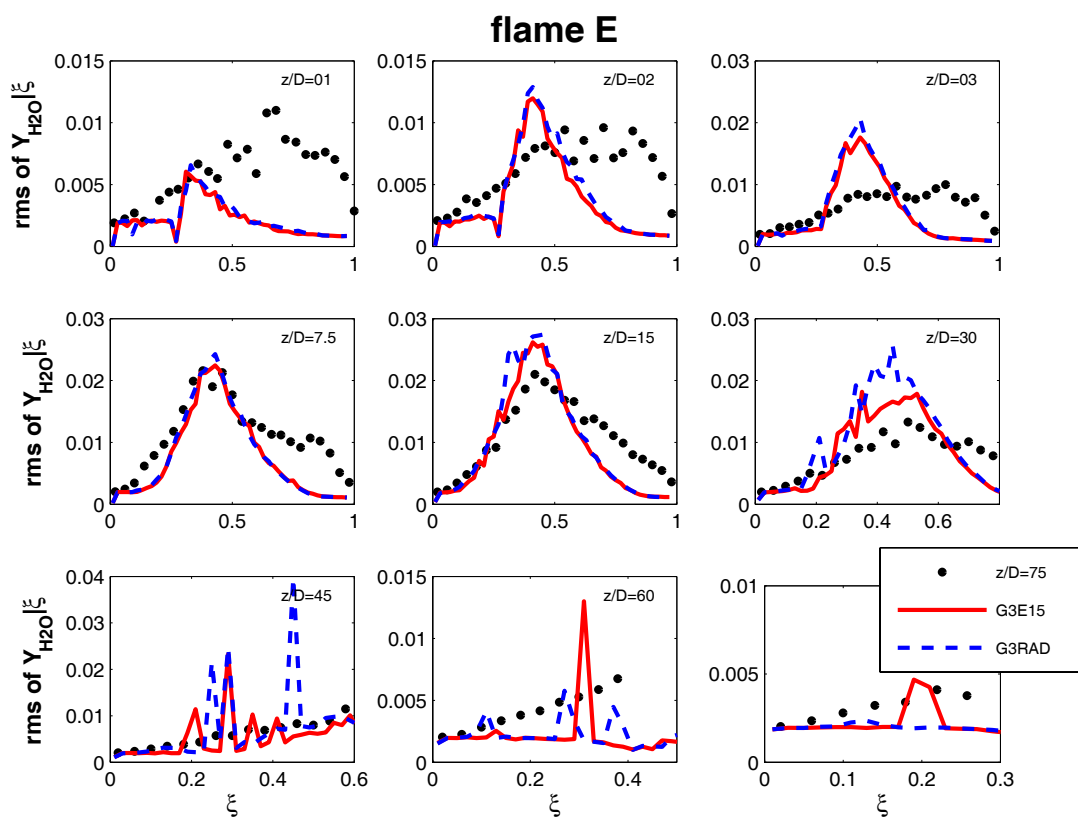
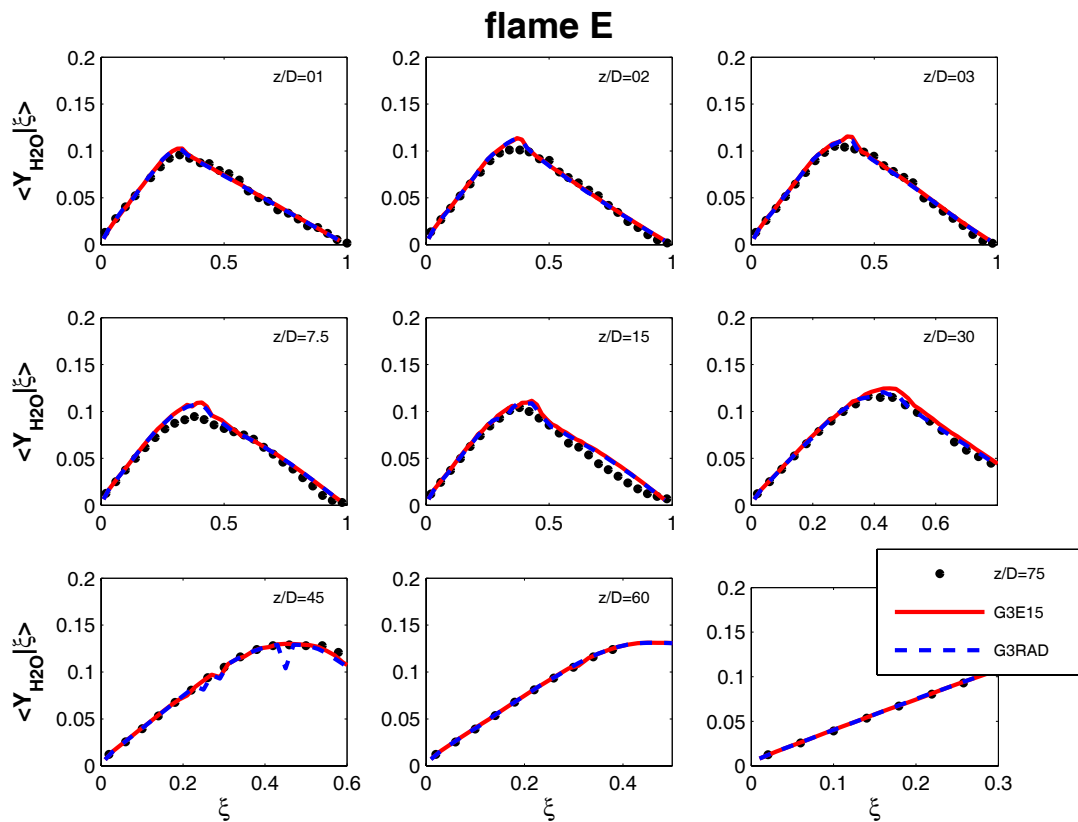


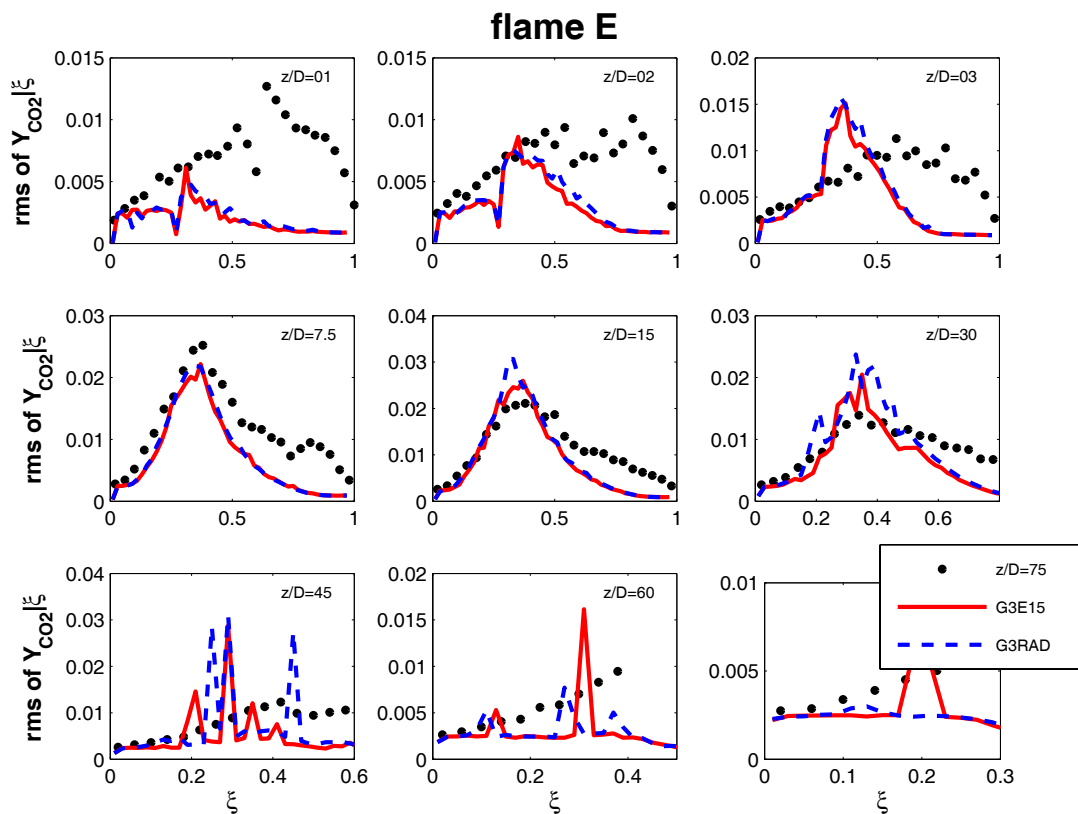
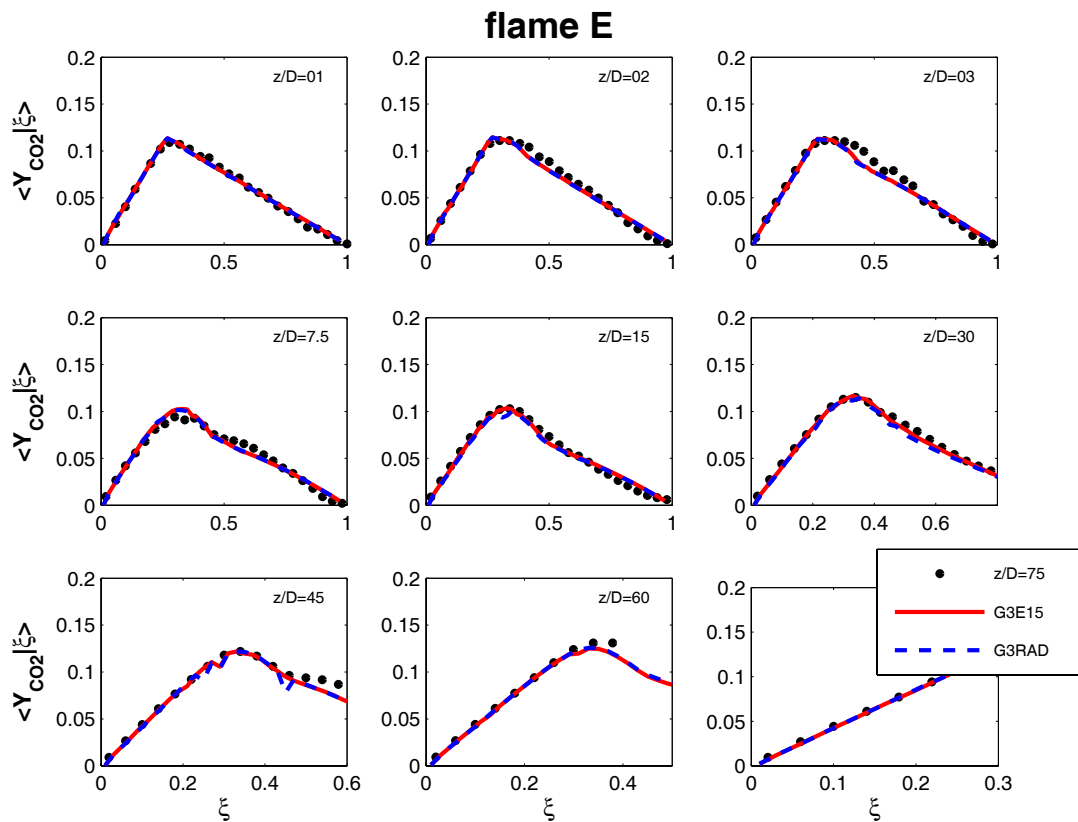


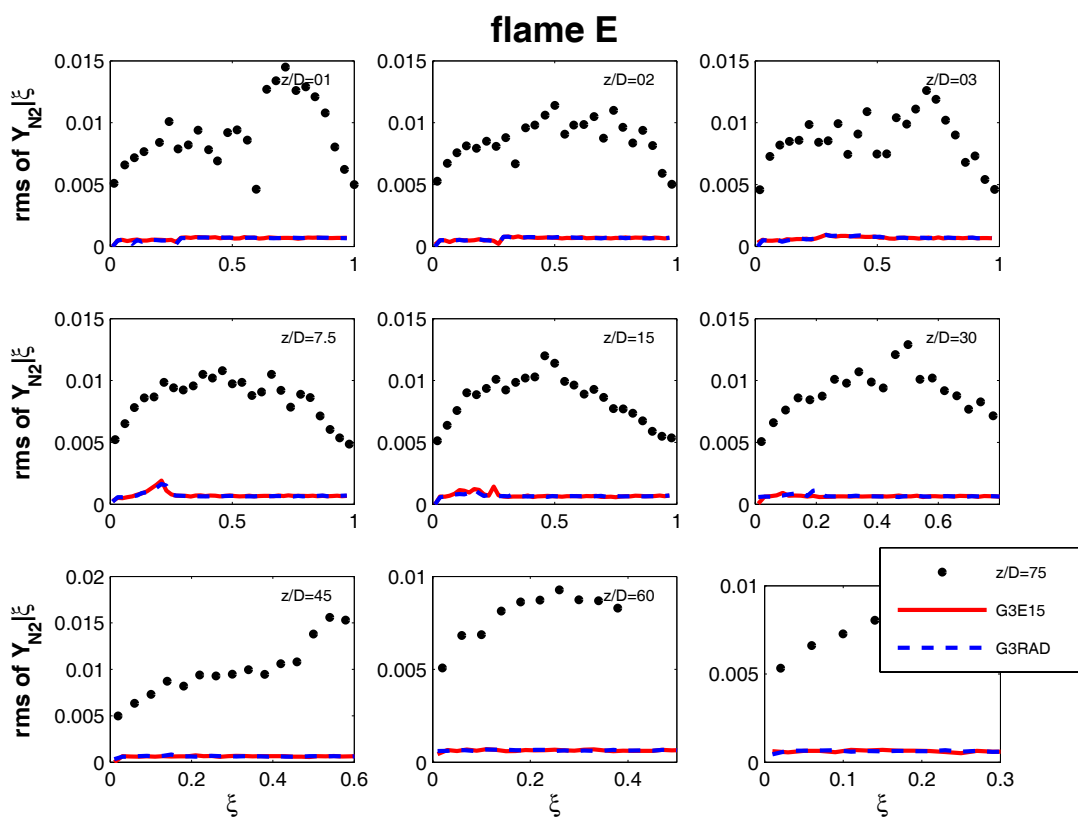
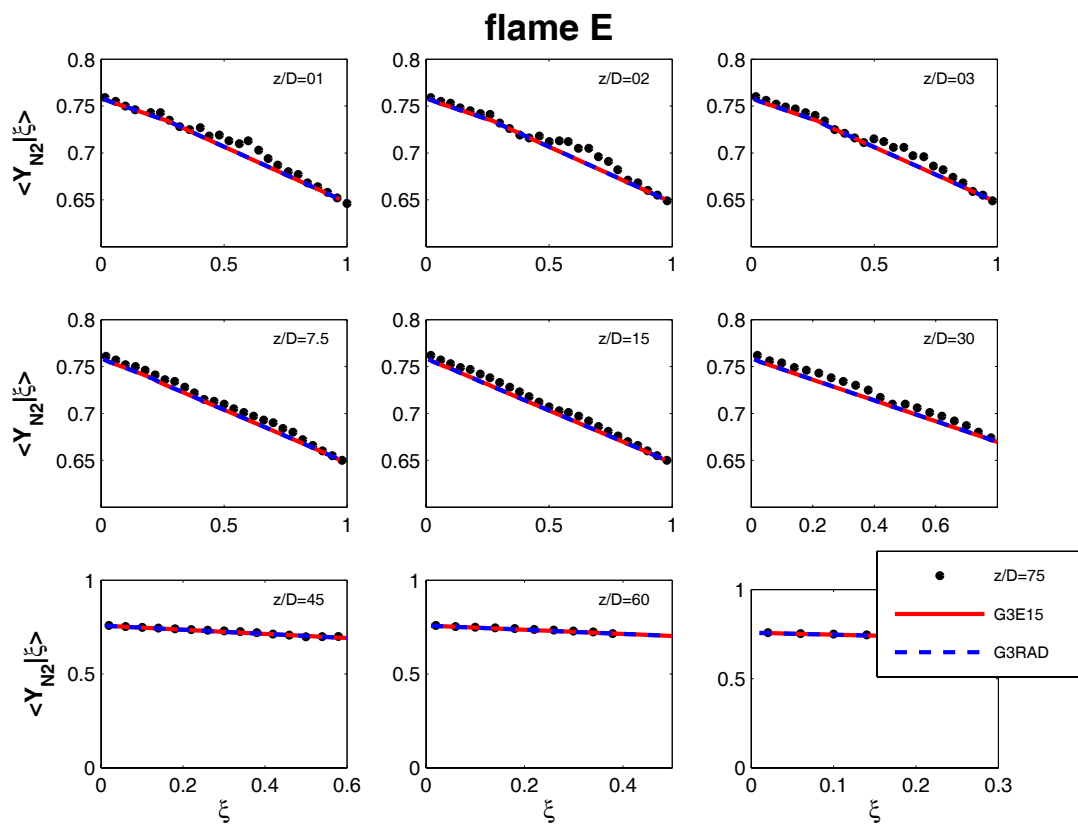


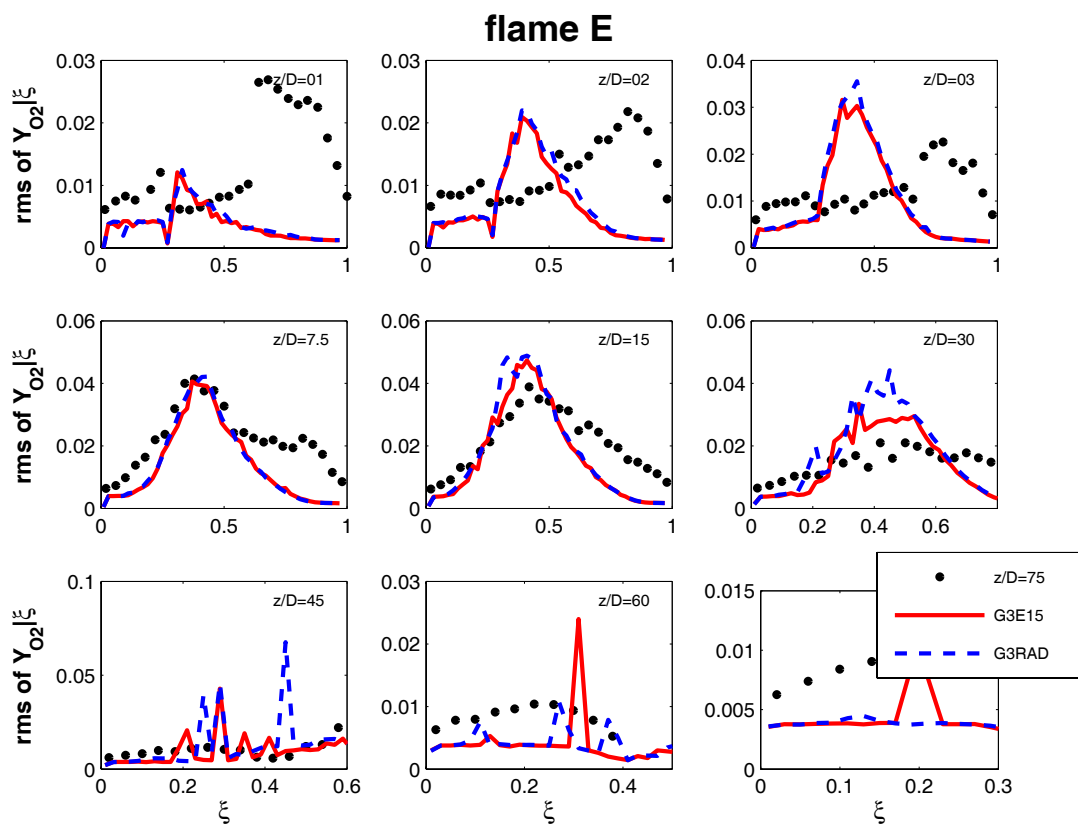
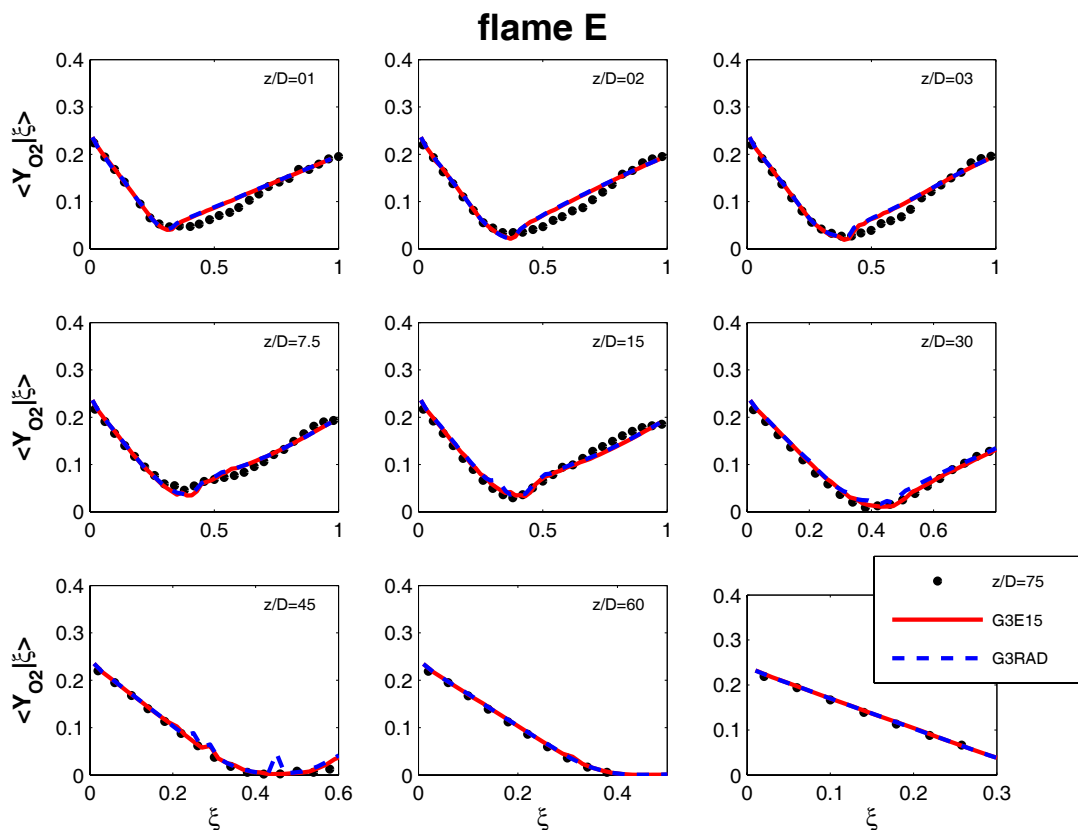
(4) G3E15 and G3RAD

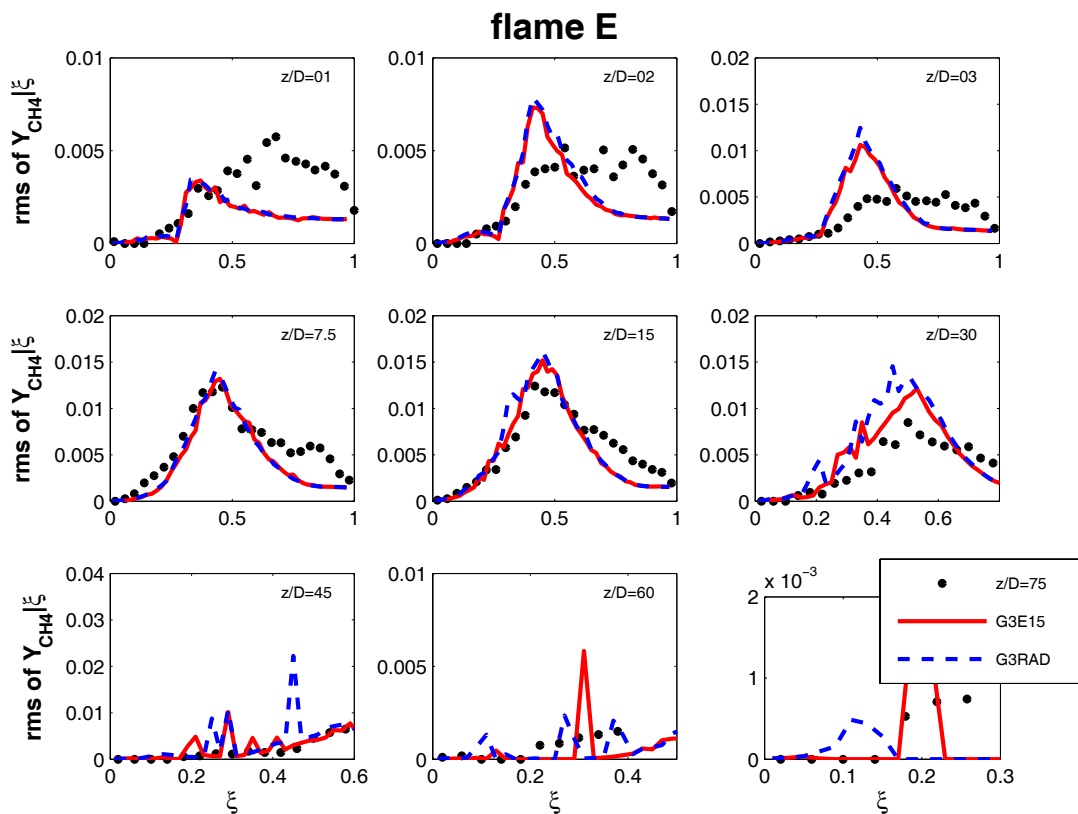
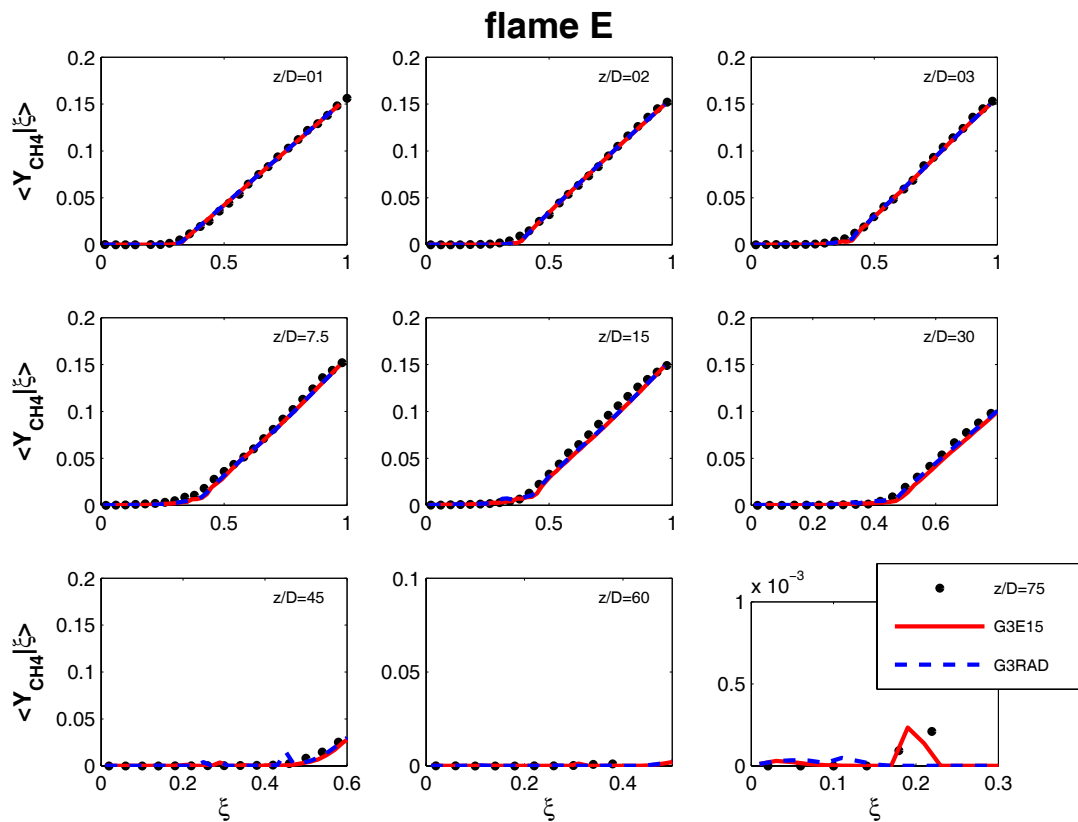


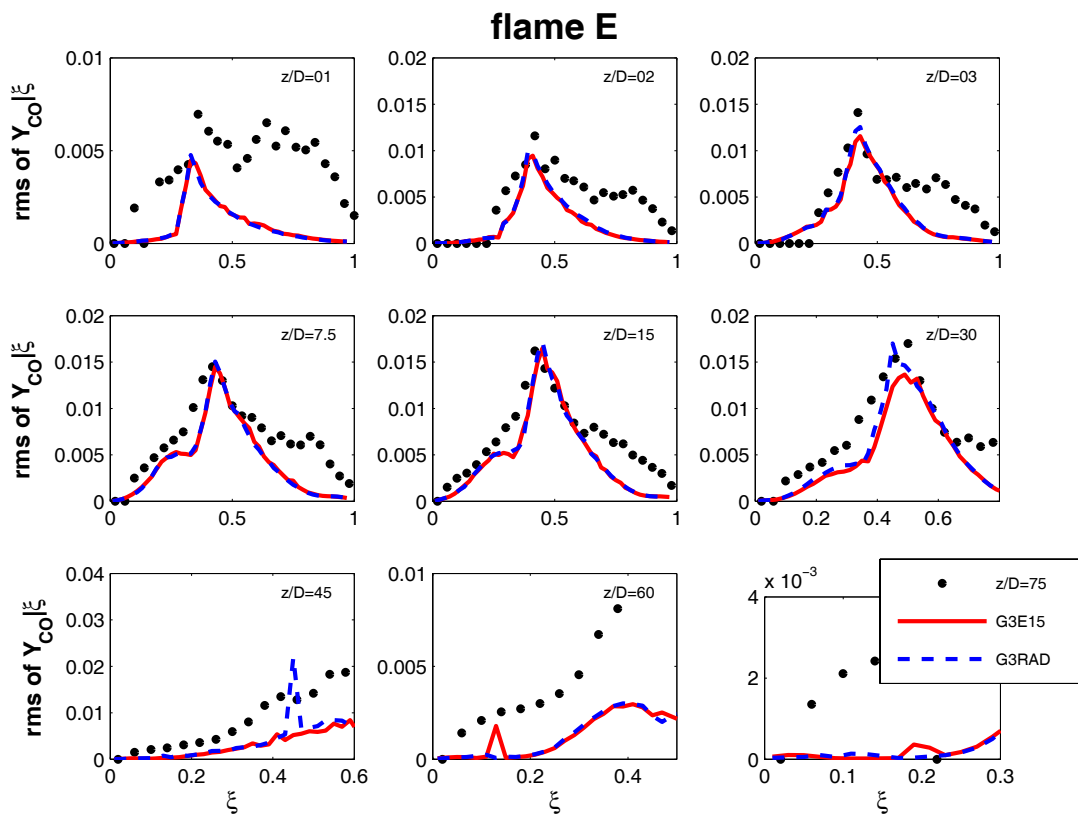
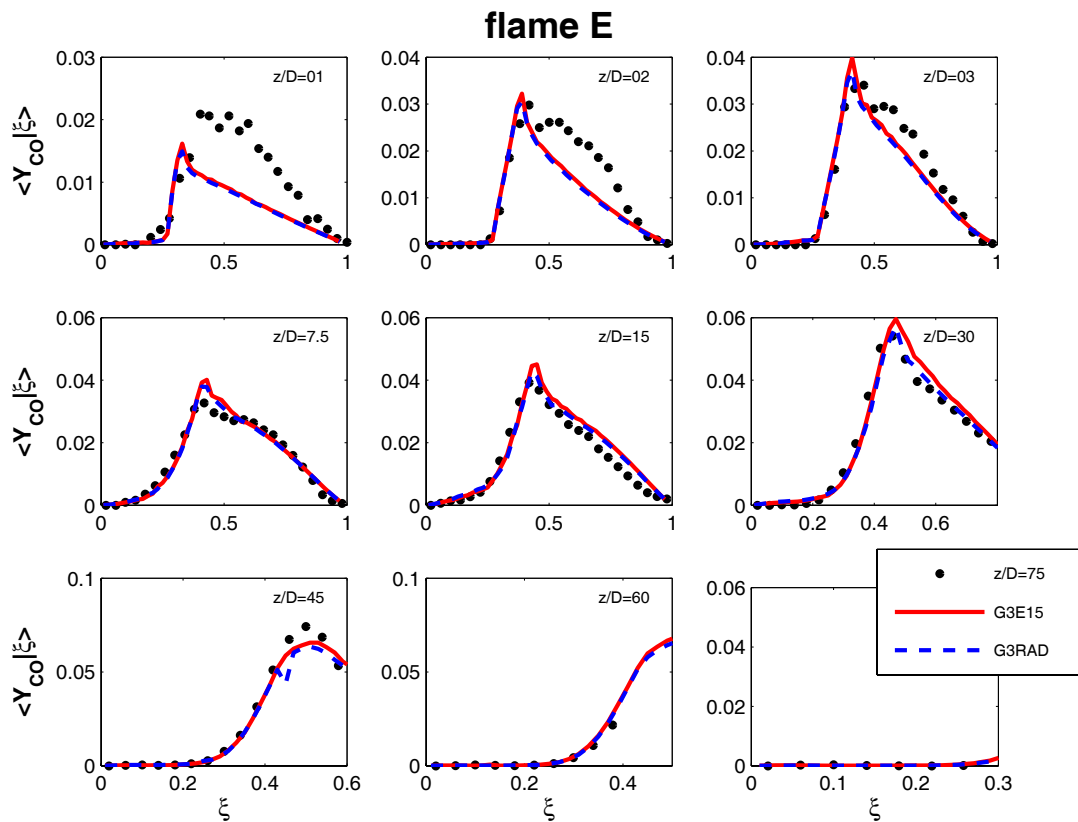


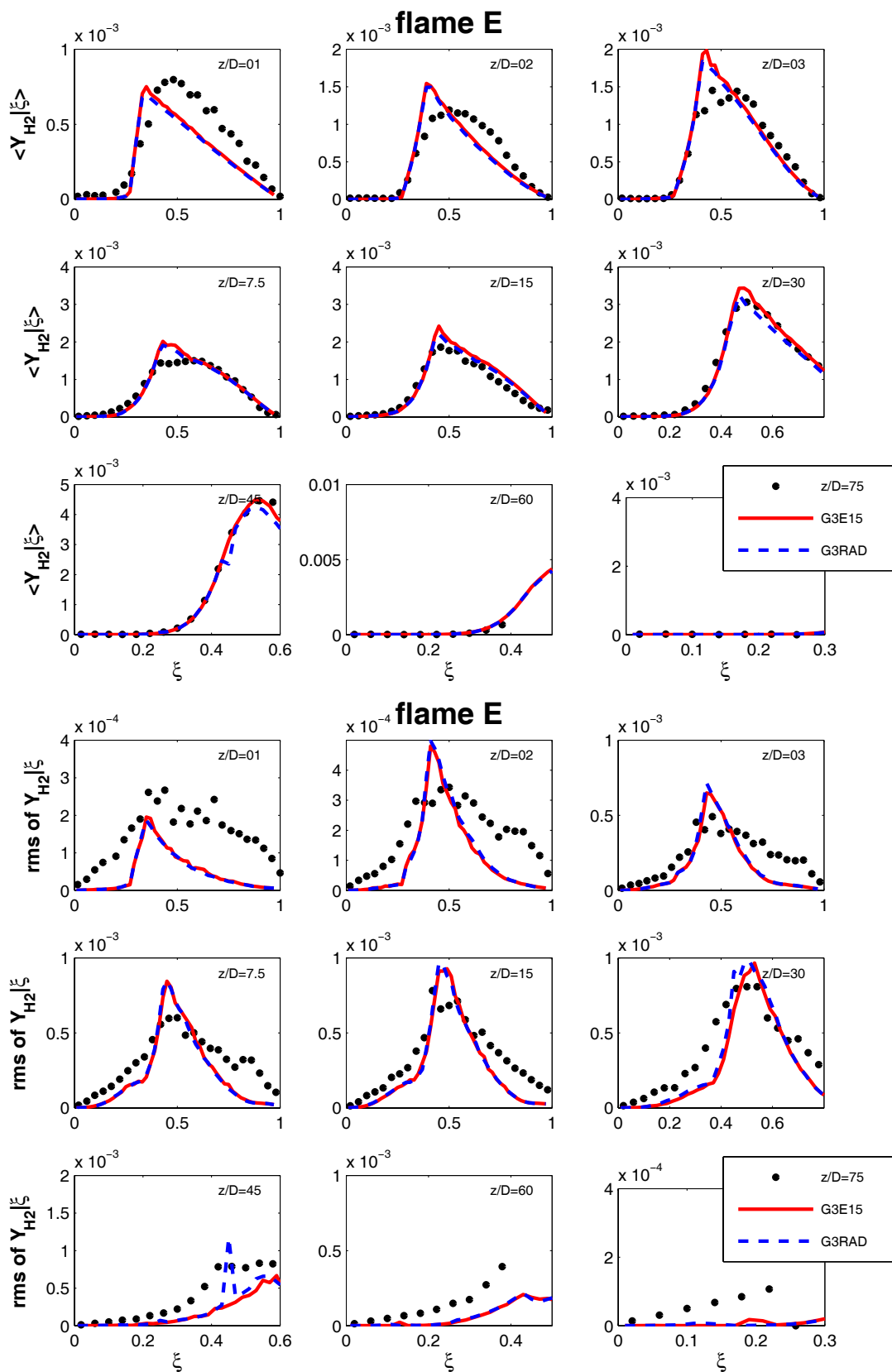


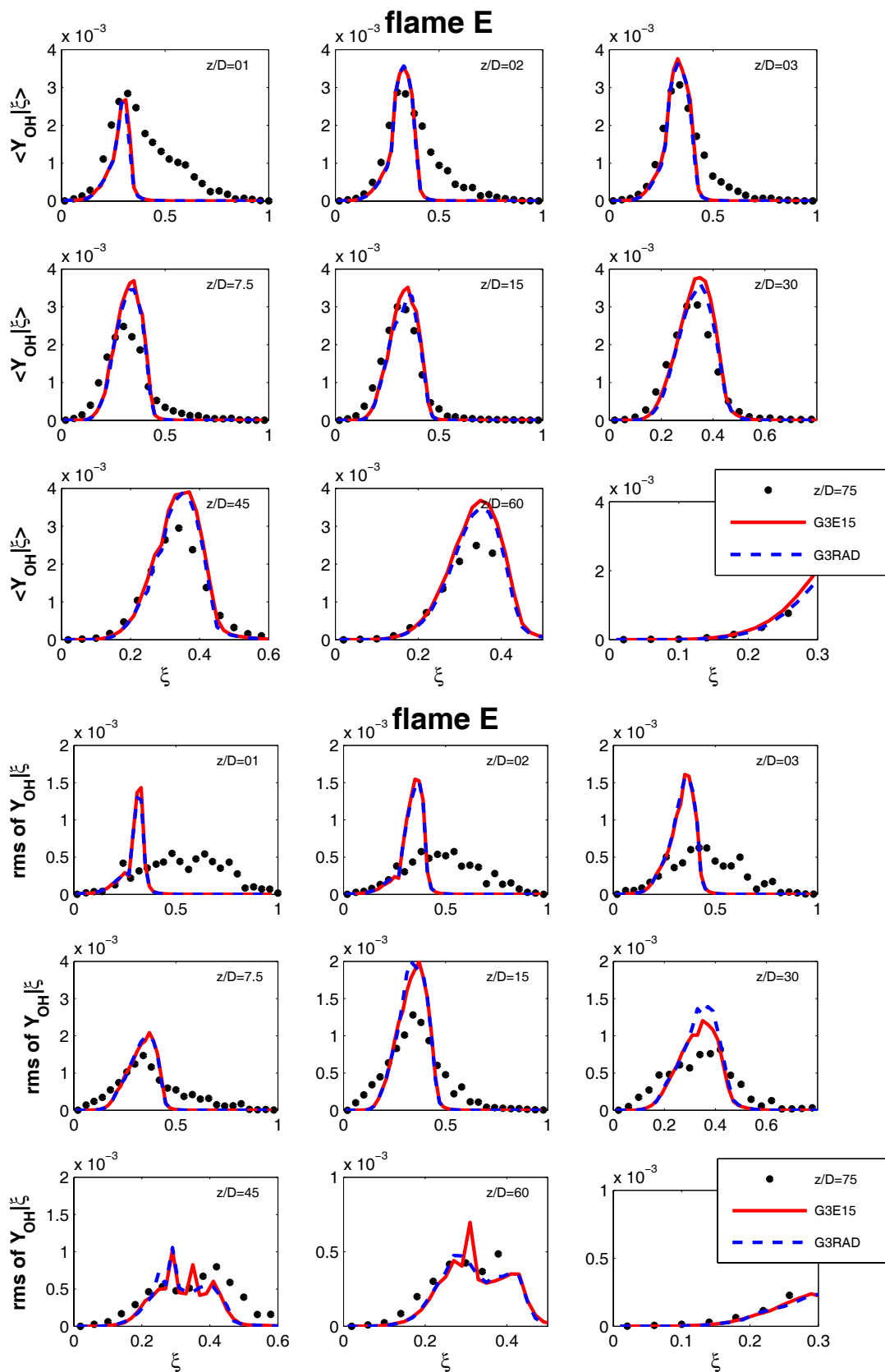


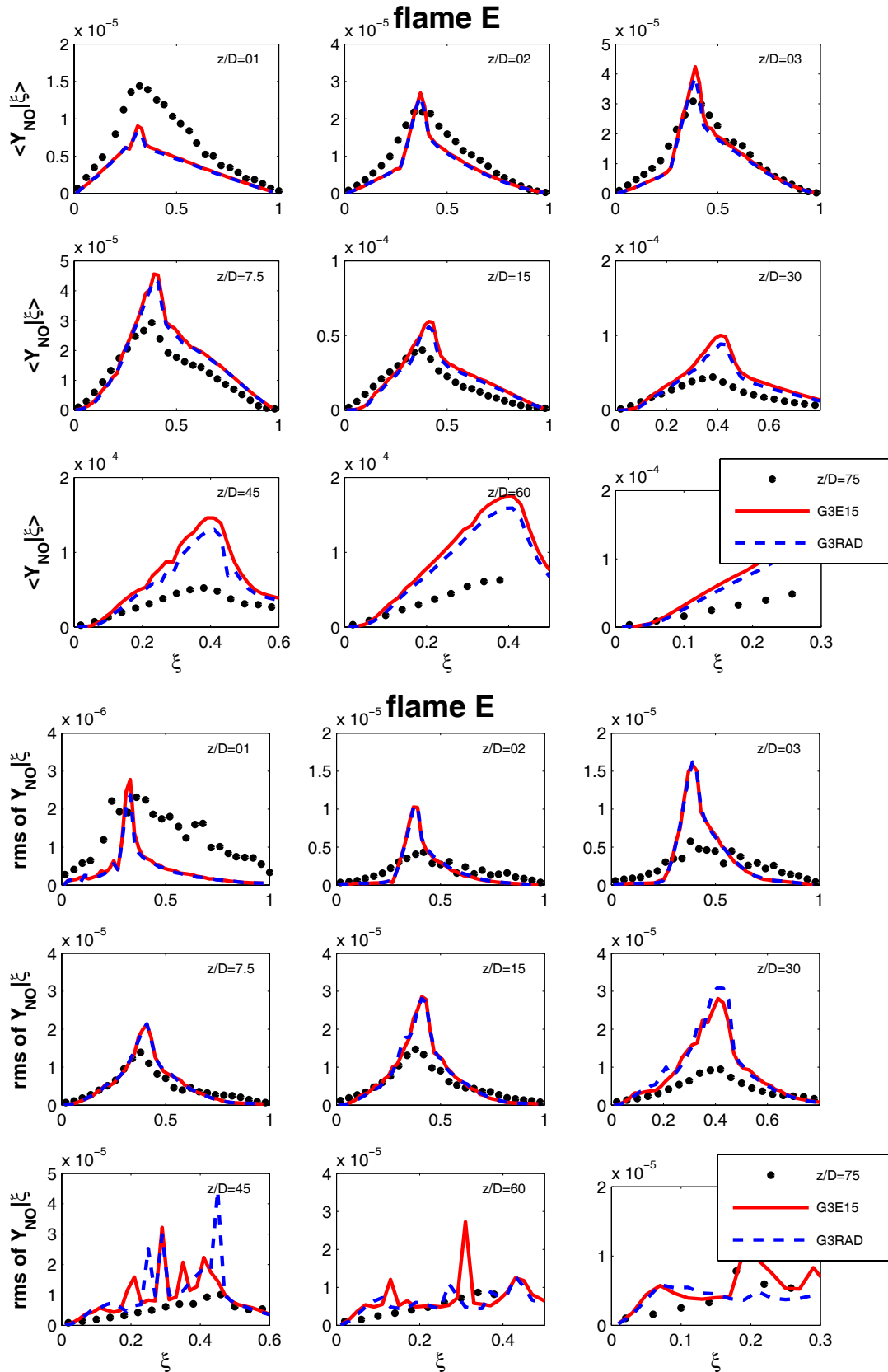




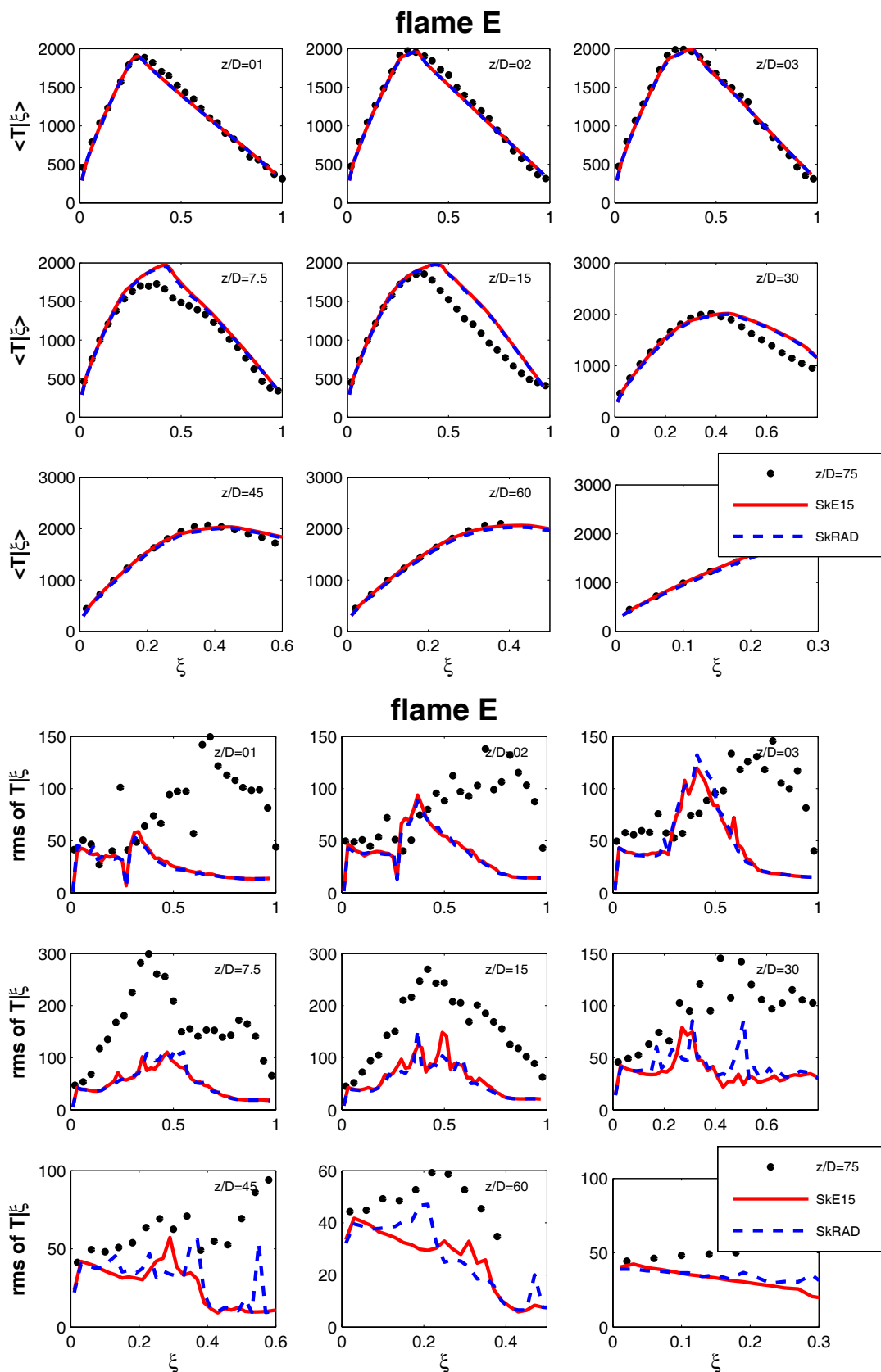


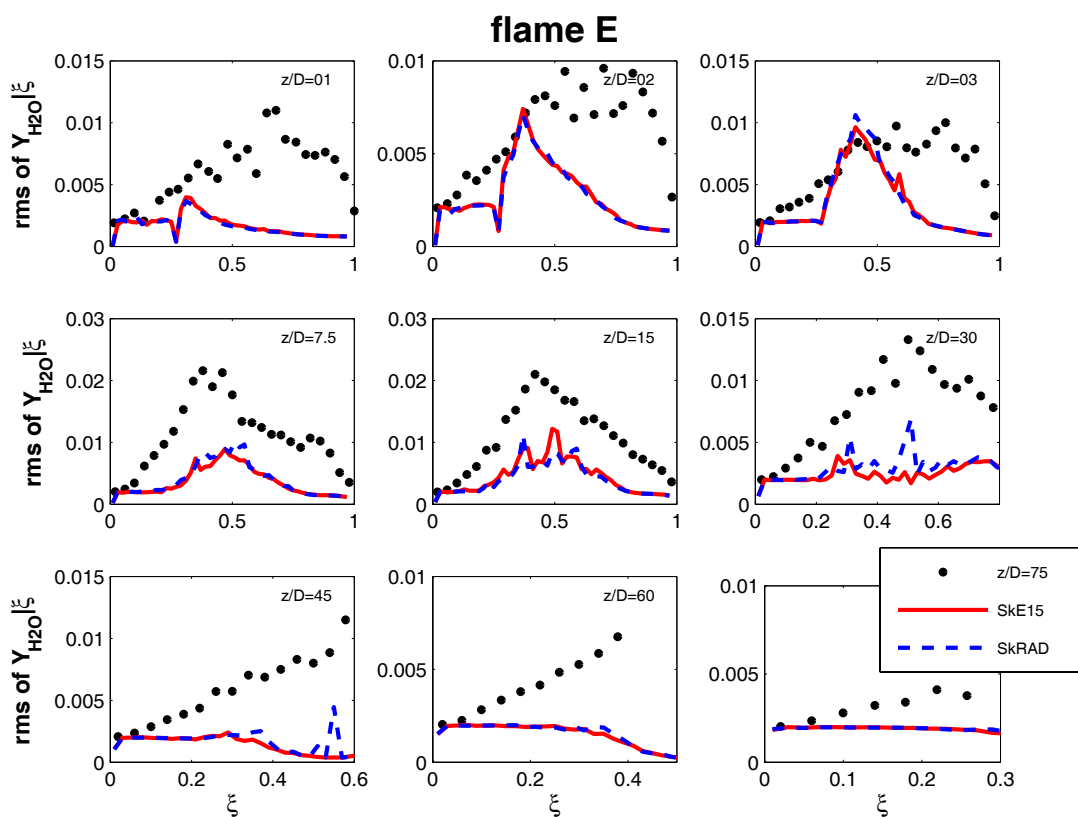
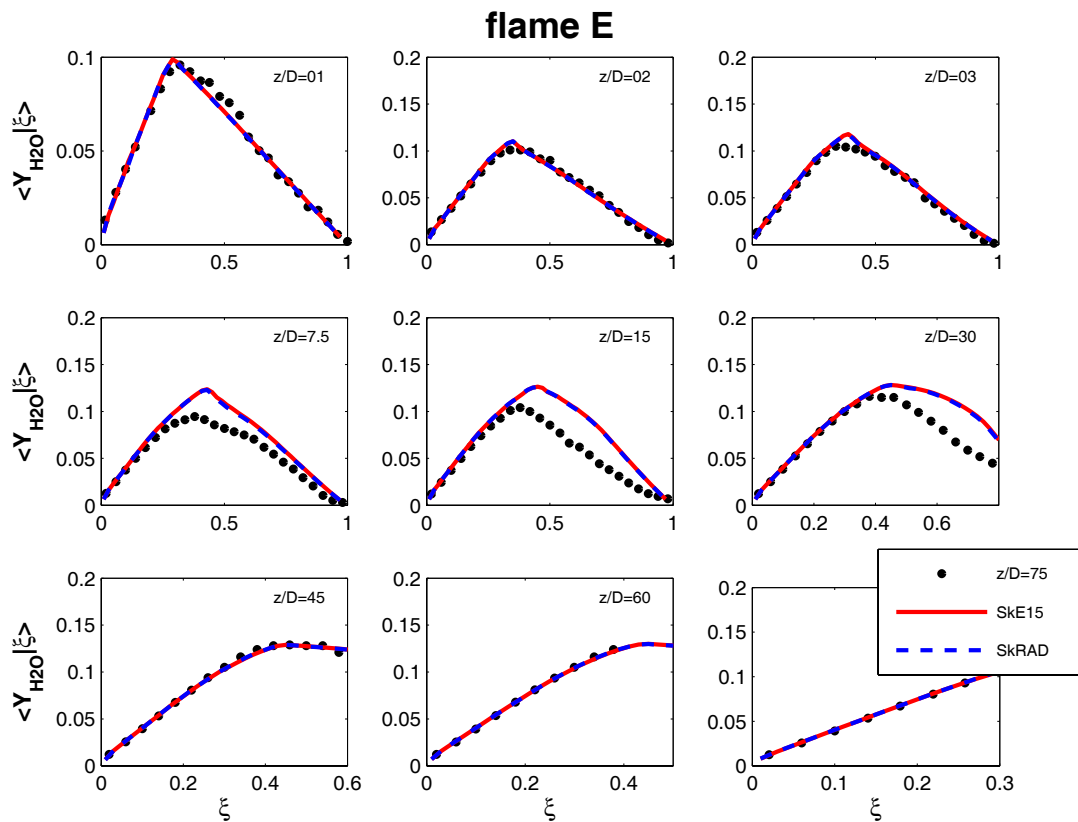


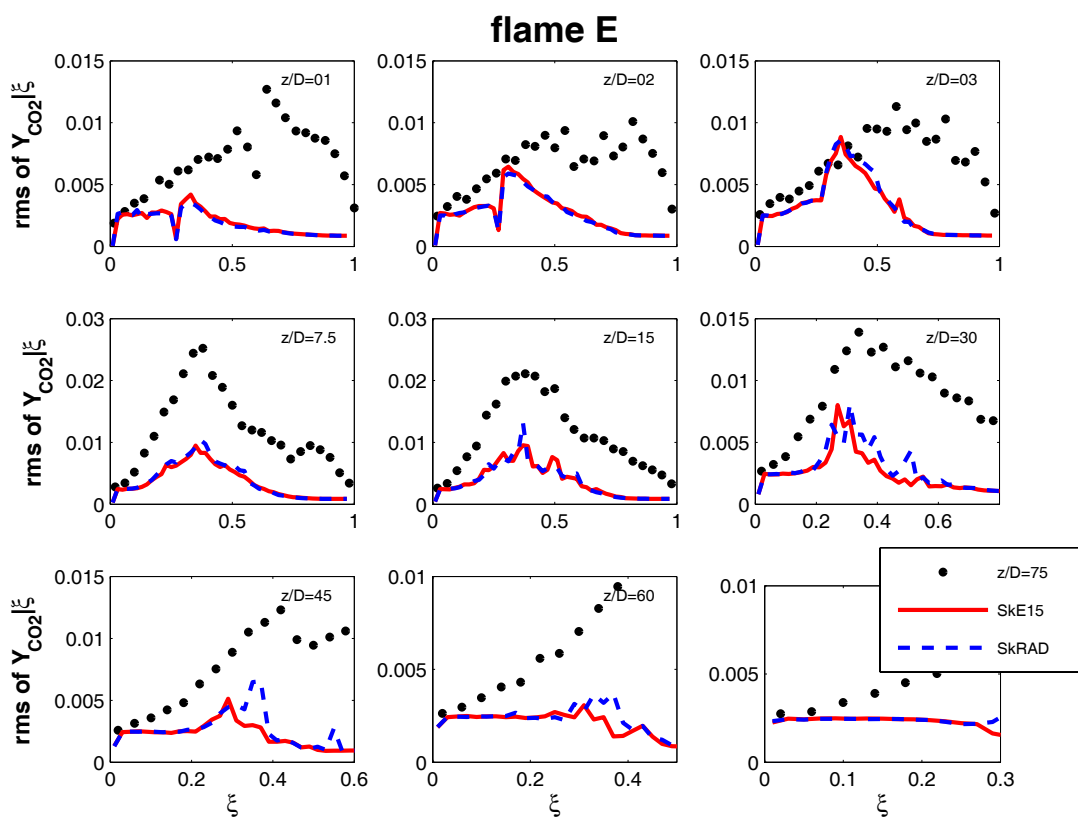
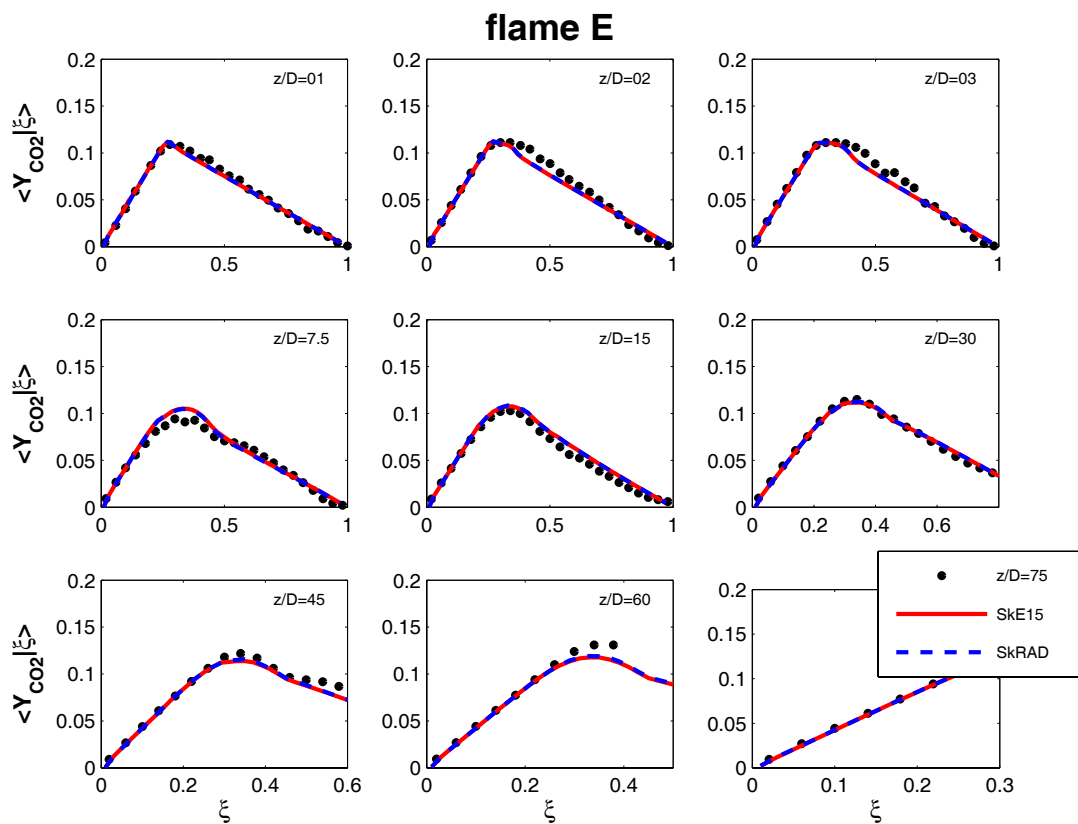


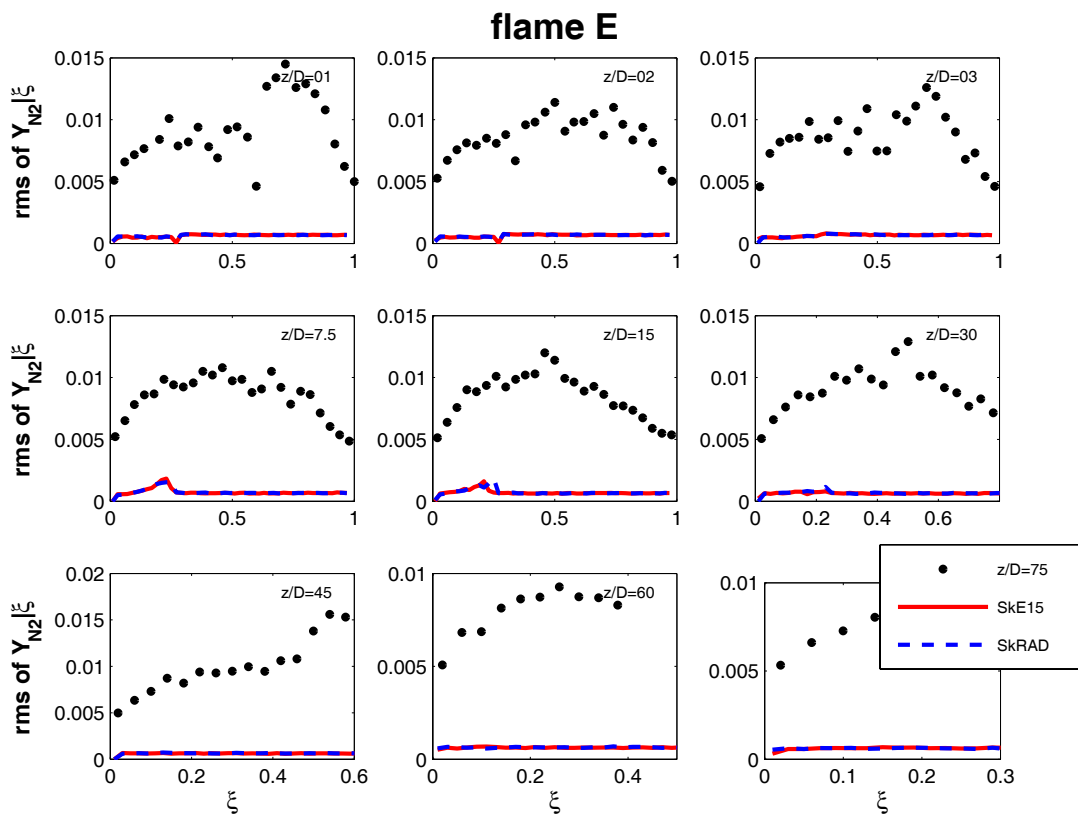
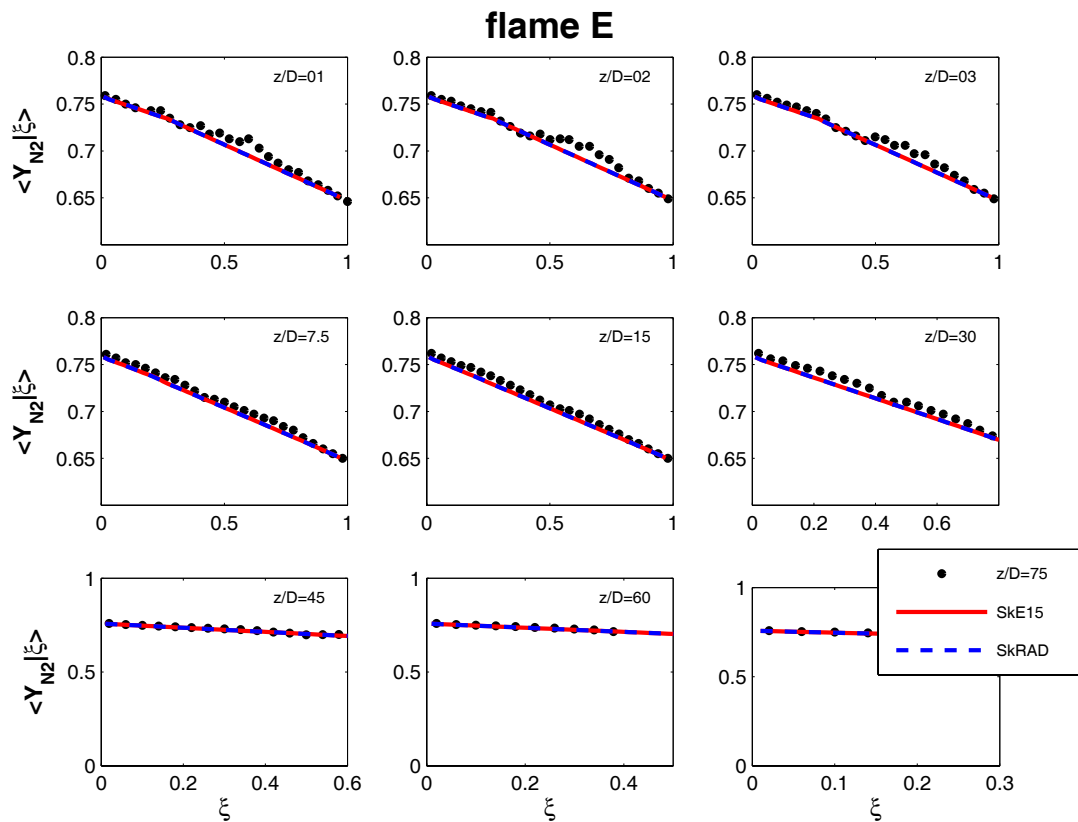


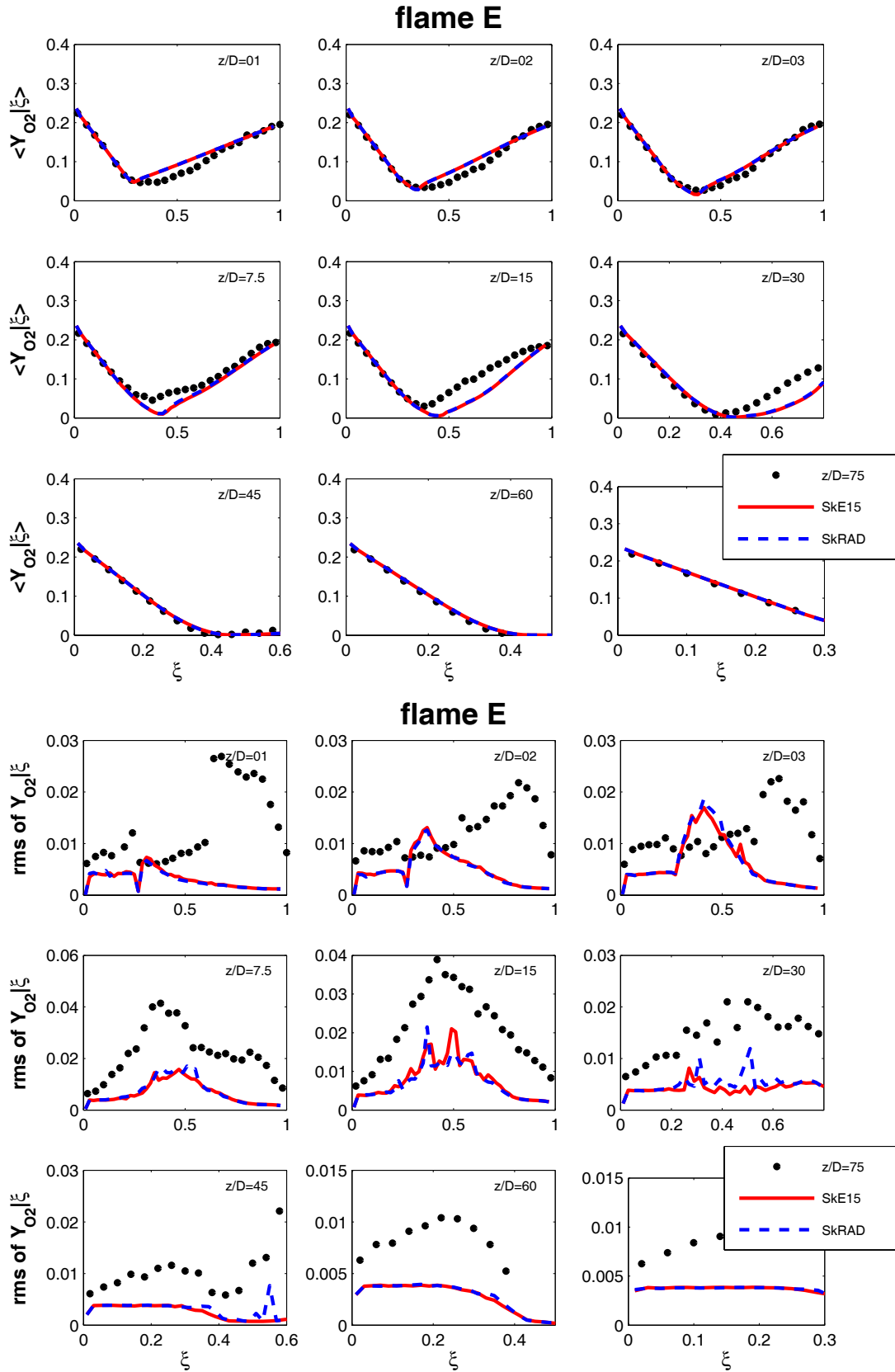
(5) SkE15 and SkRAD

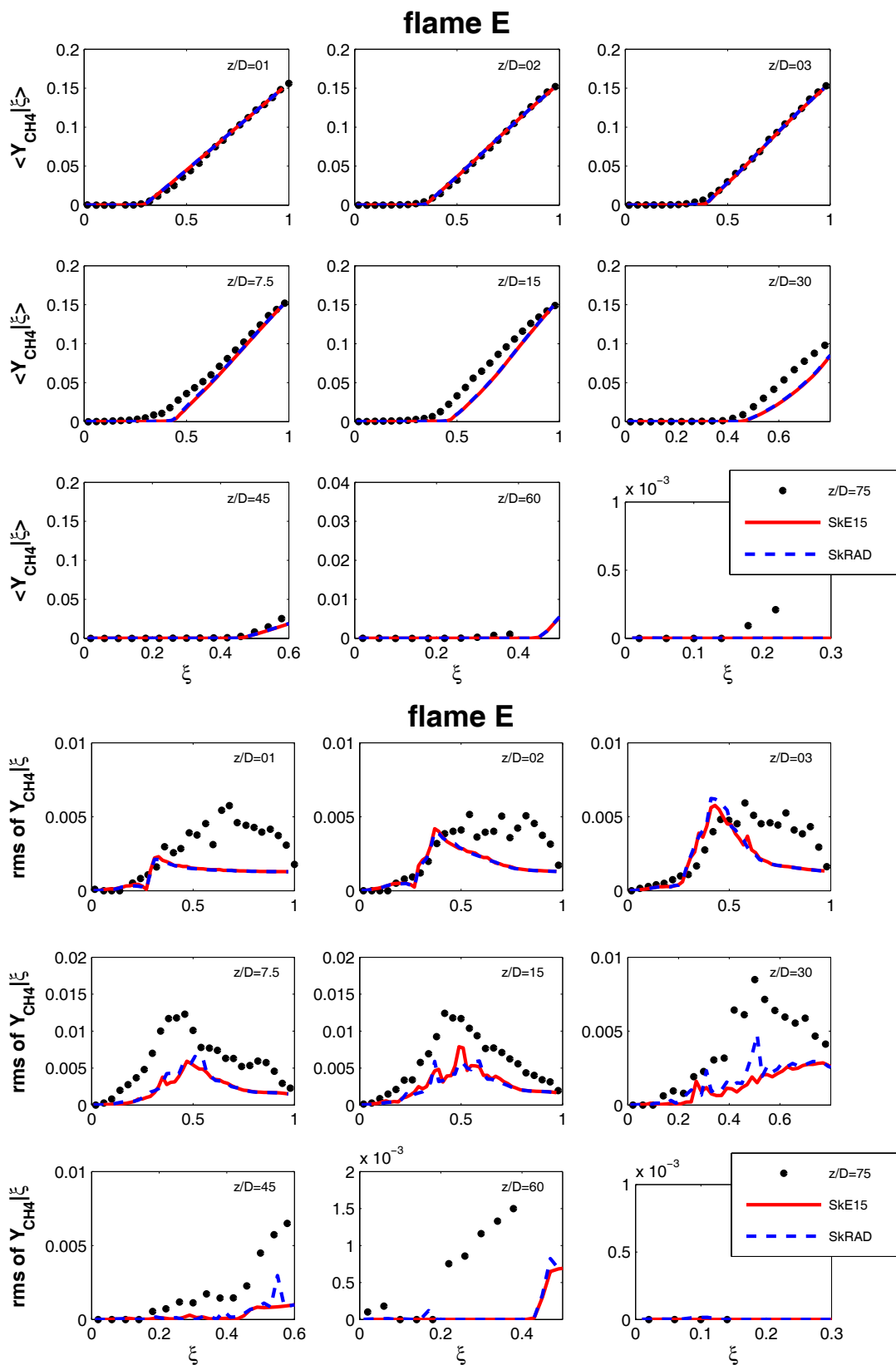


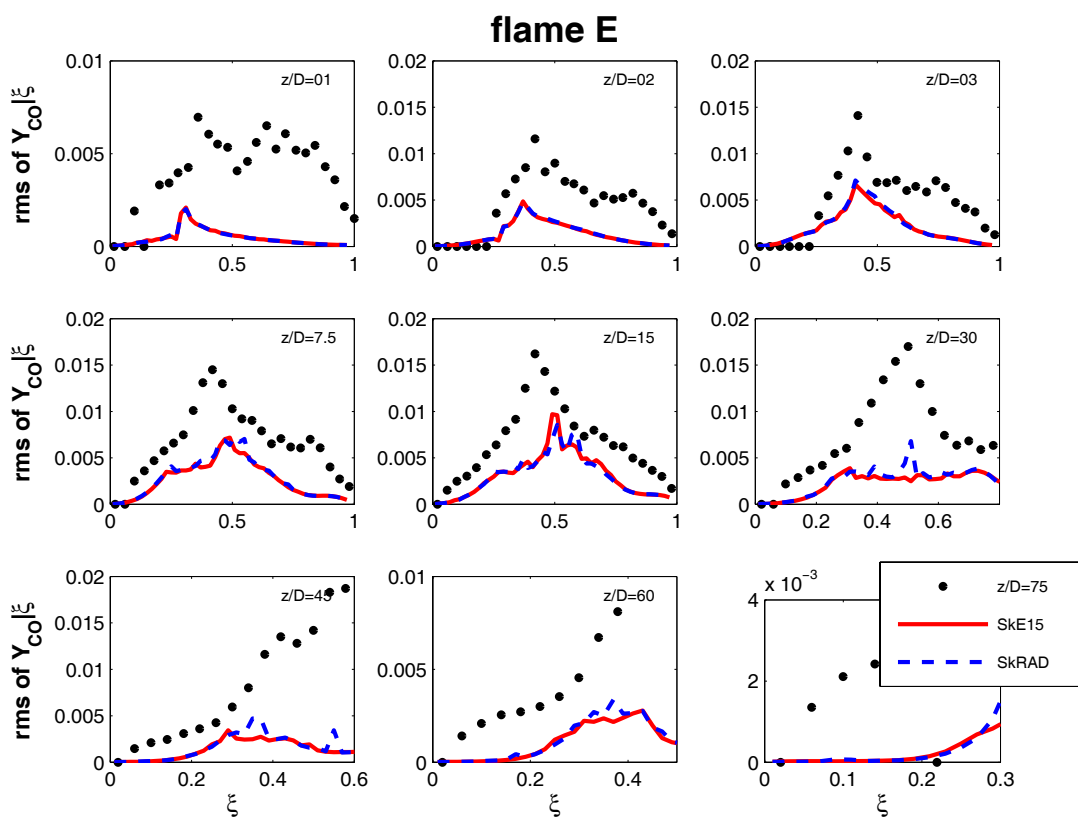
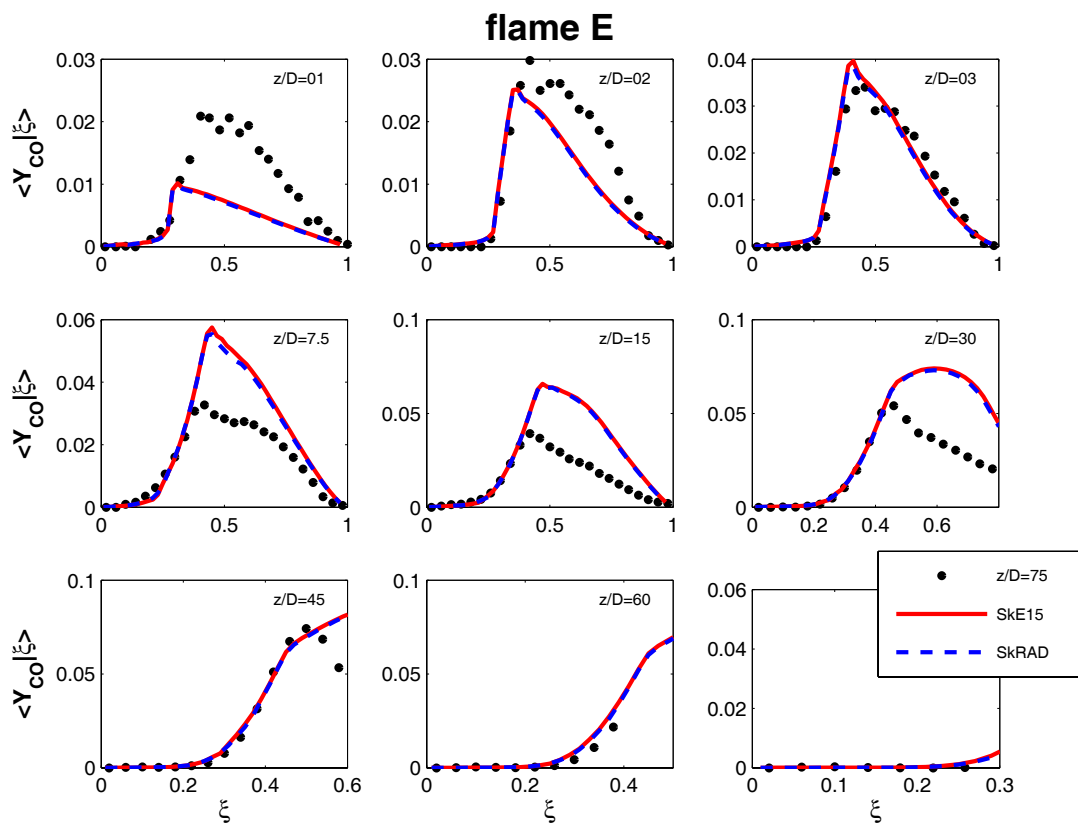


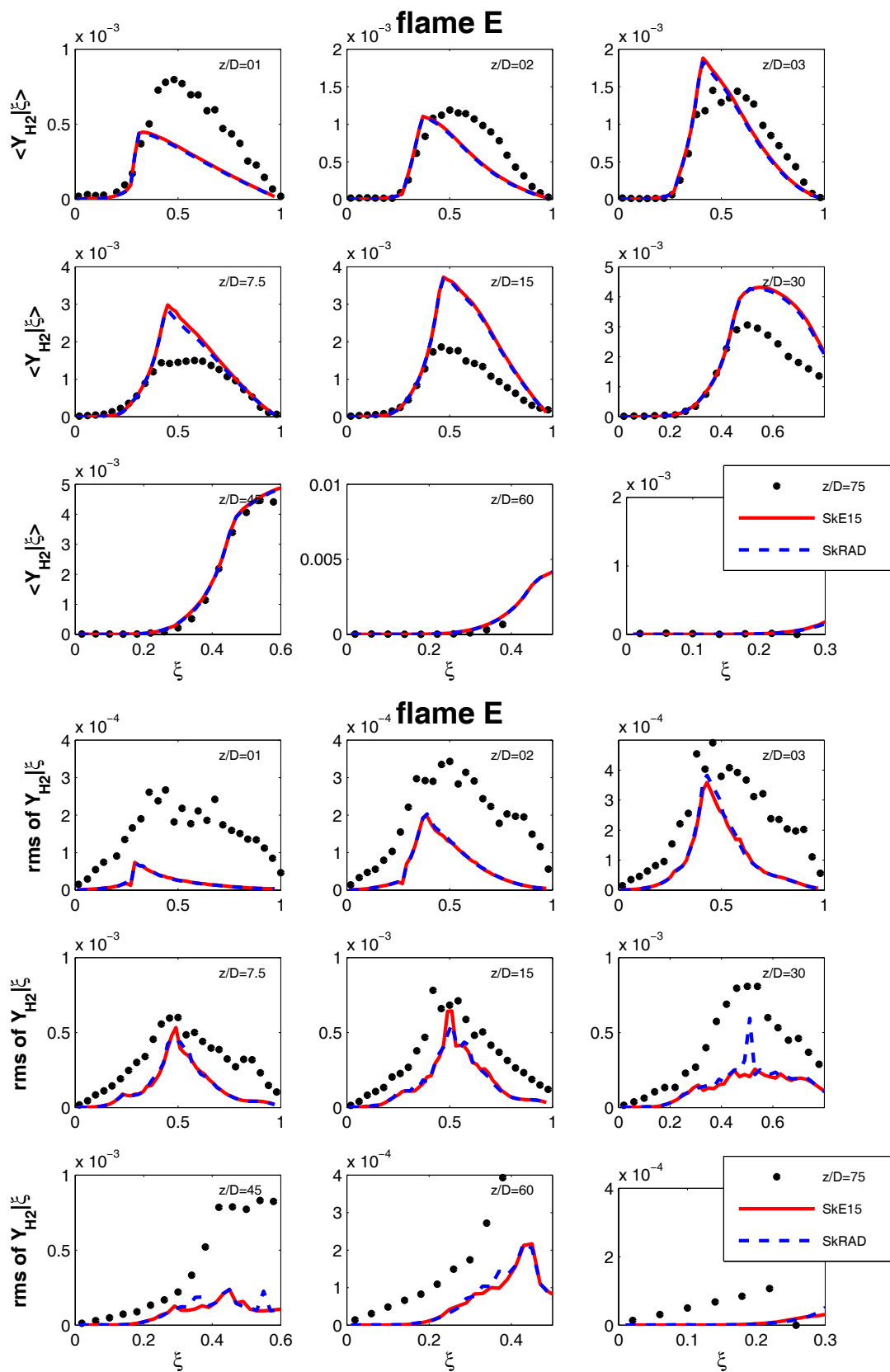


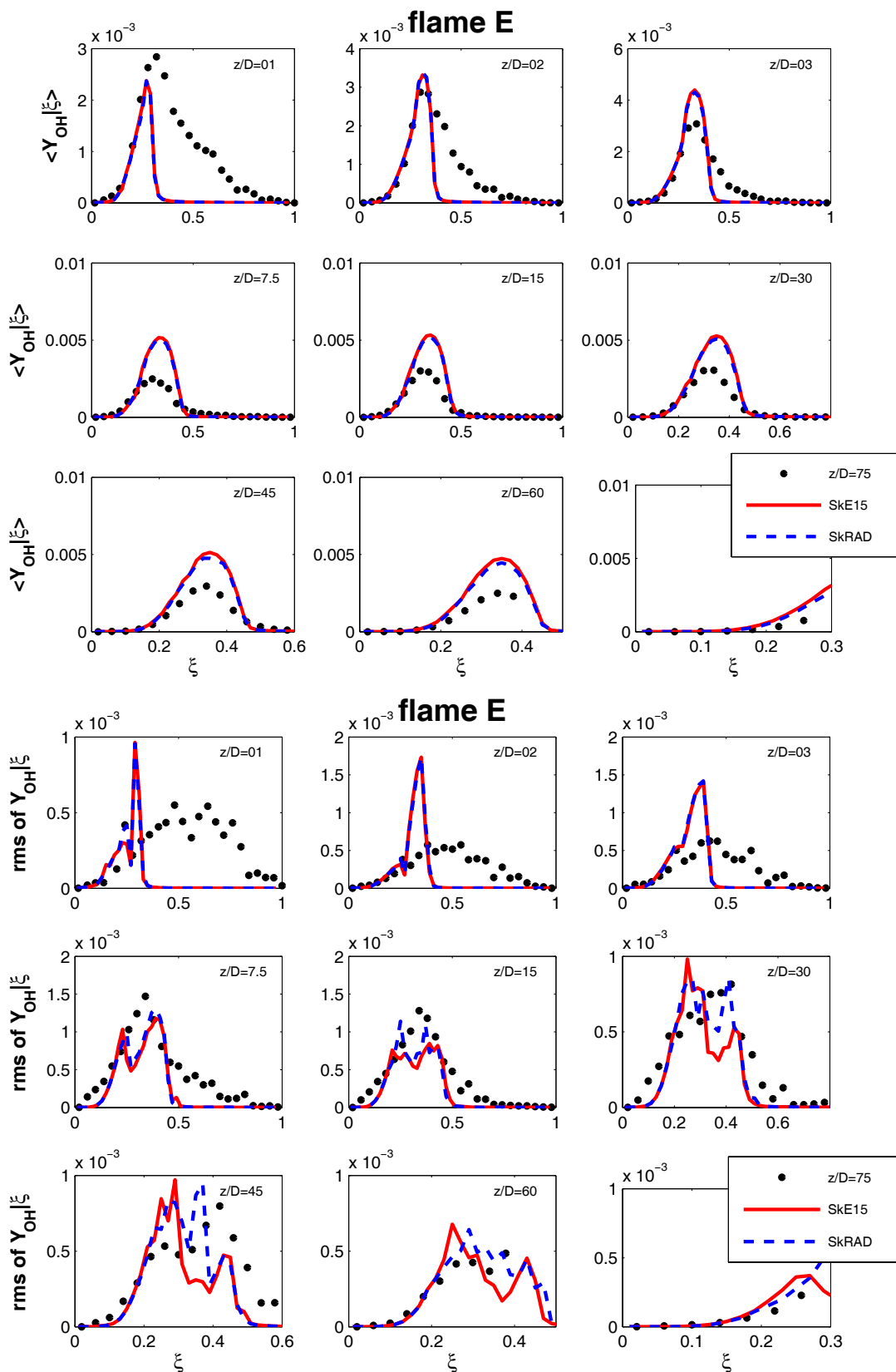




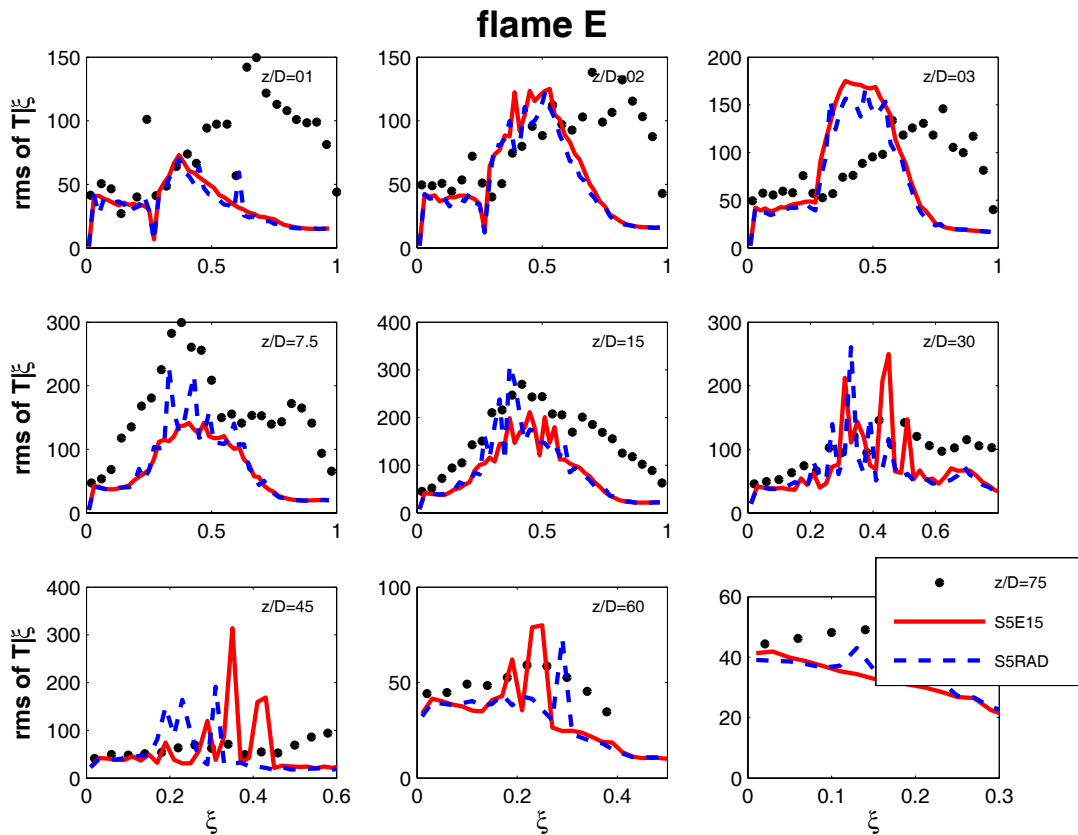
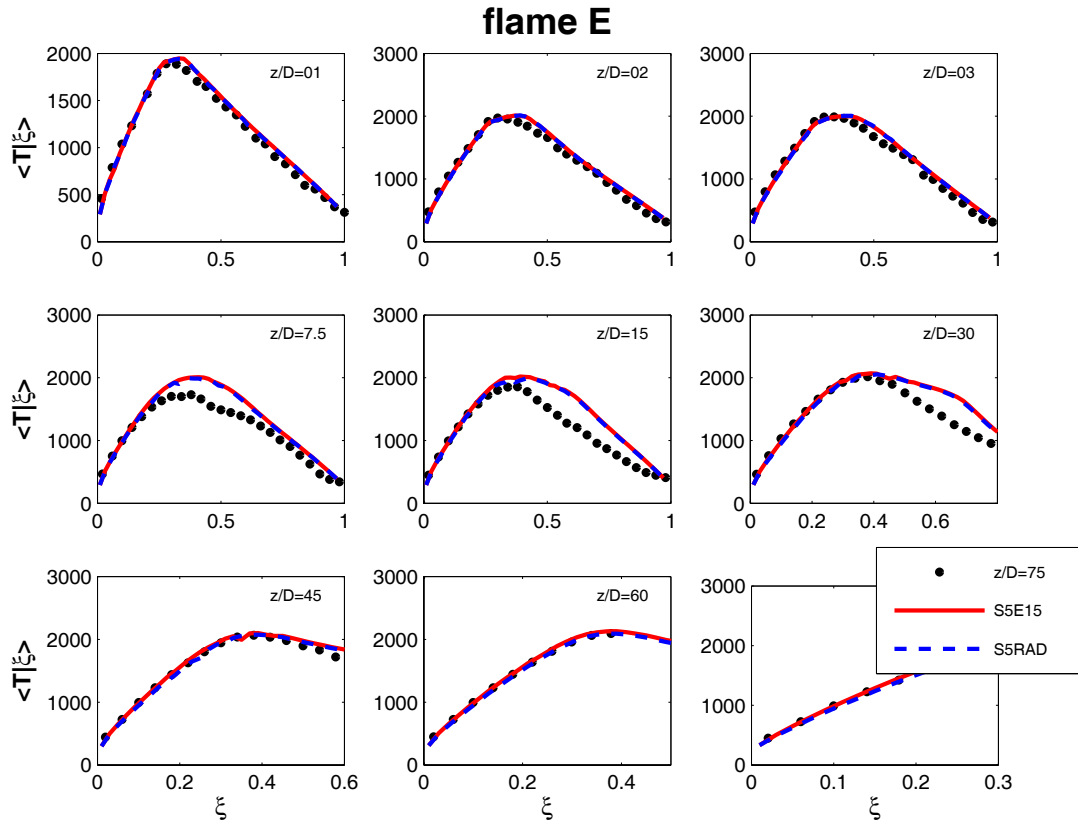


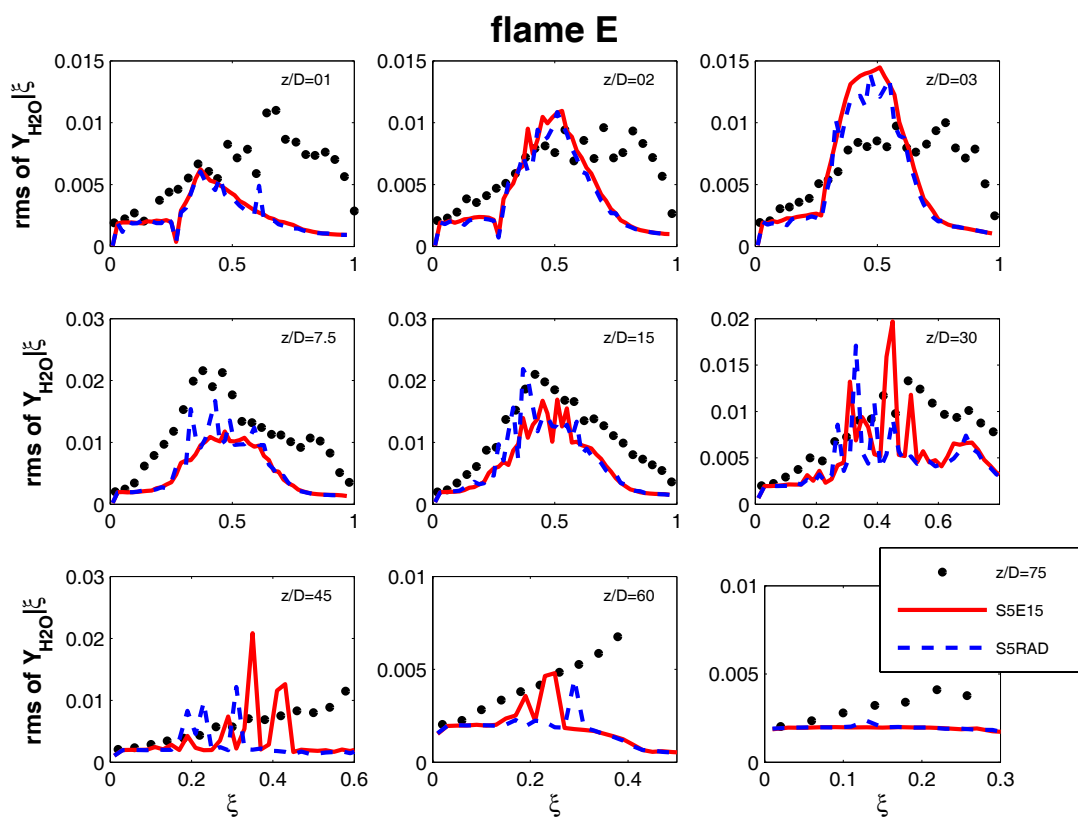
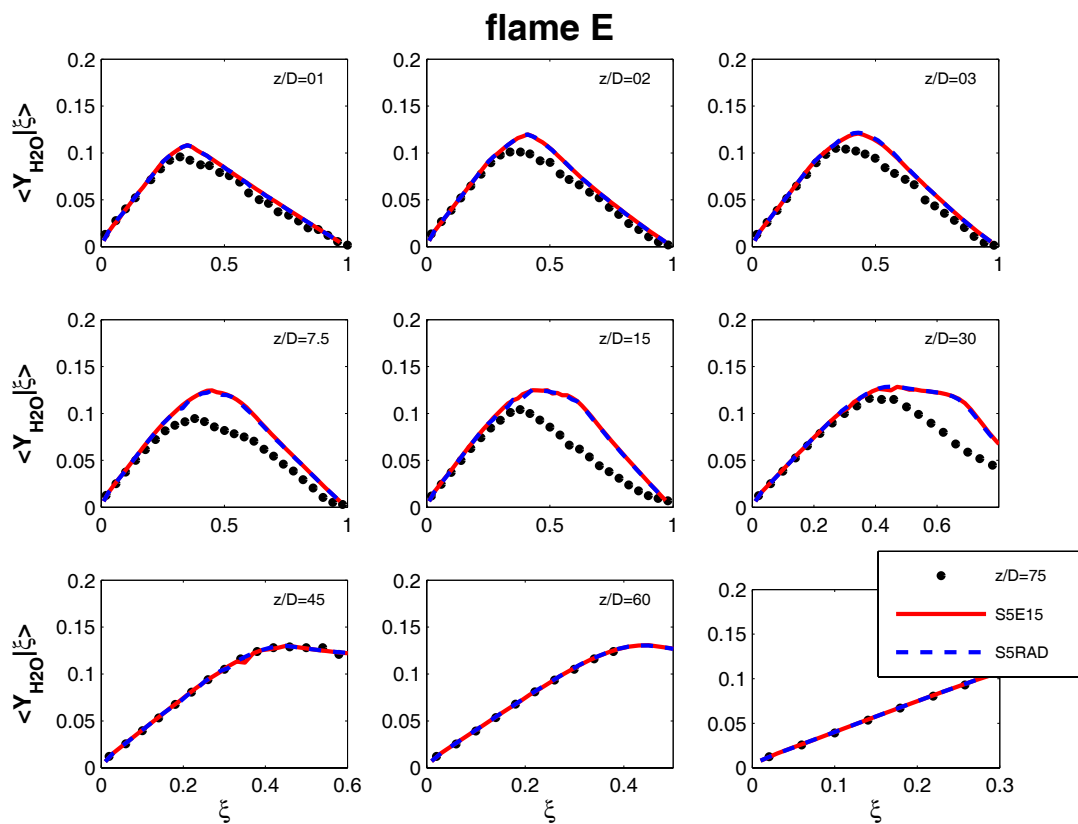


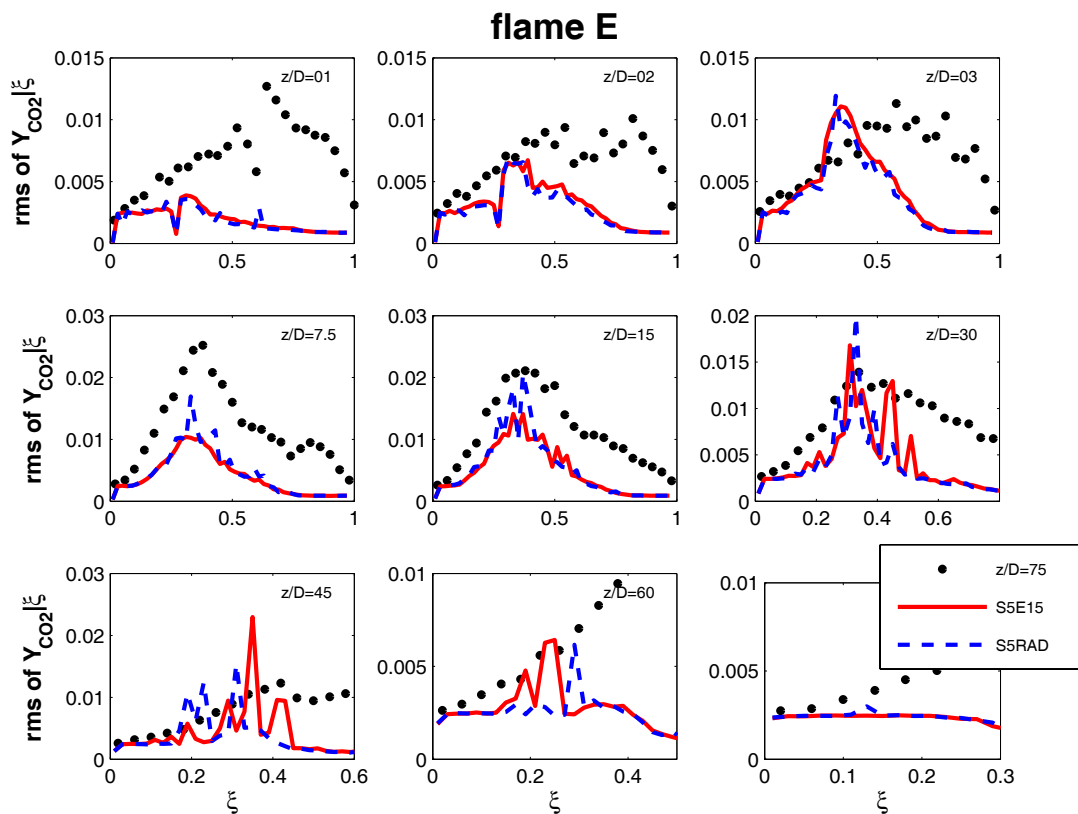
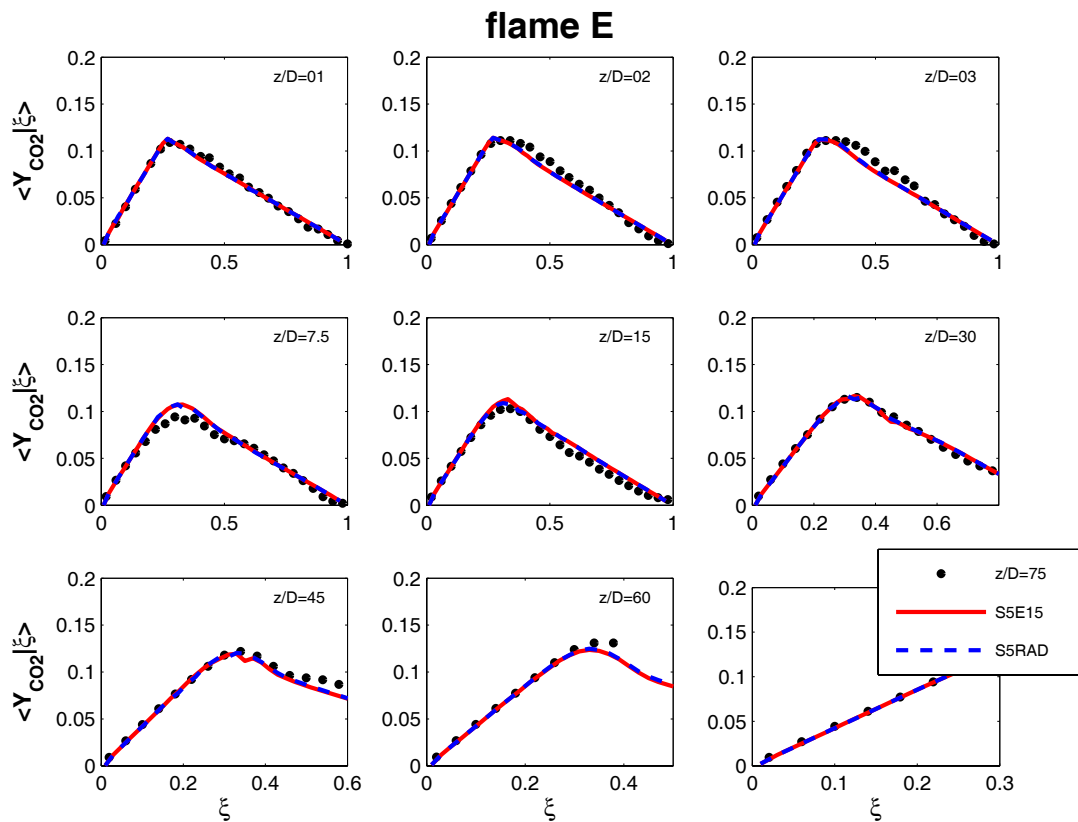


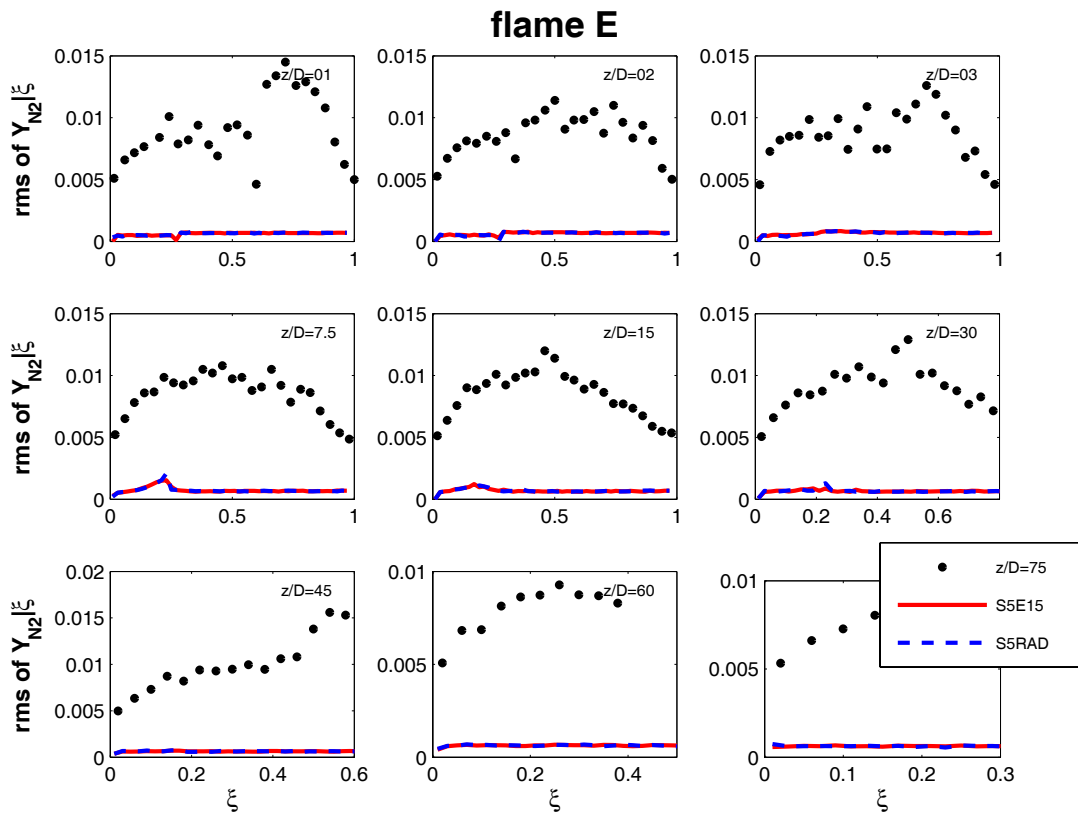
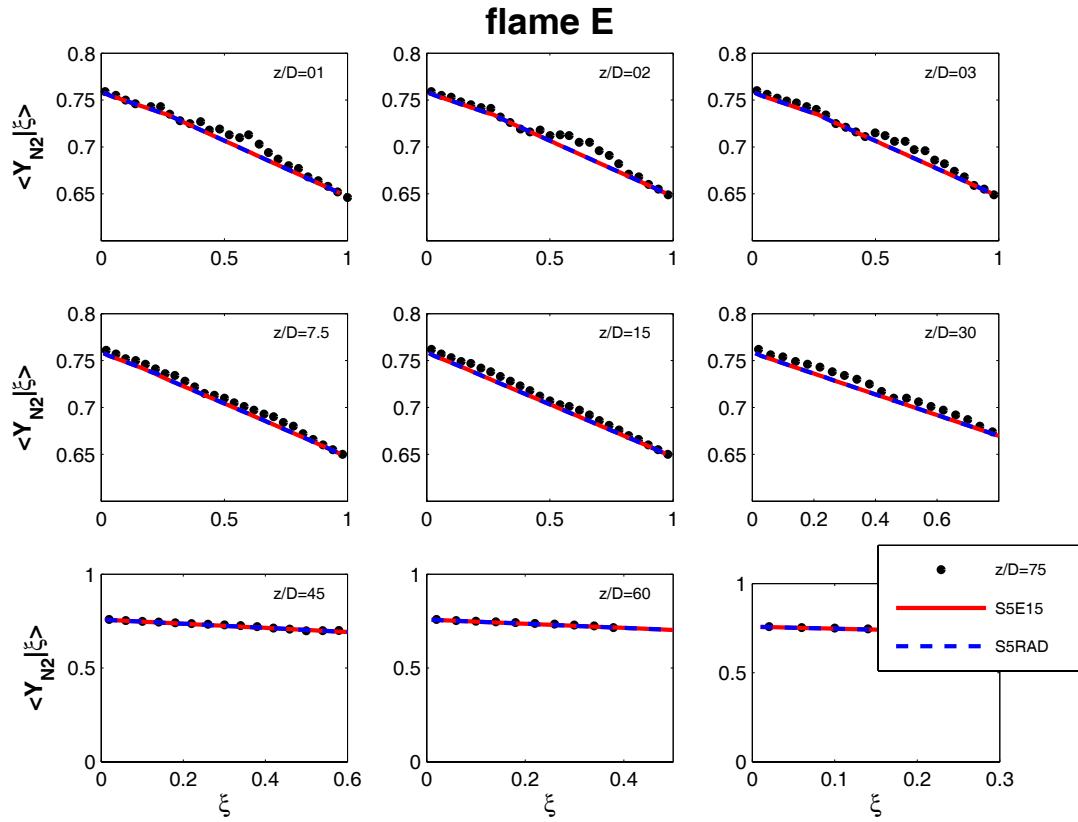


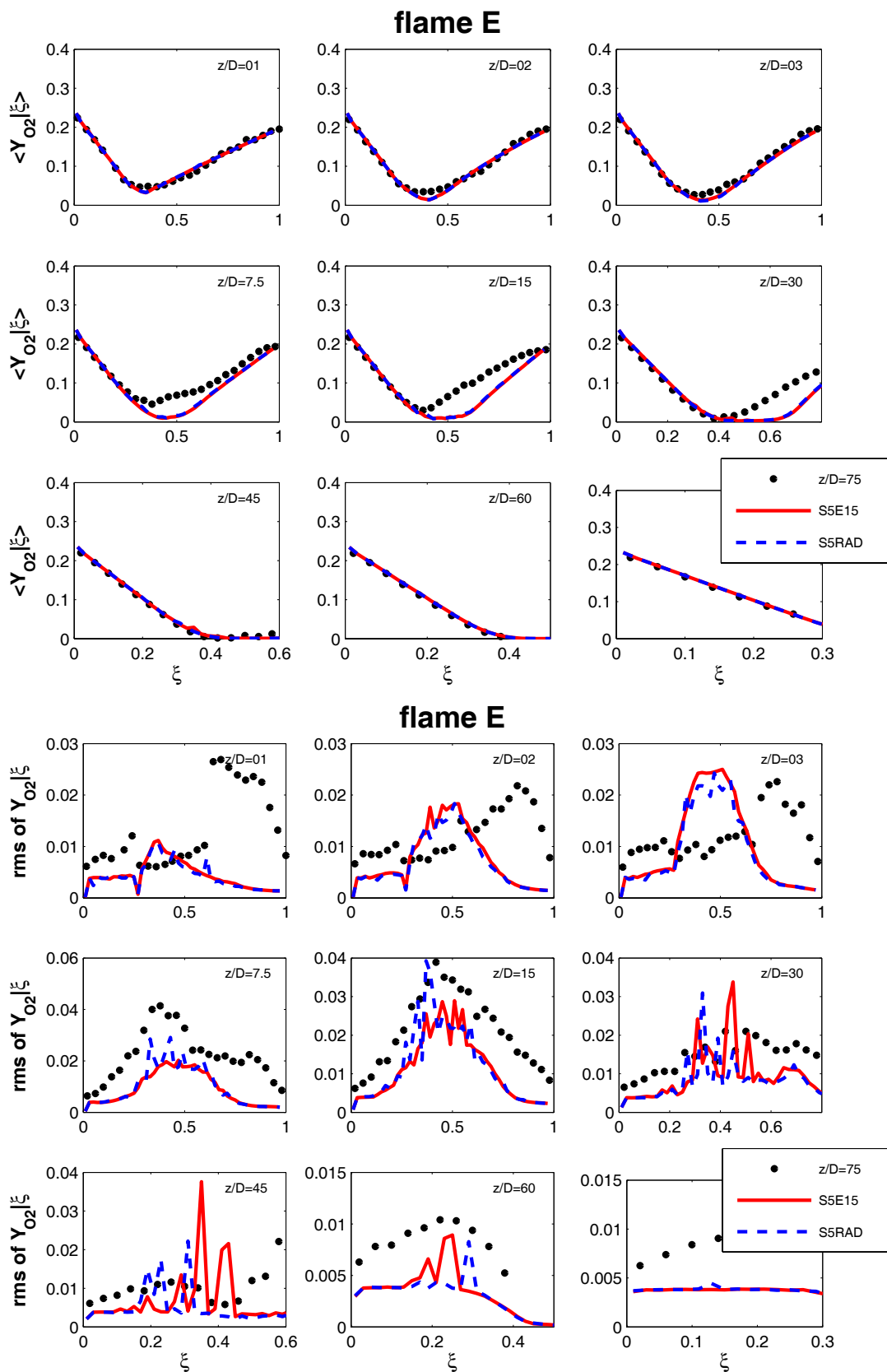
(6) S5E15 and S5RAD

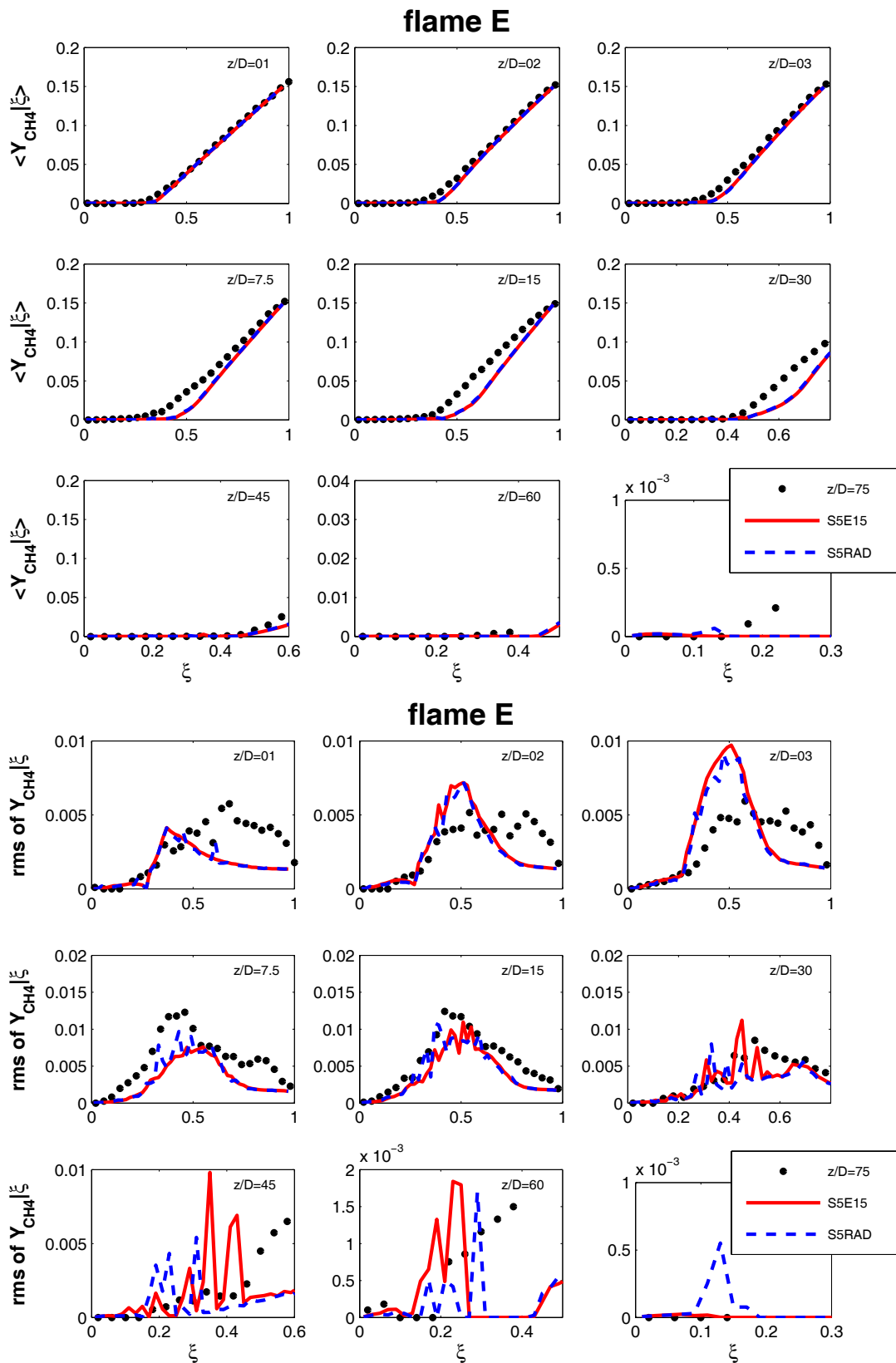


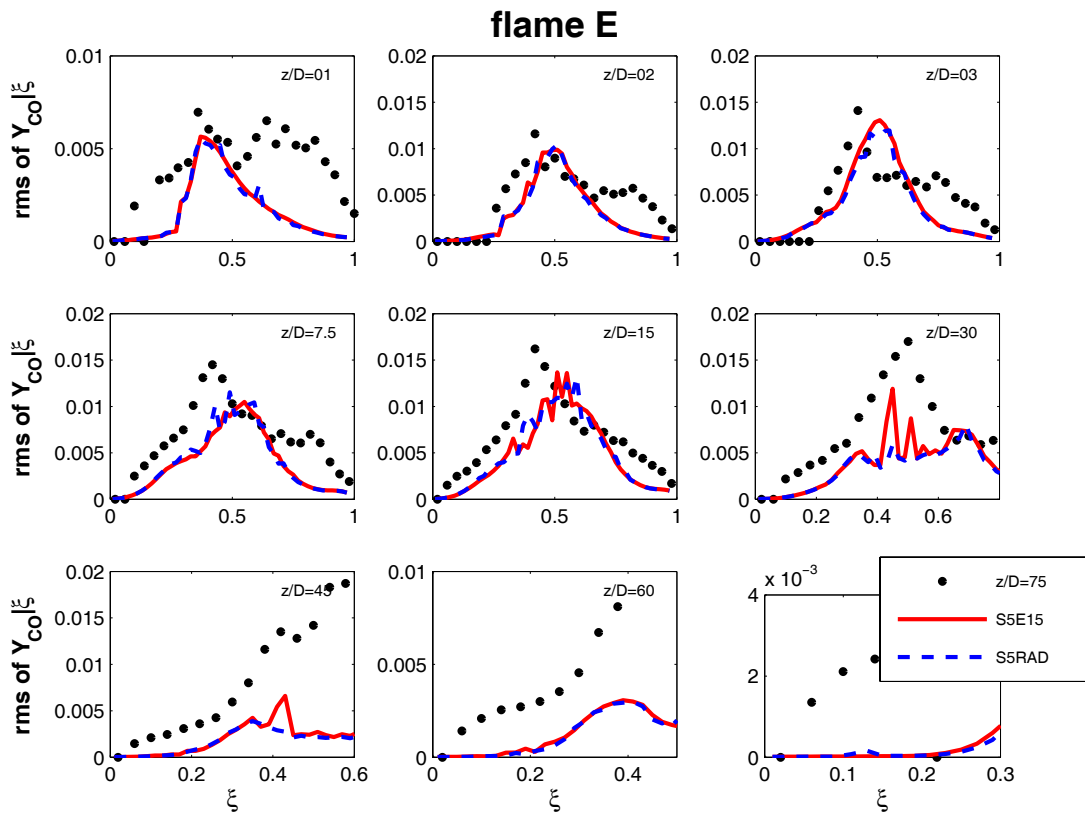
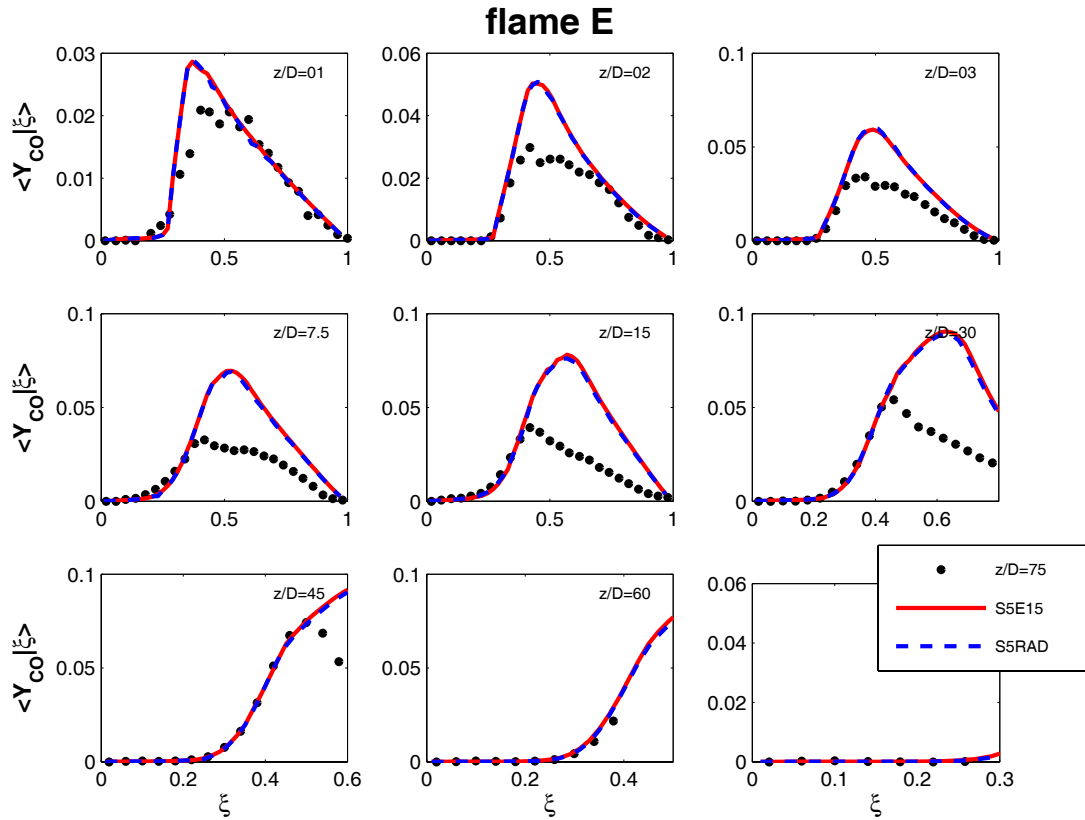


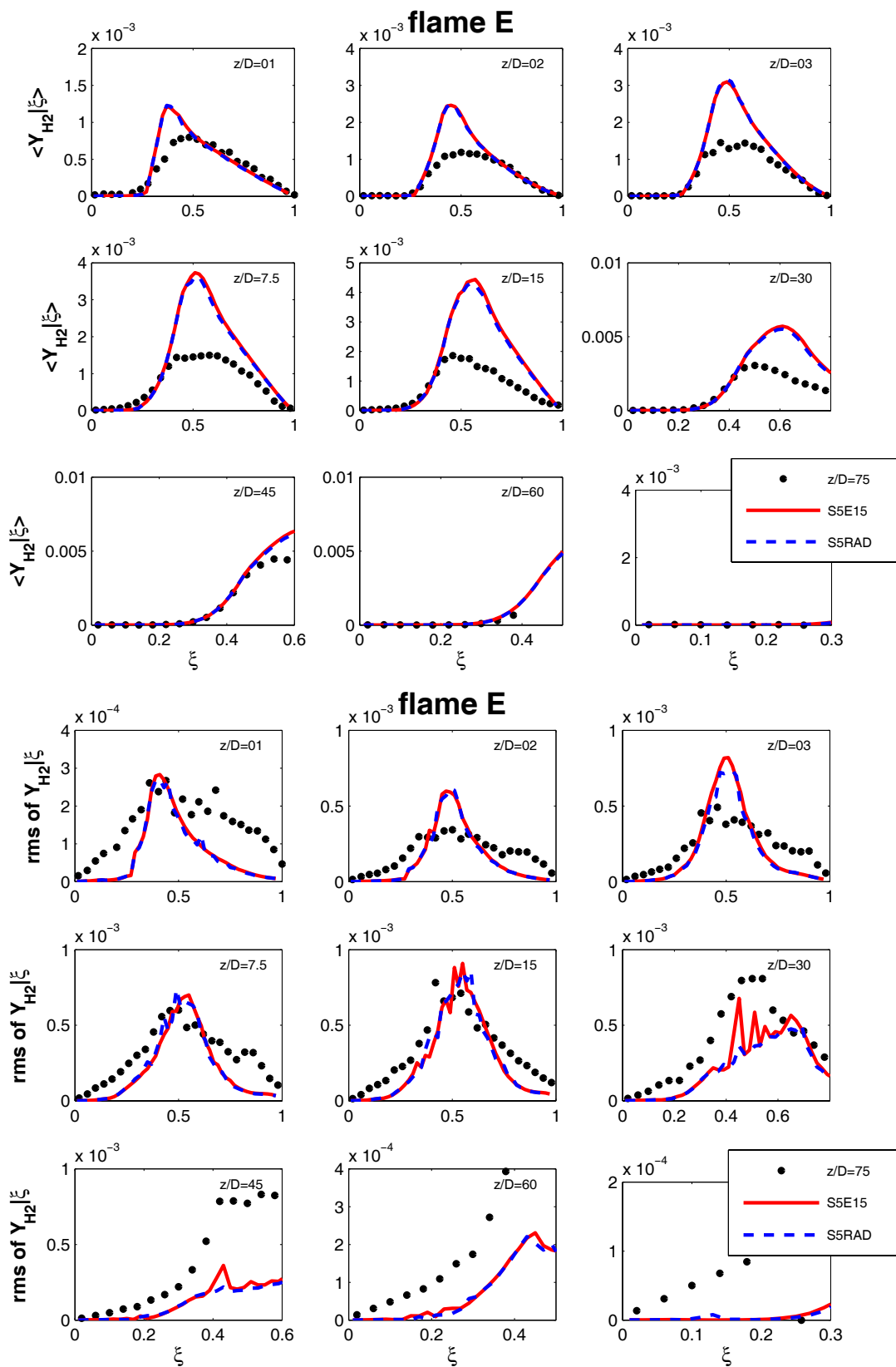


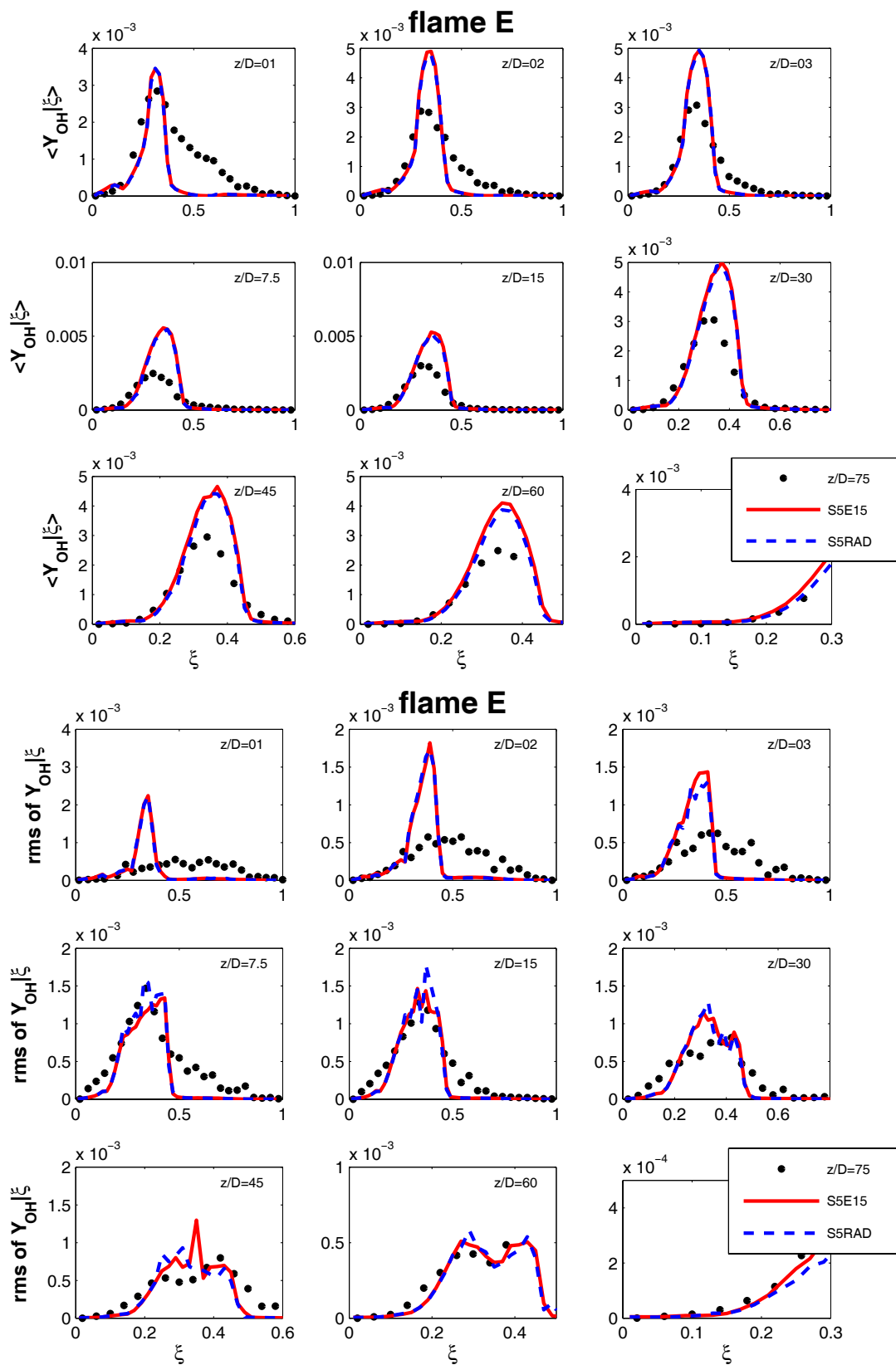


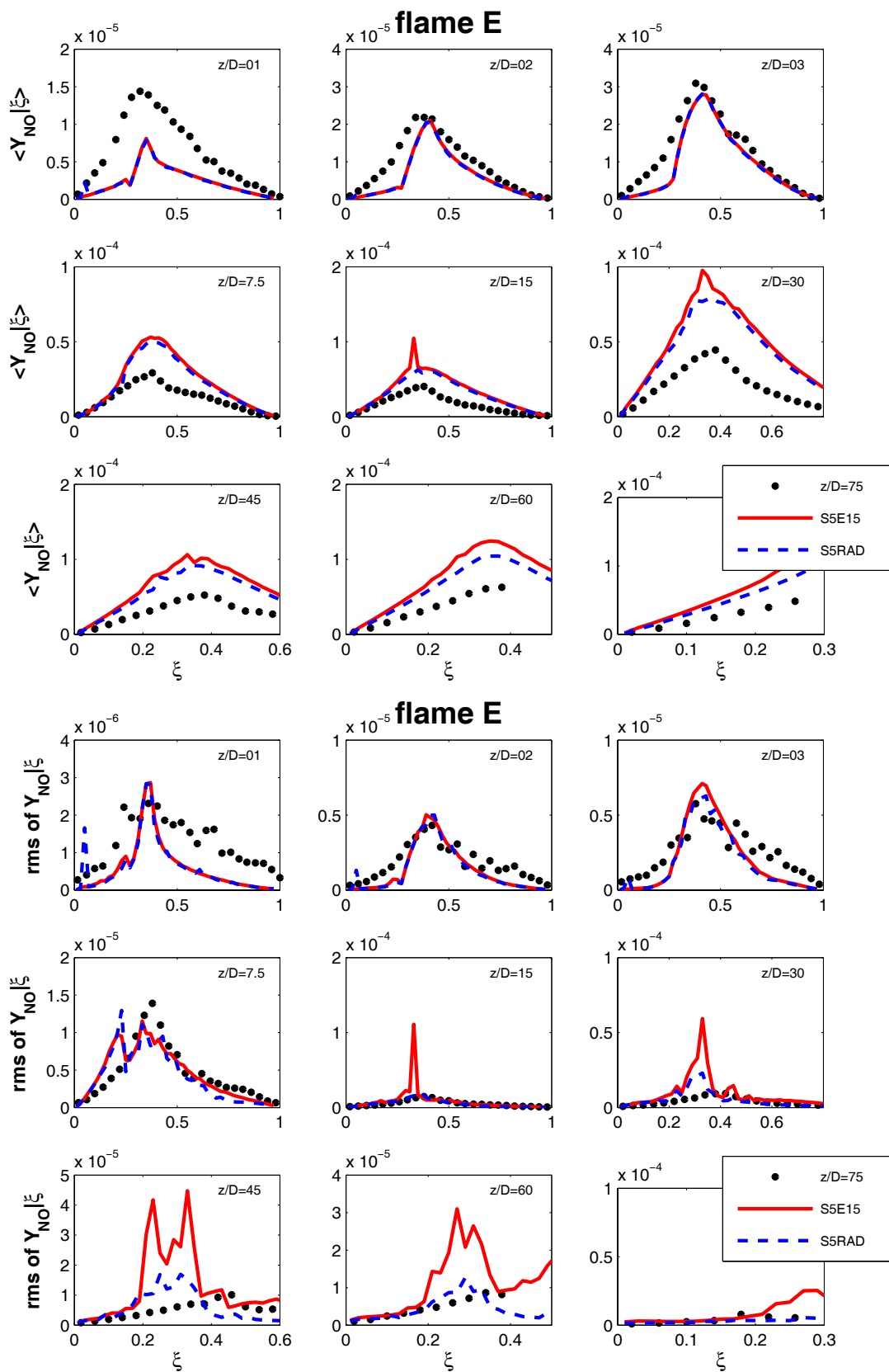




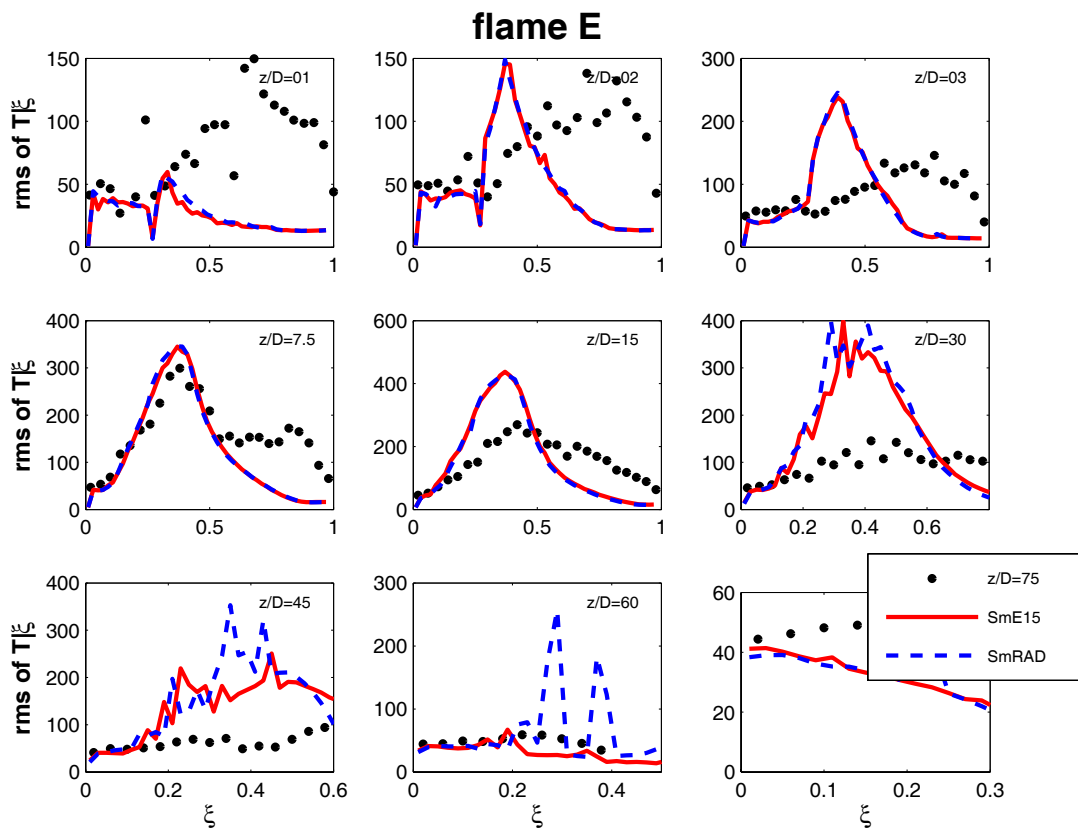
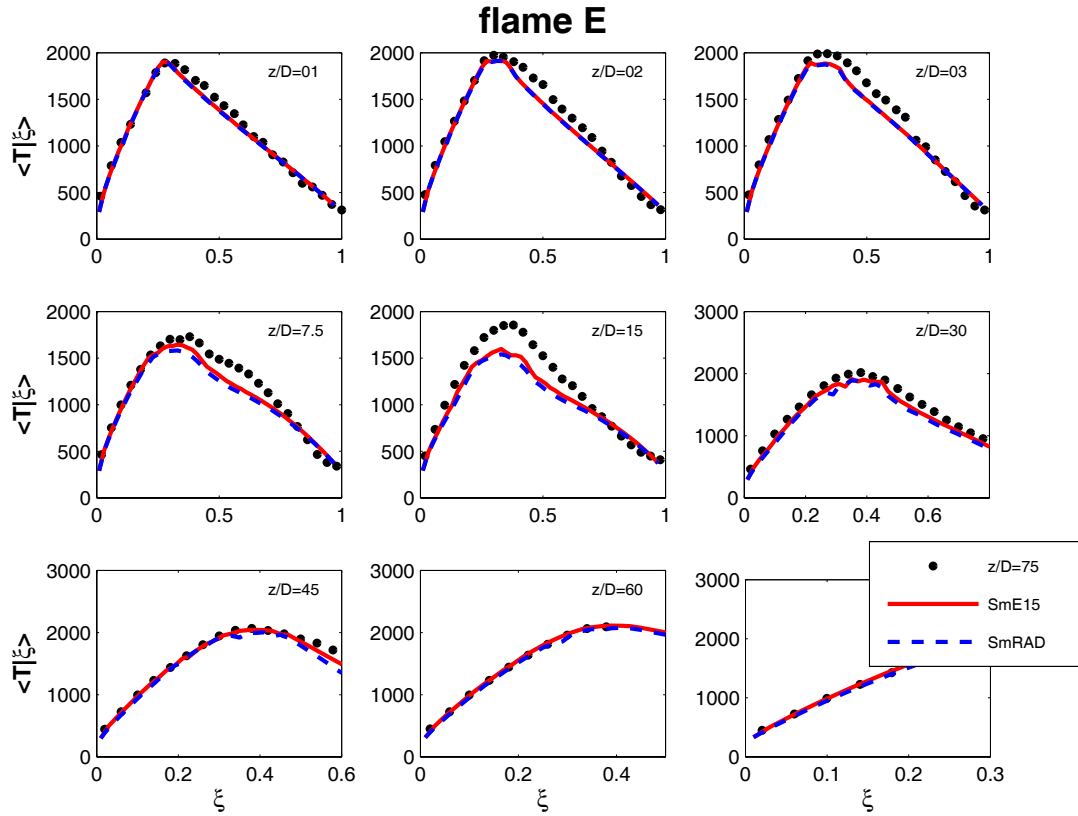


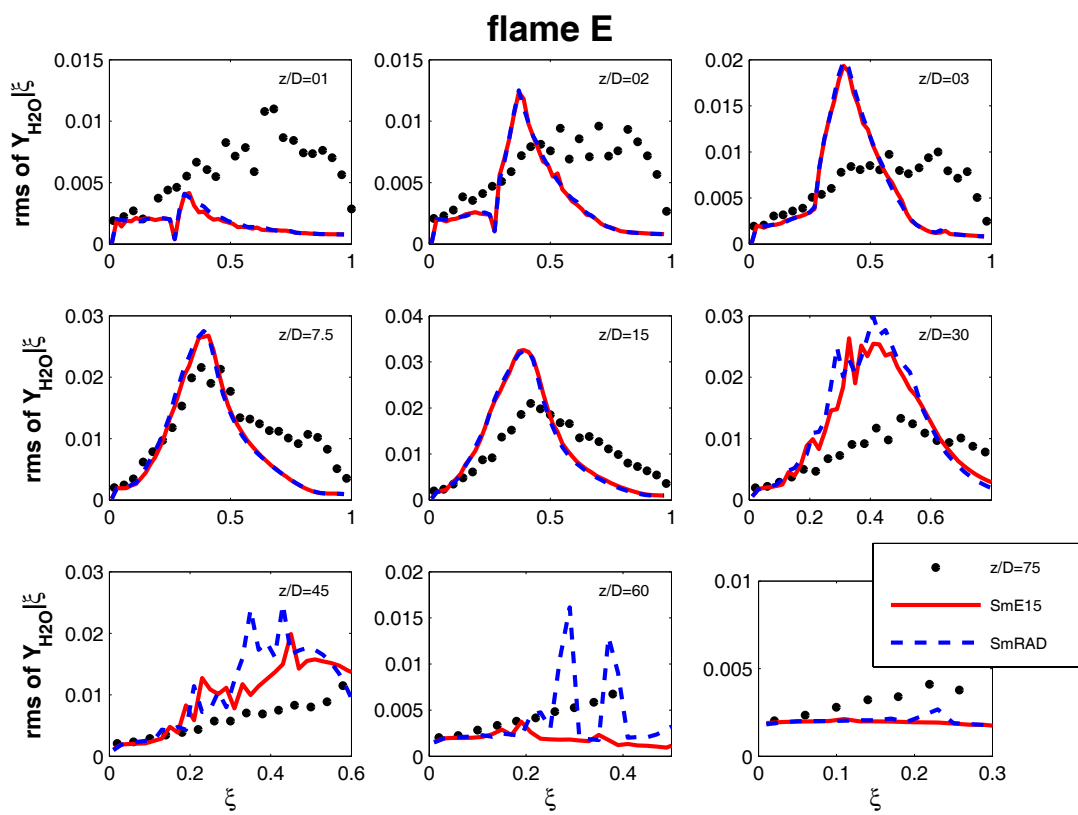
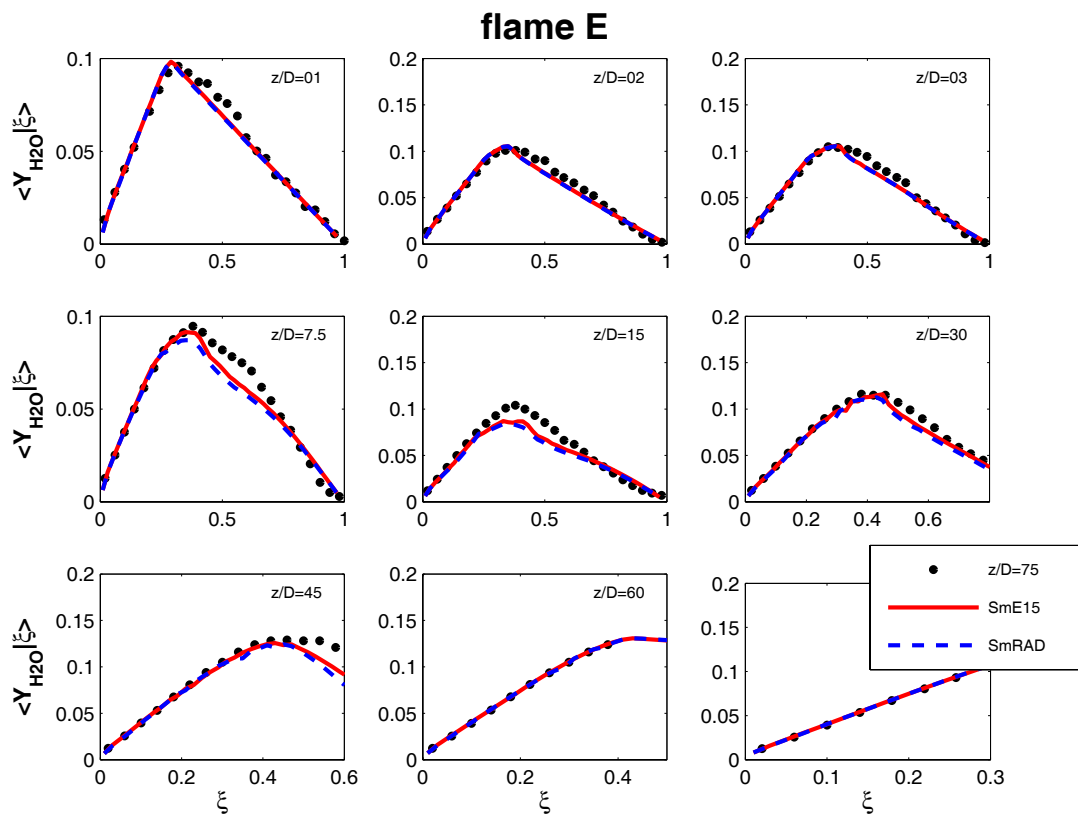


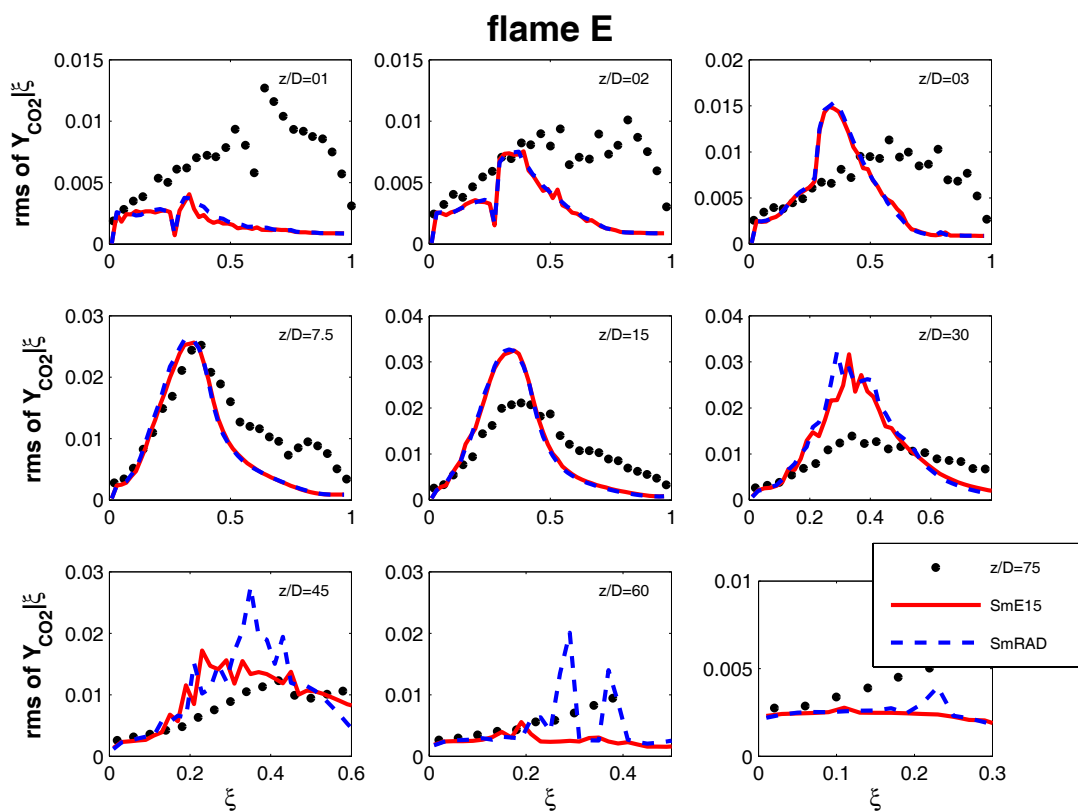
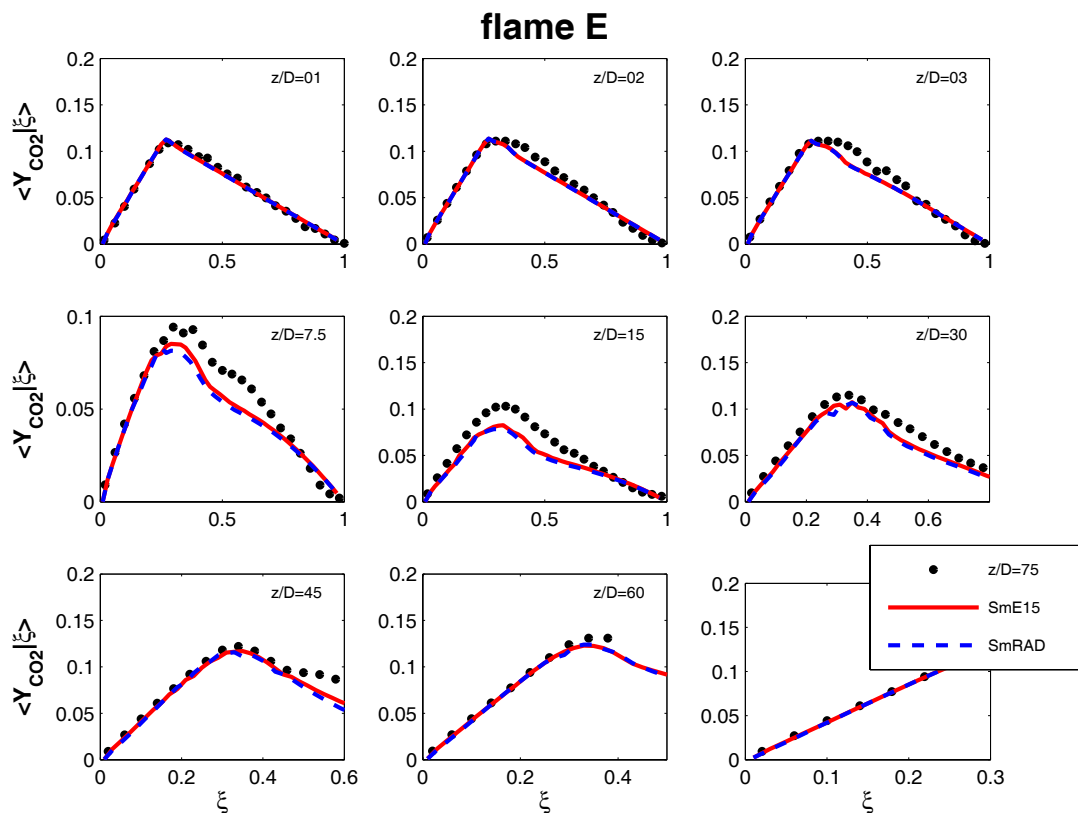


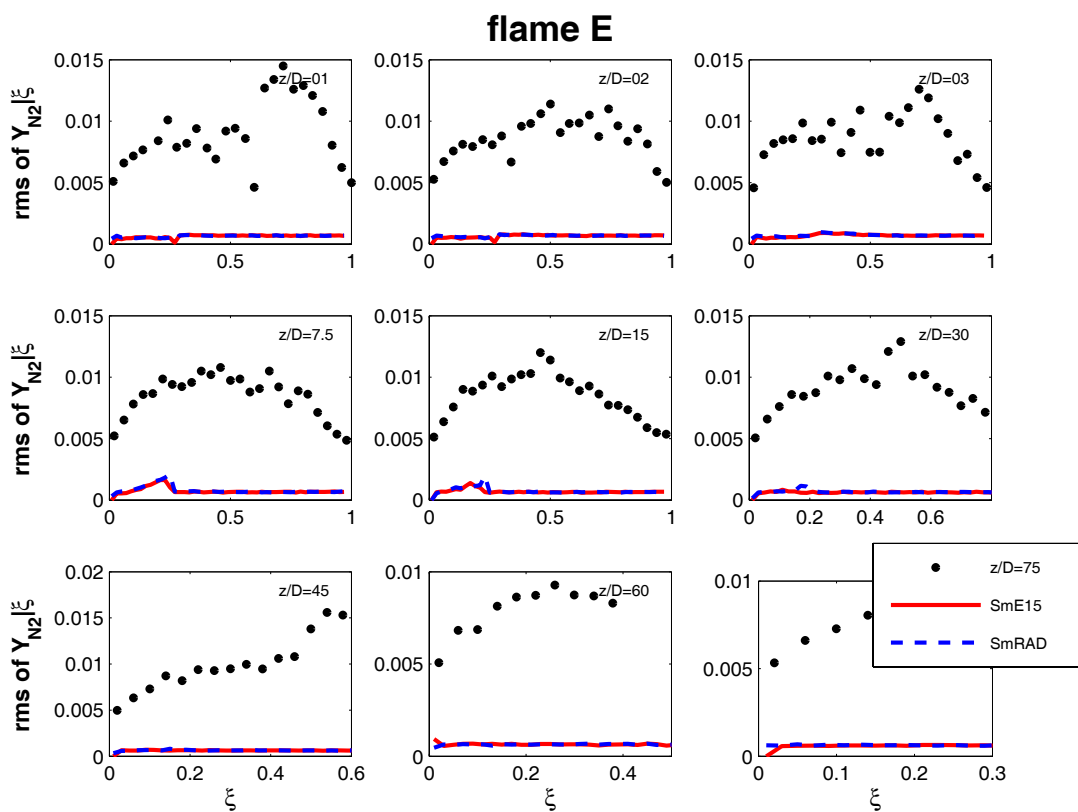
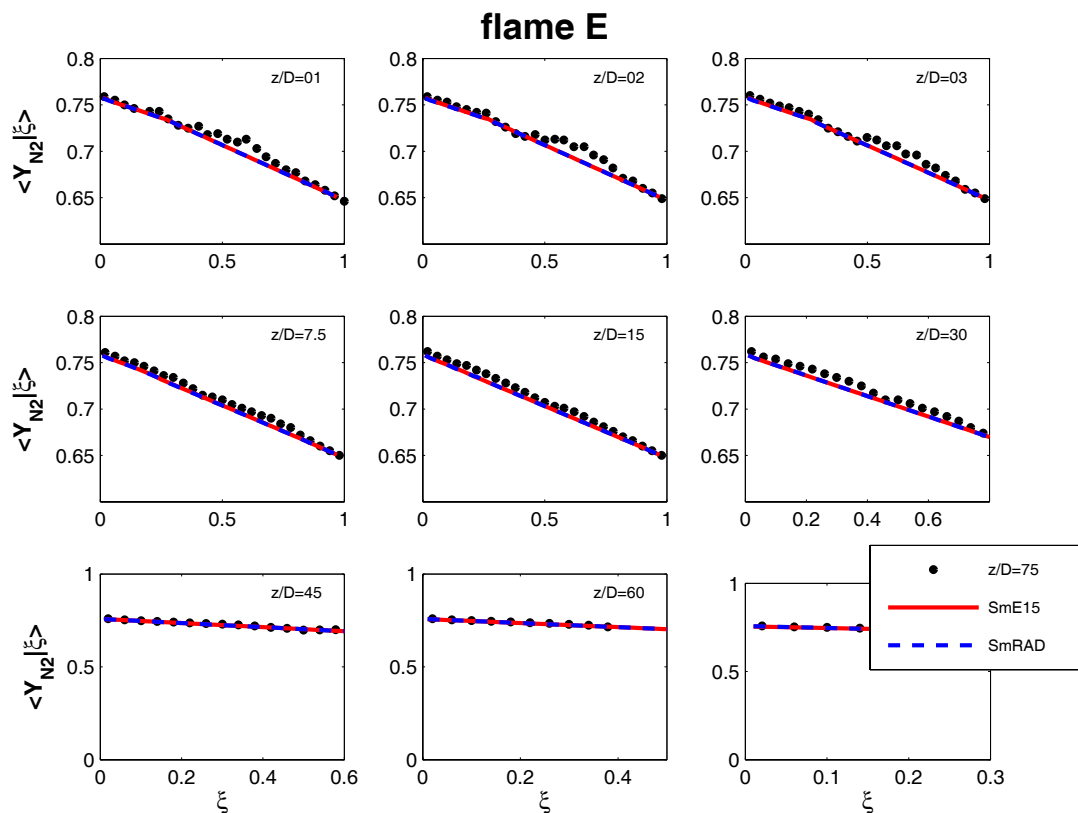


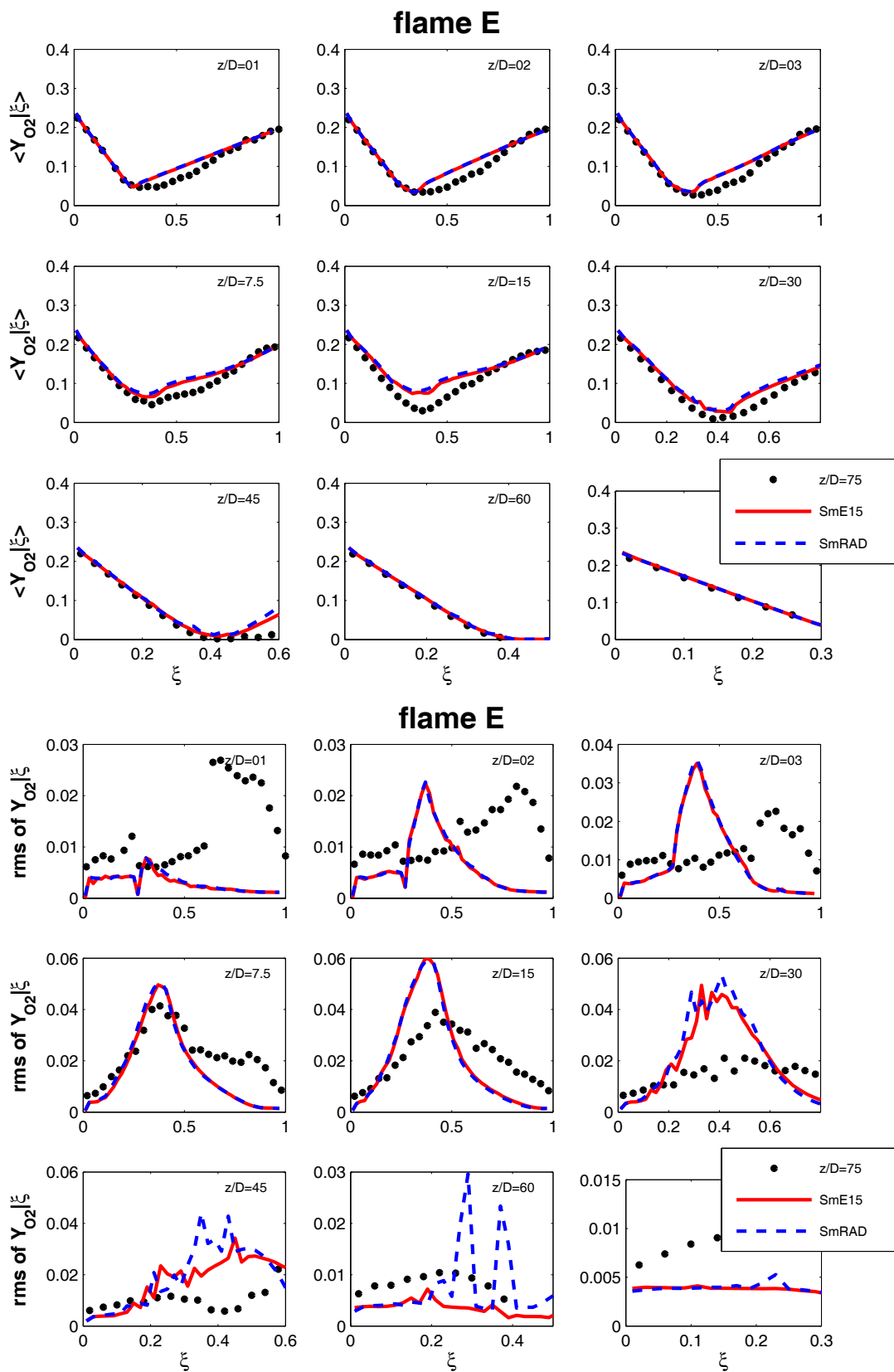
(7) SmE15 and SmRAD

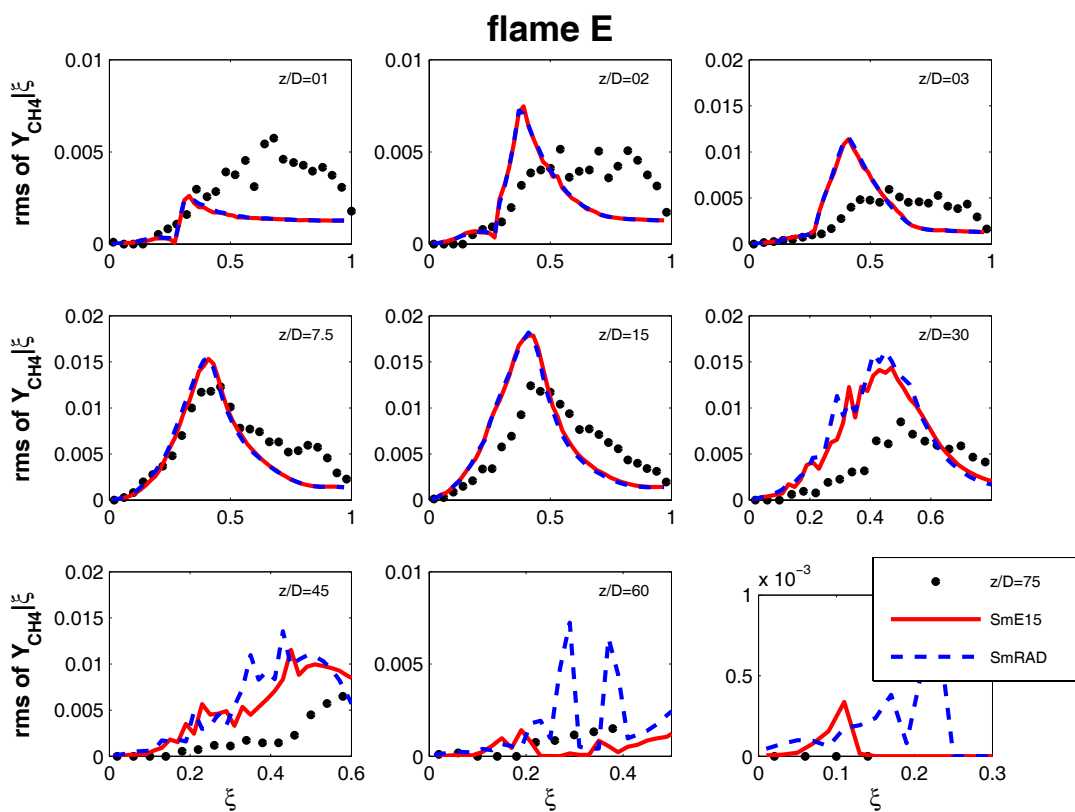
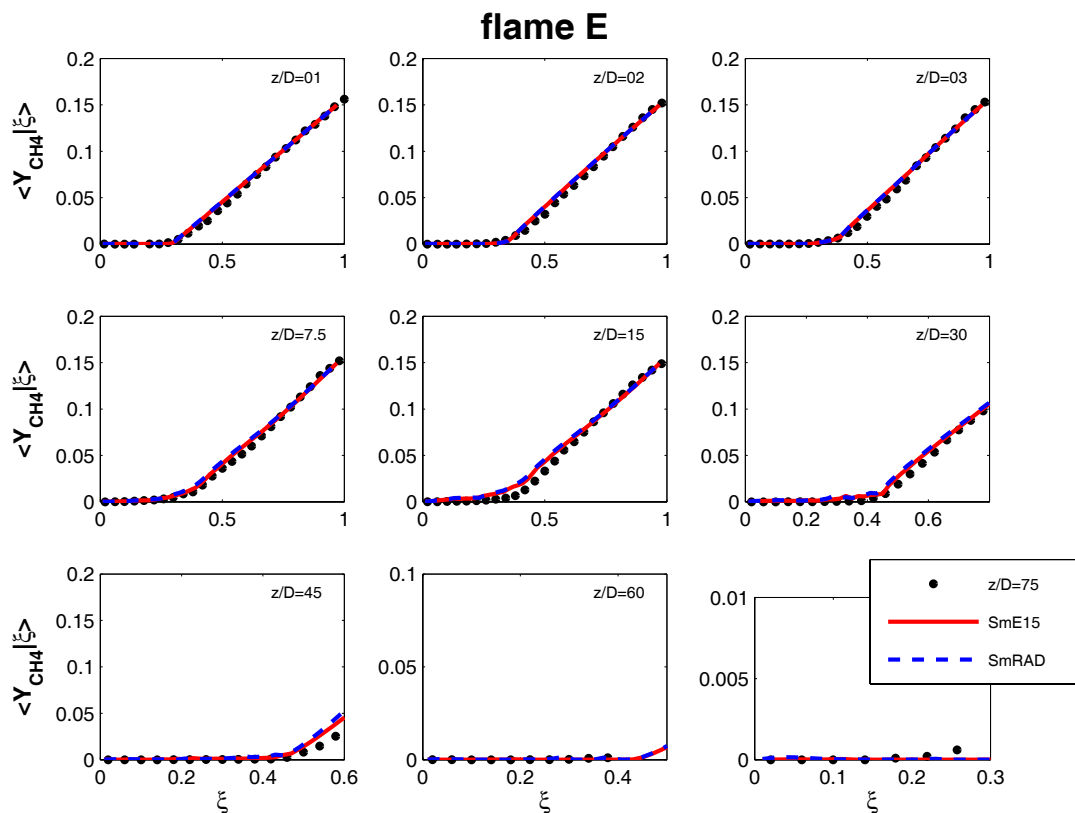


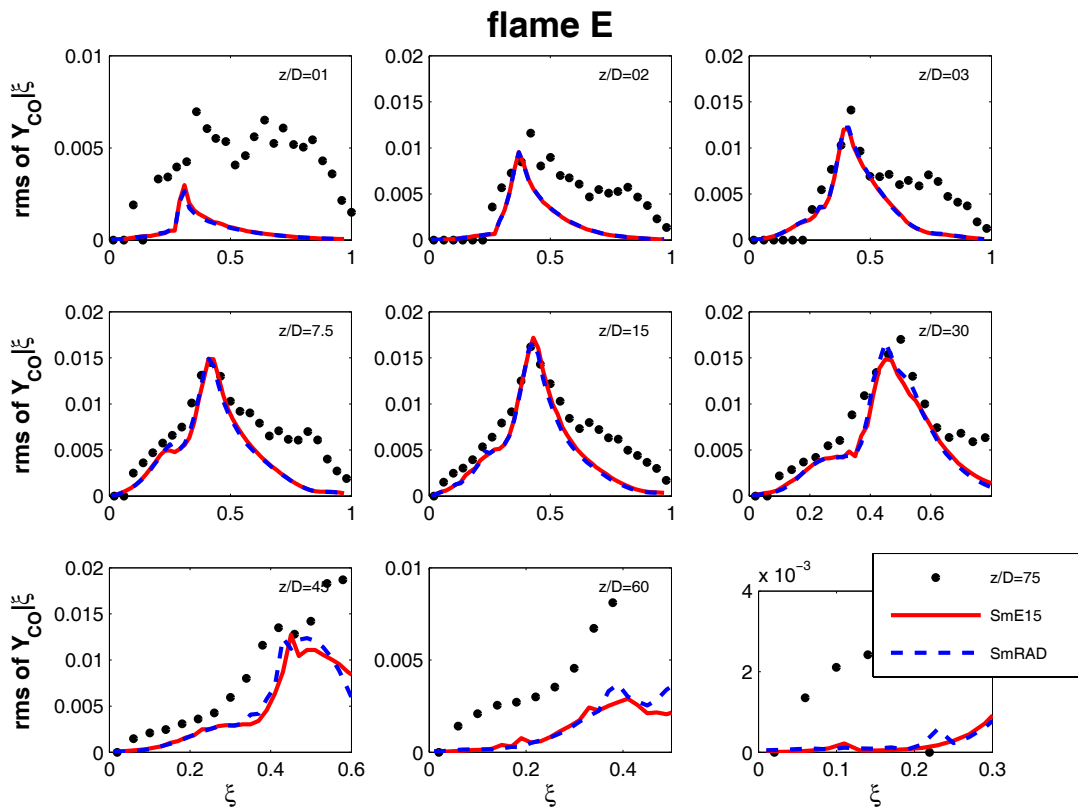
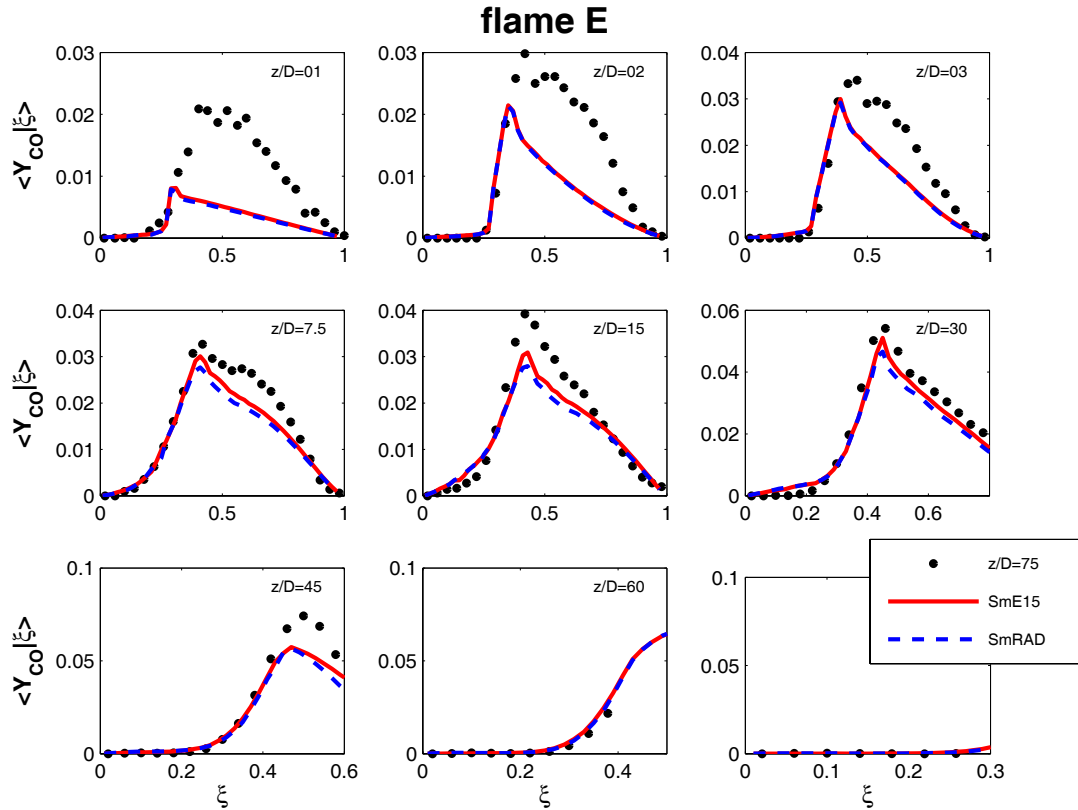


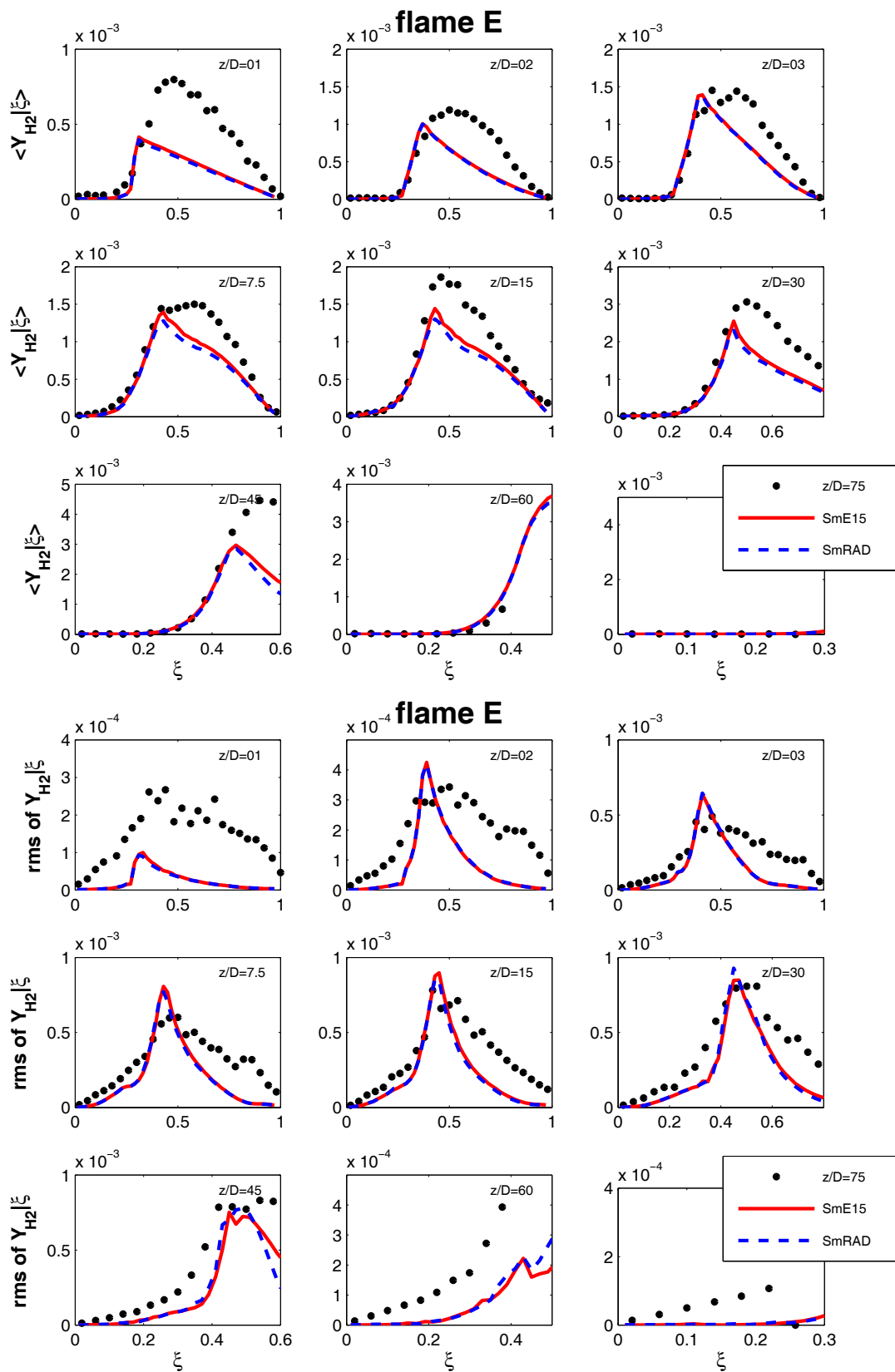


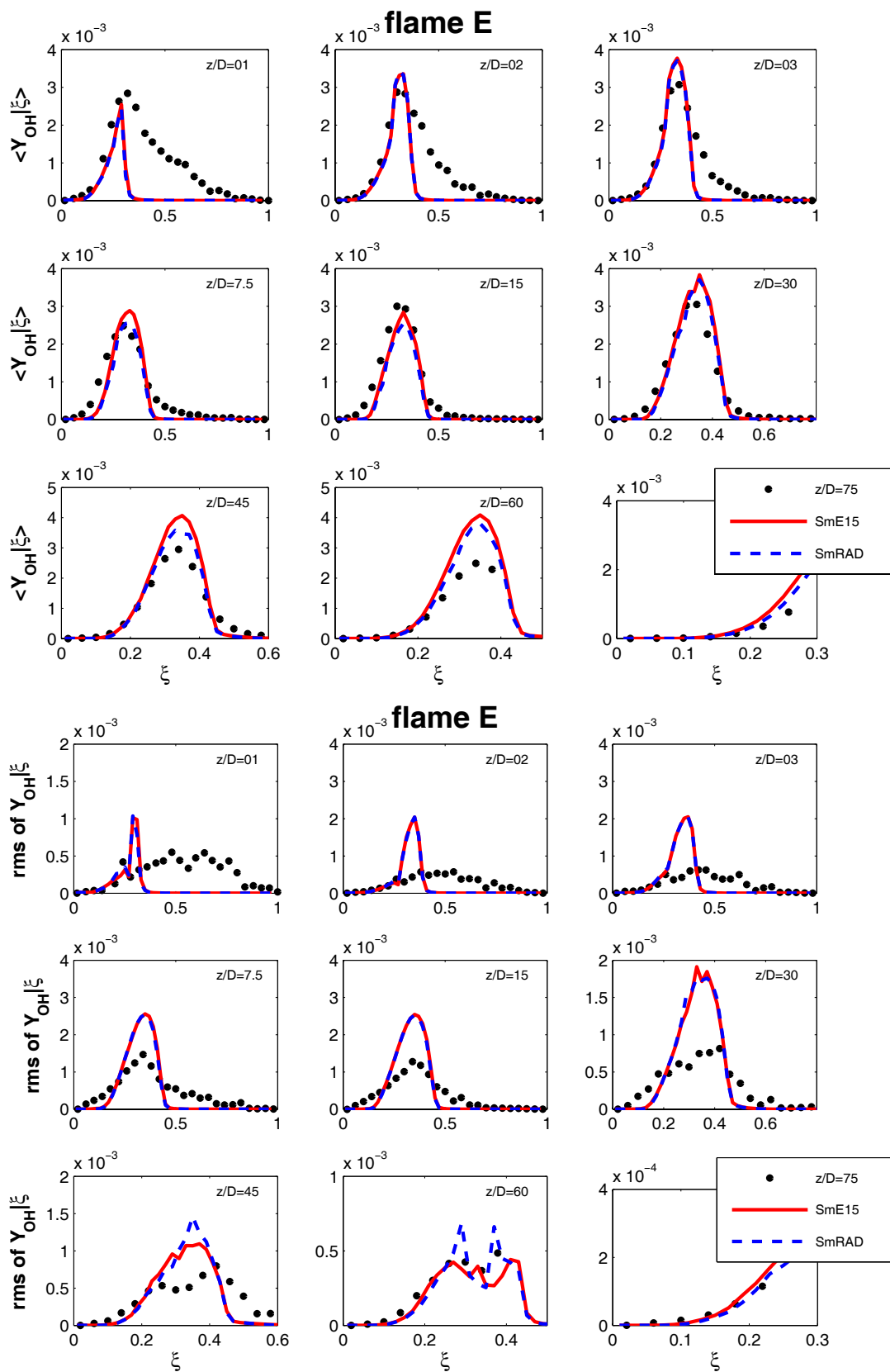






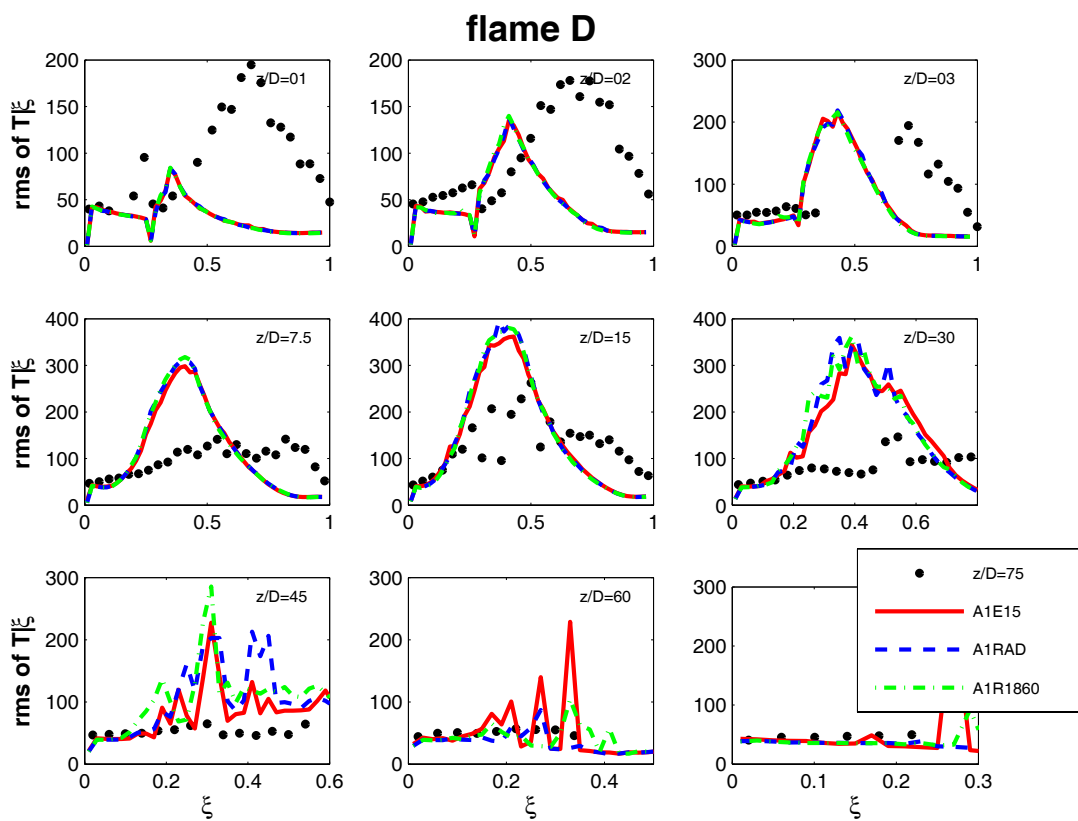
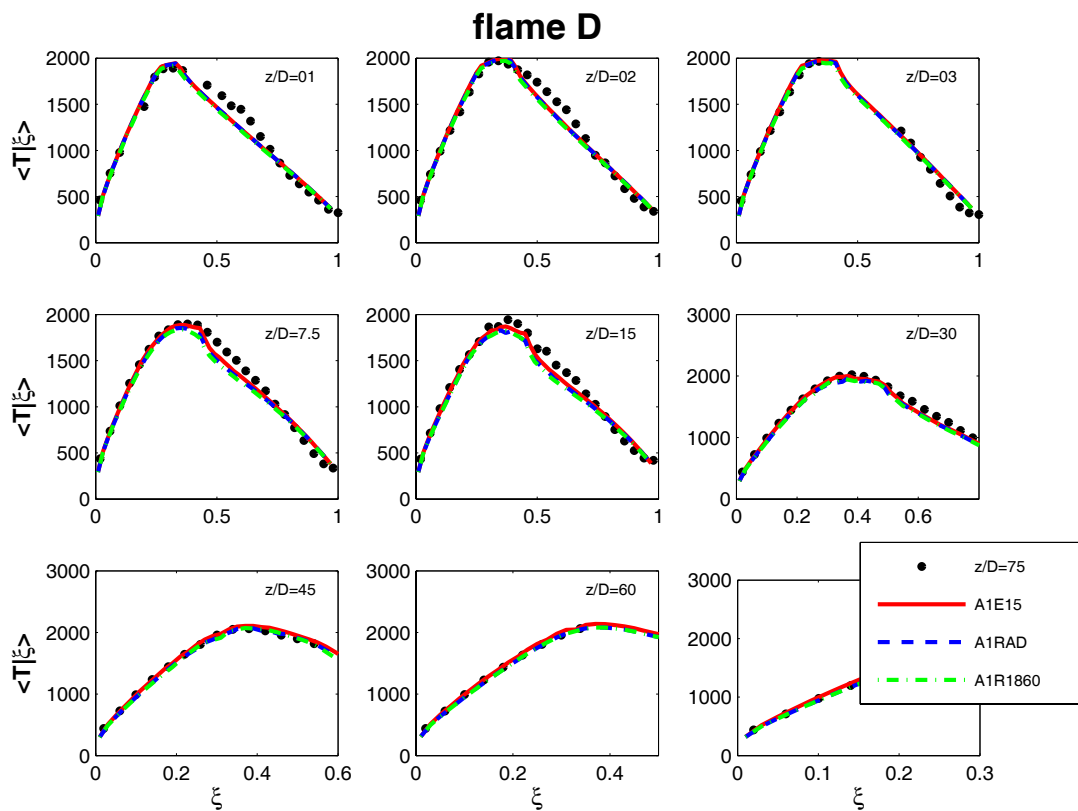


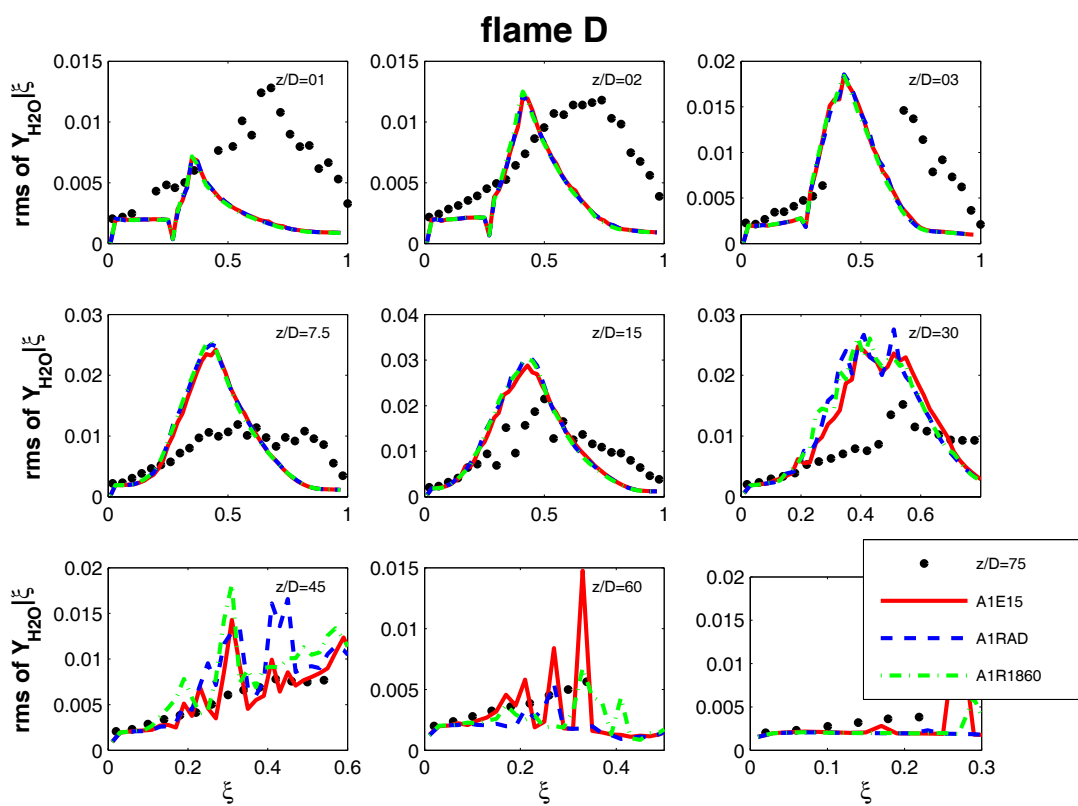
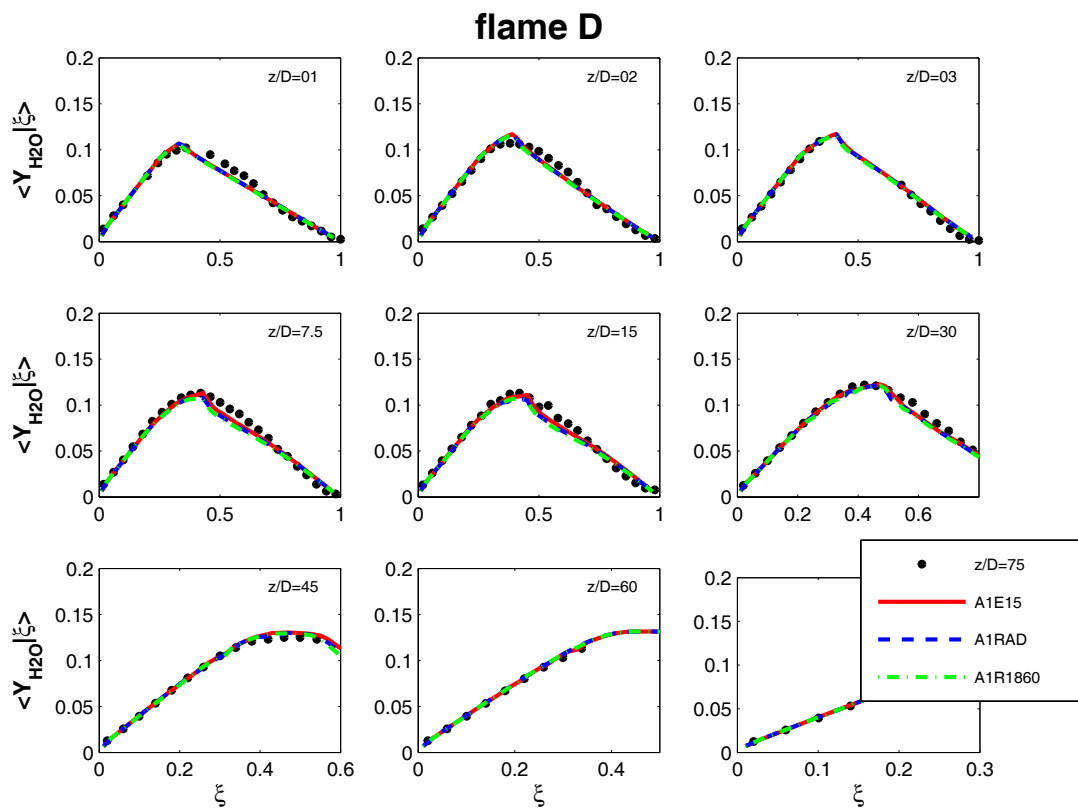


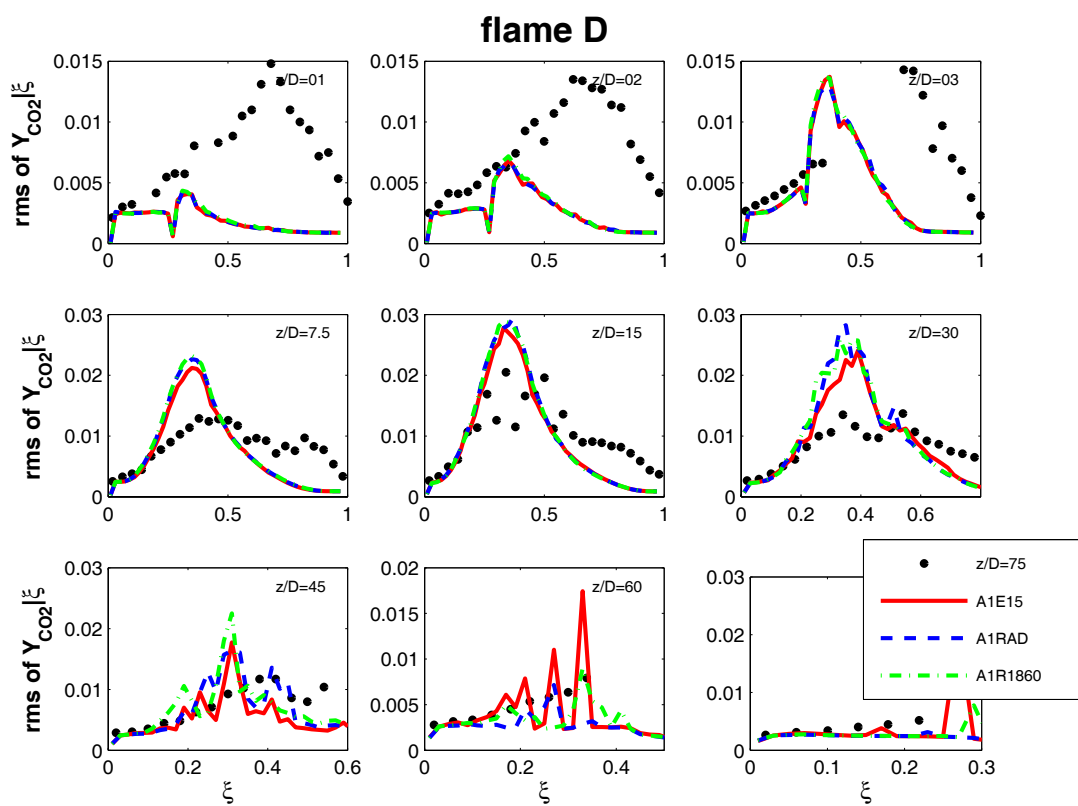
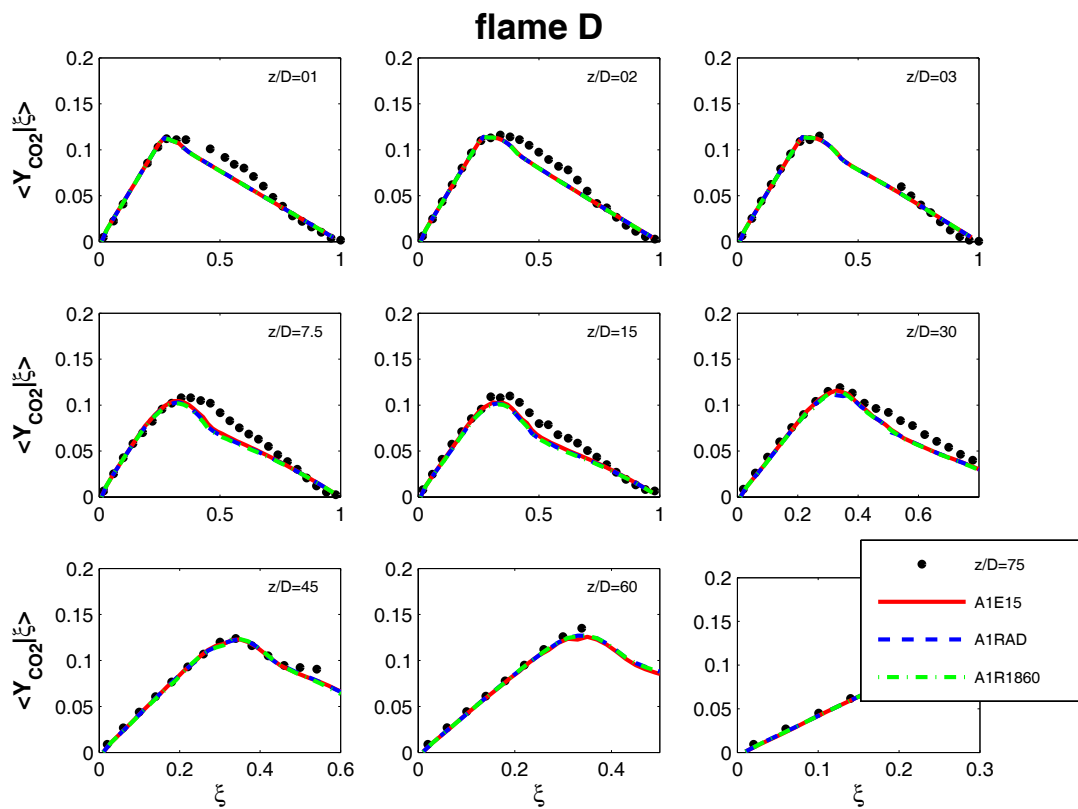


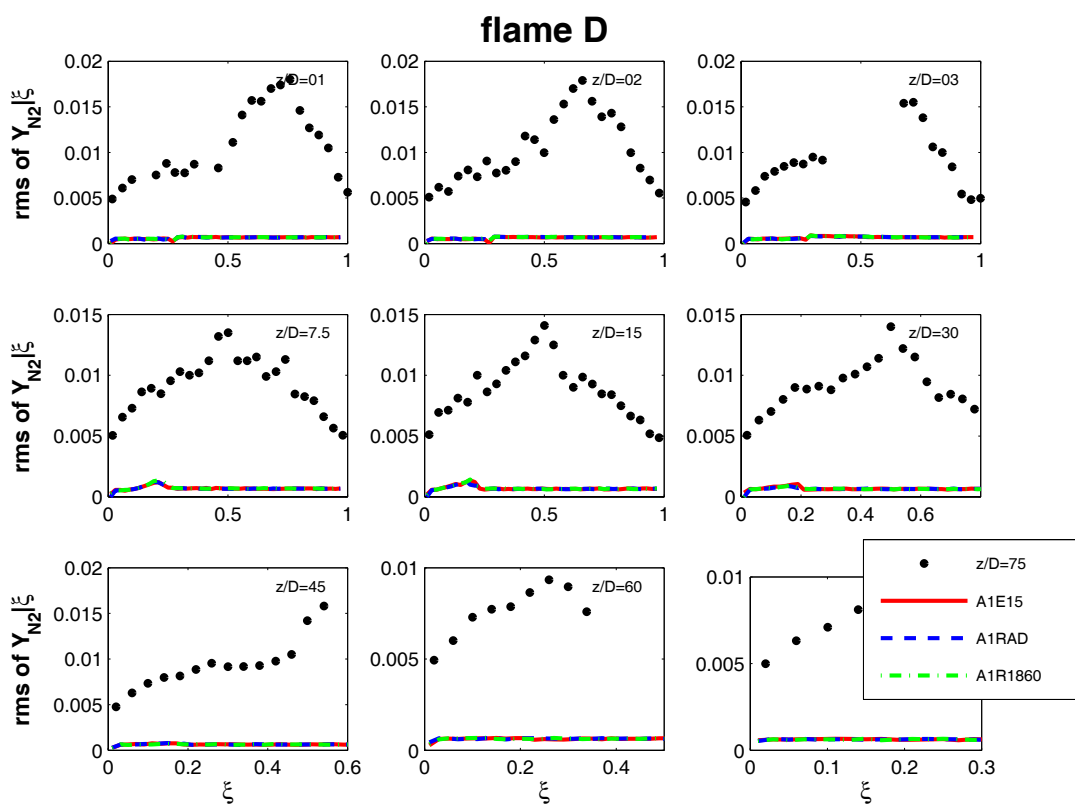
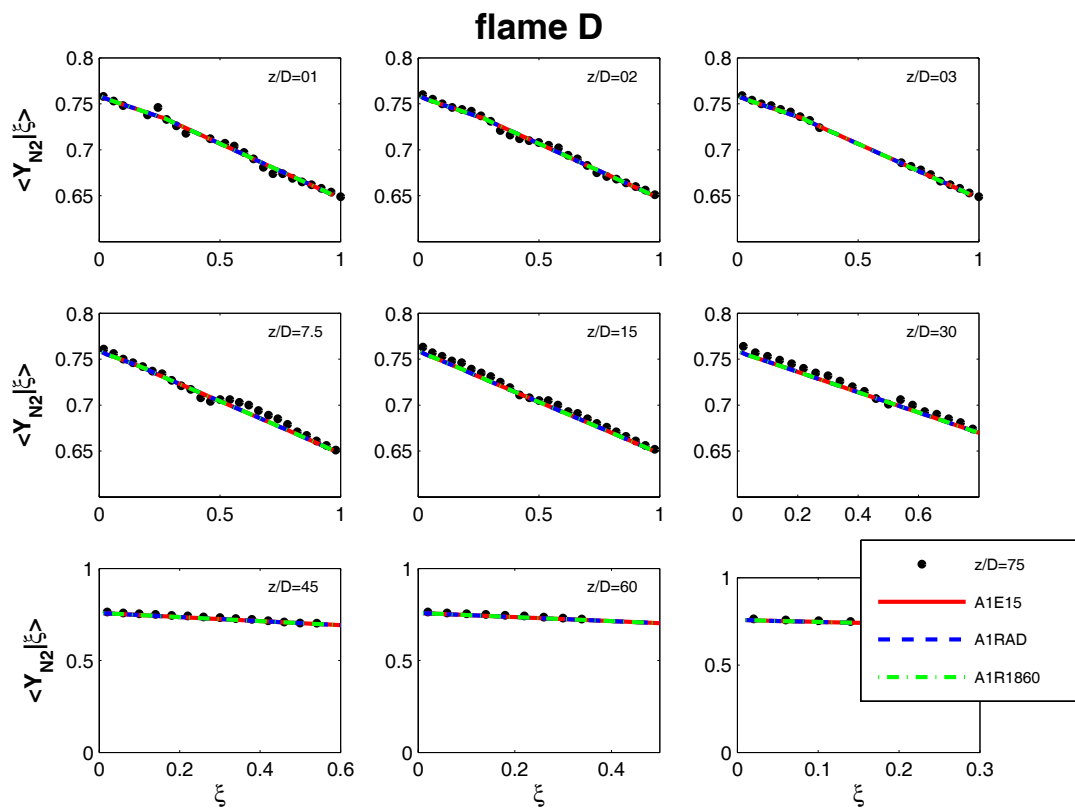
B-4 Flame D calculations

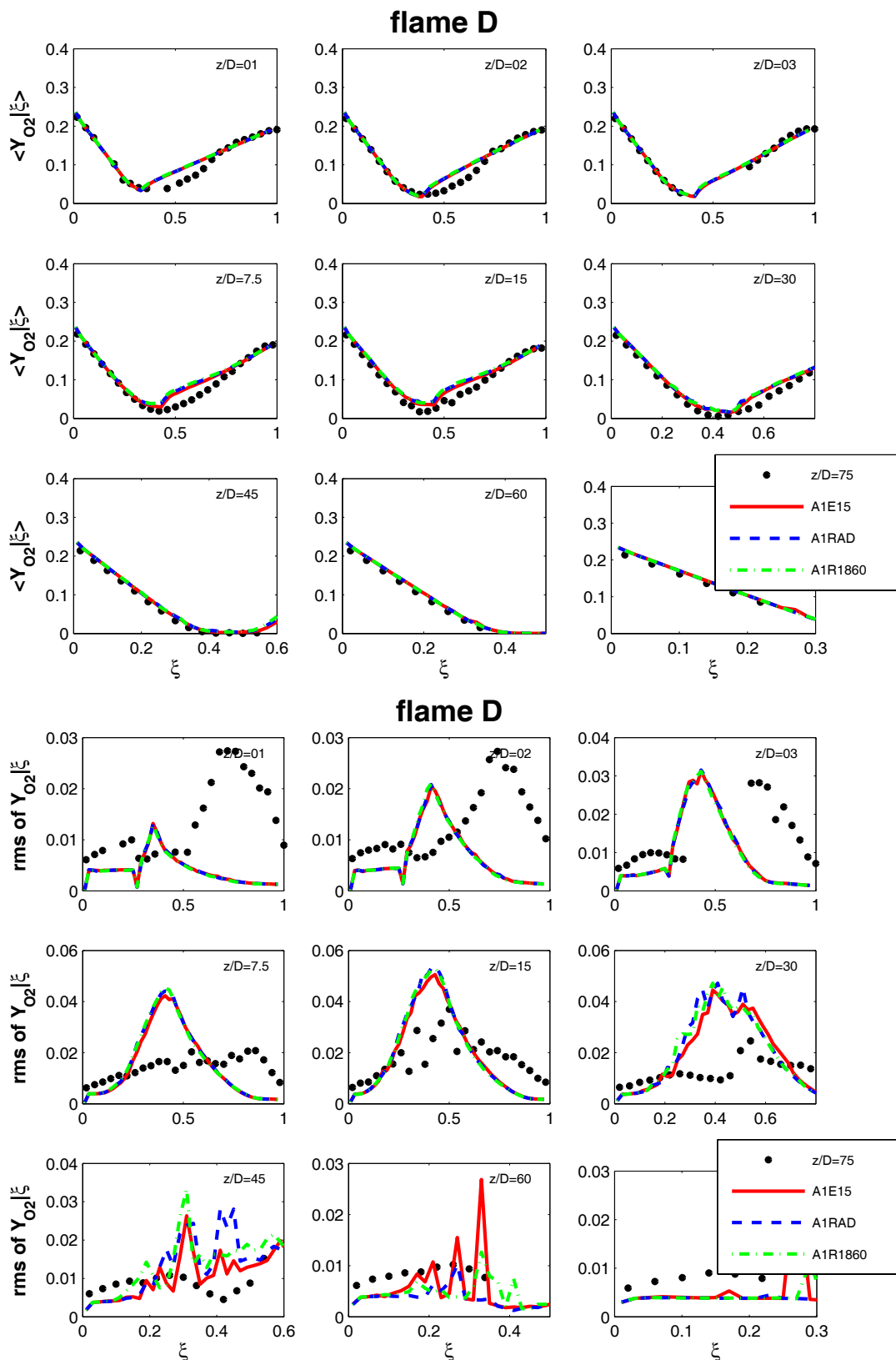
(1) A1E15, A1RAD and A1R1860

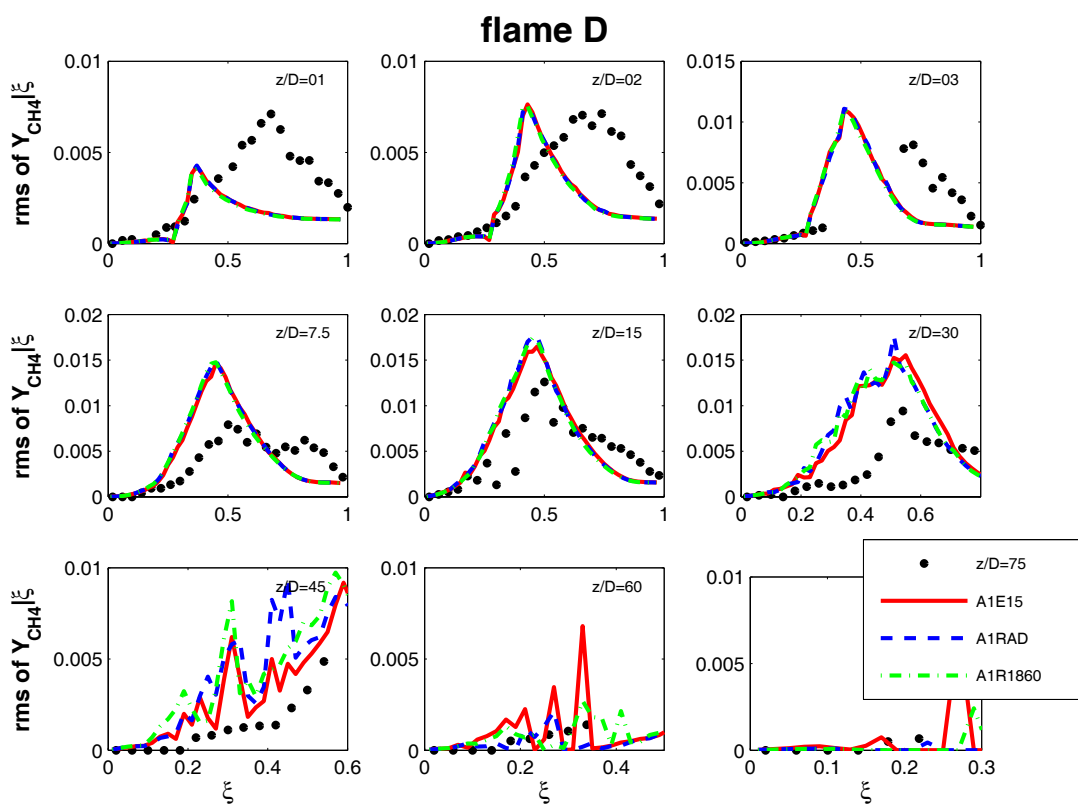
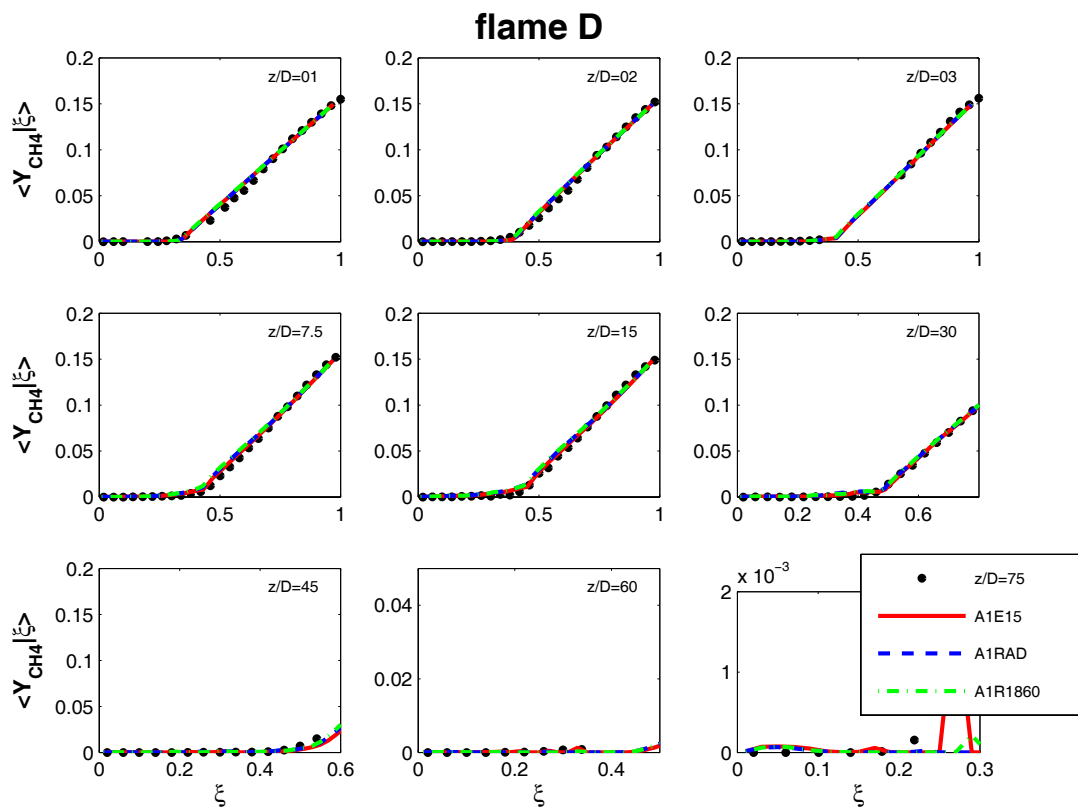


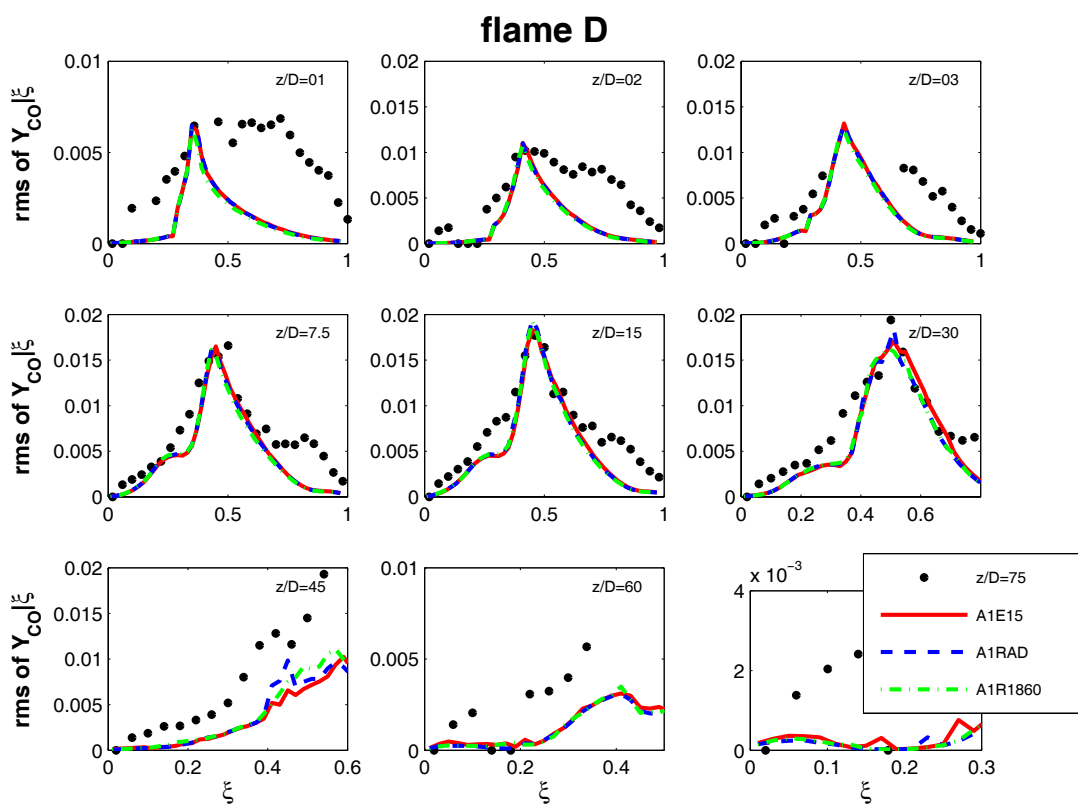
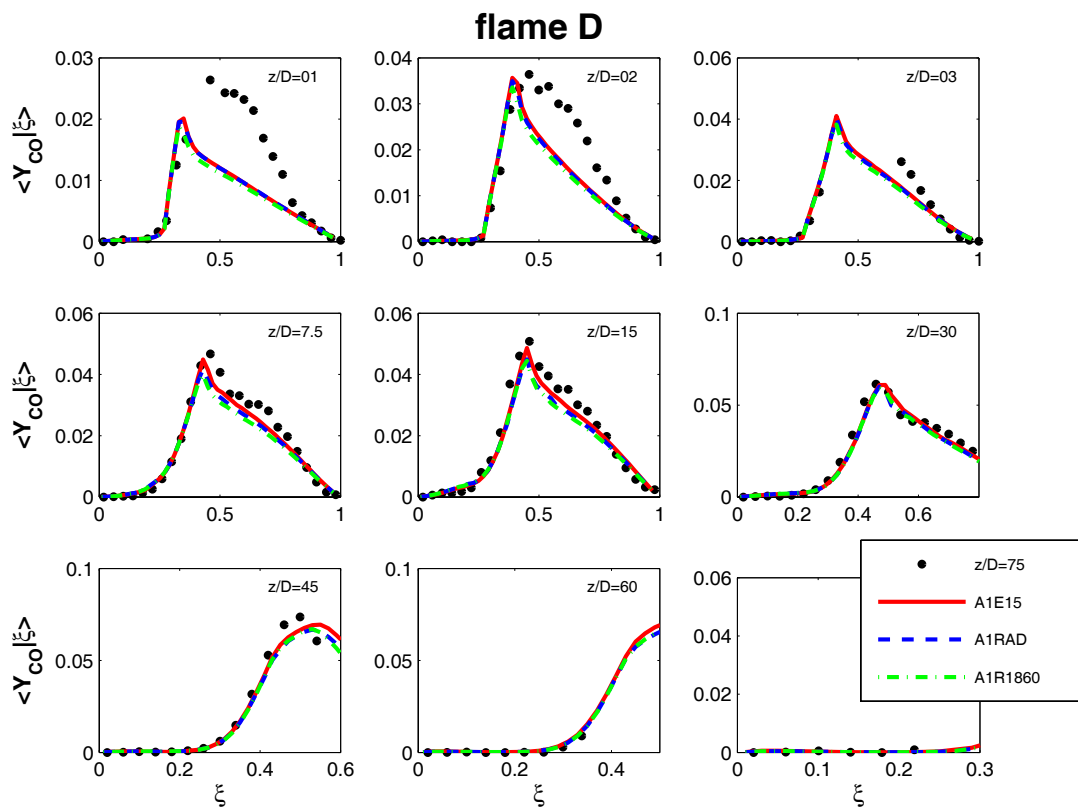


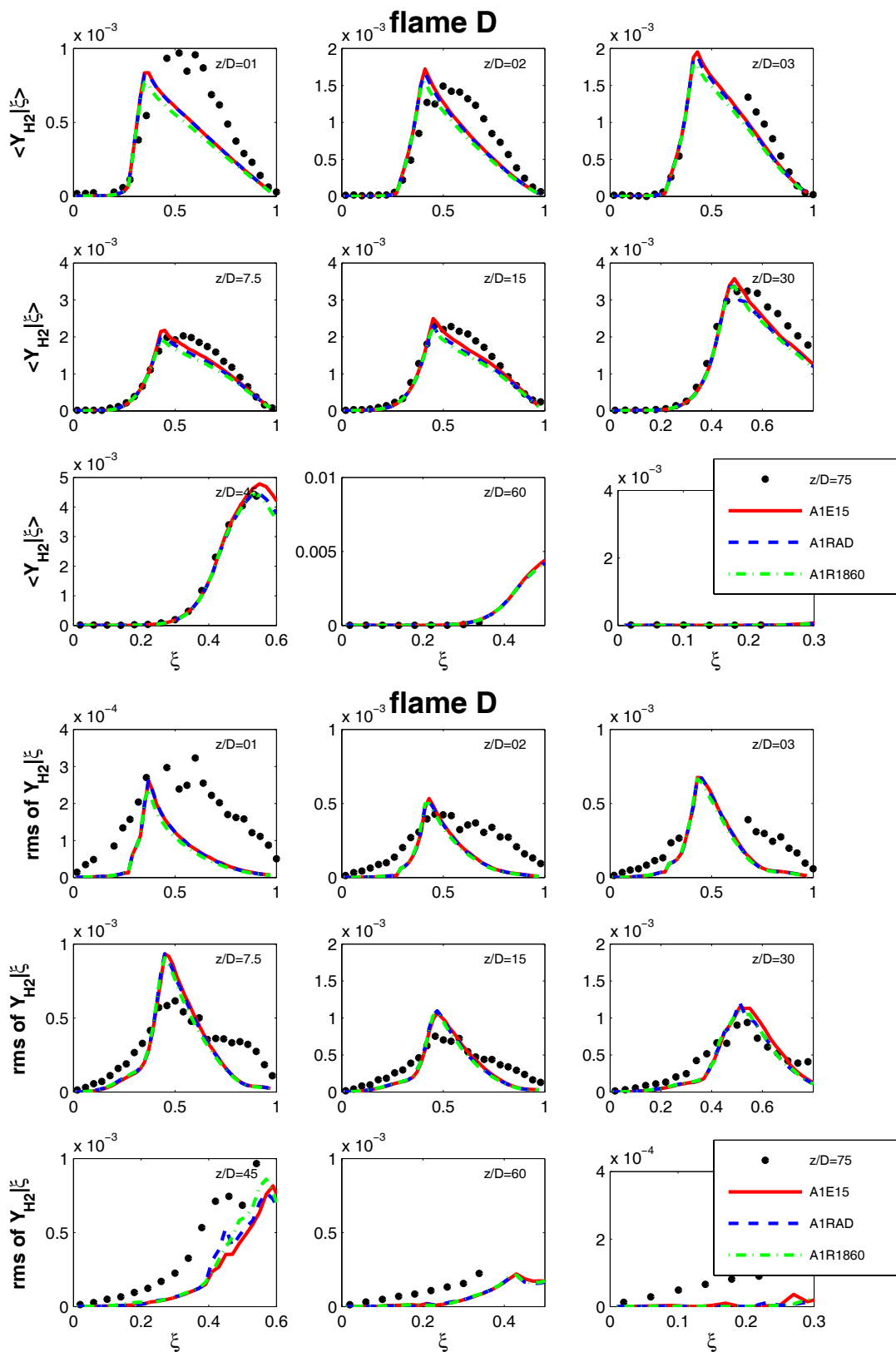


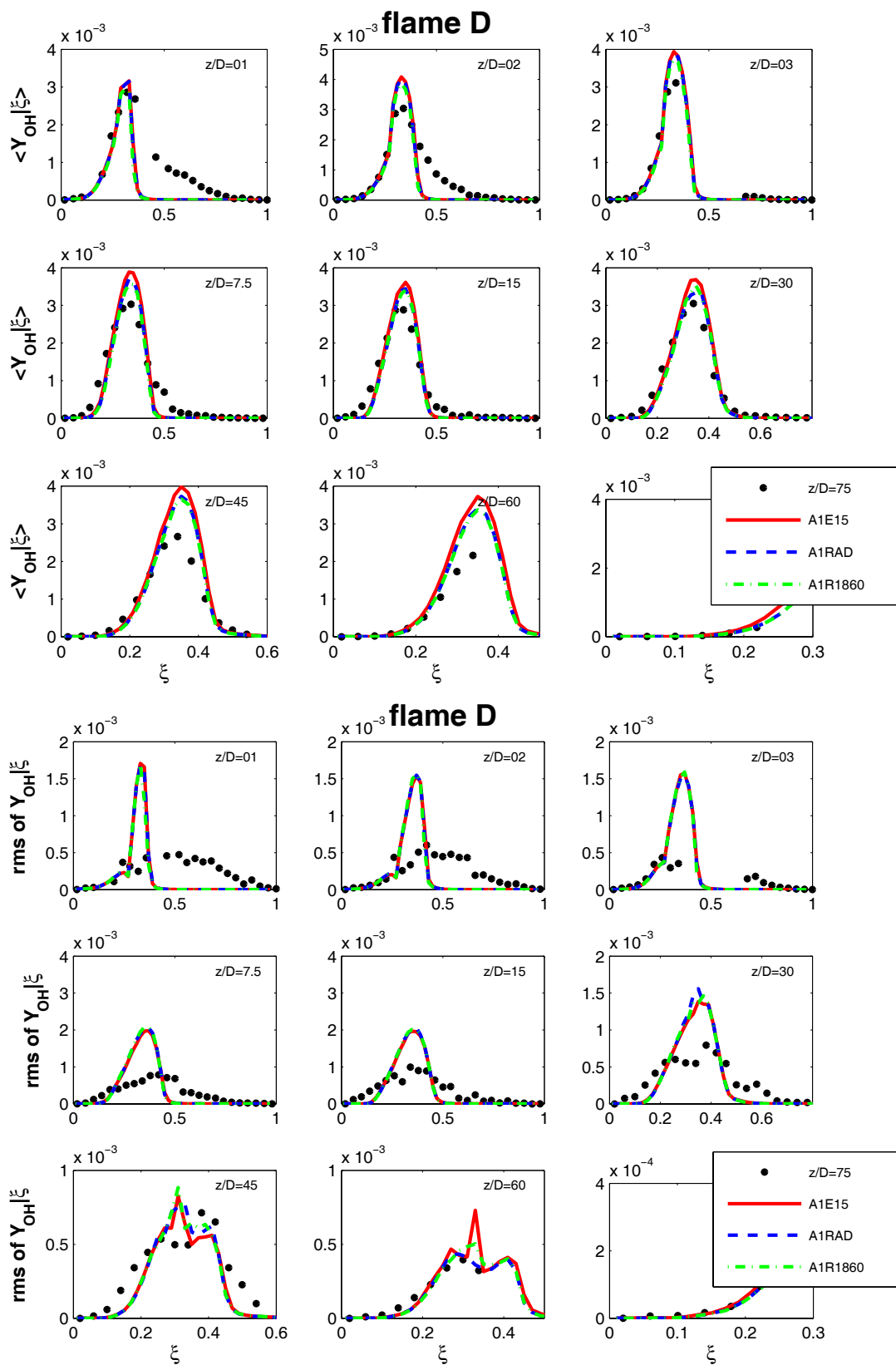




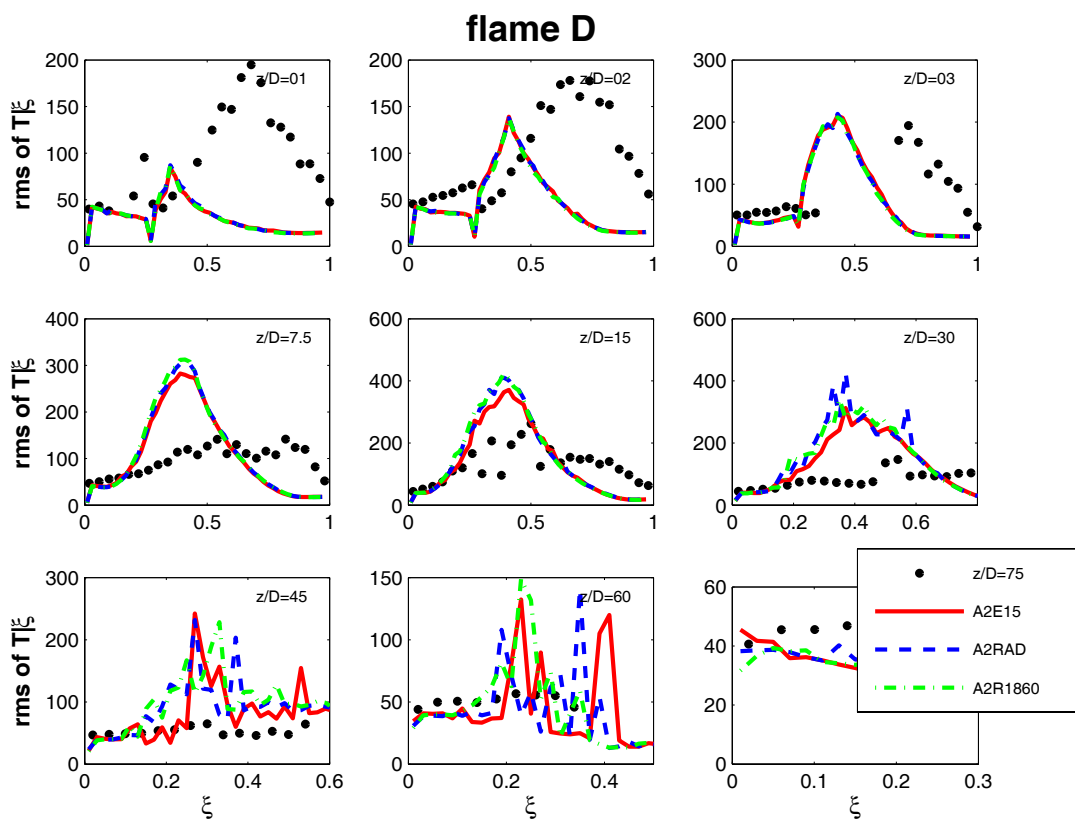
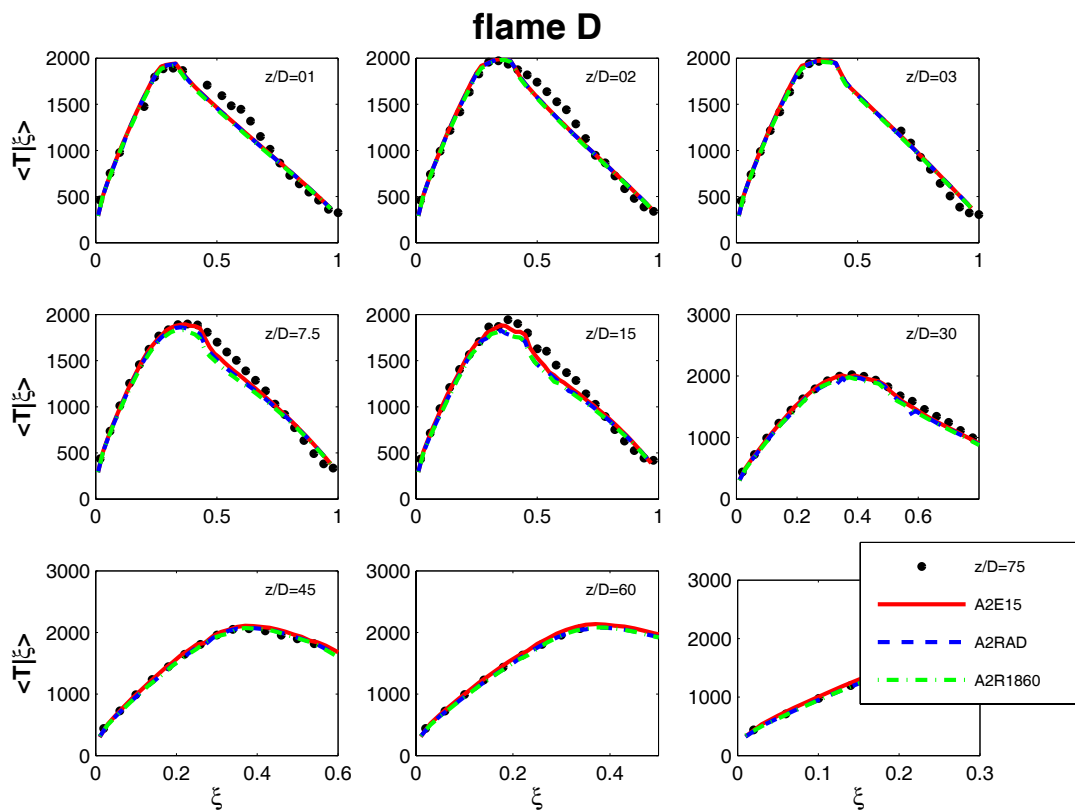


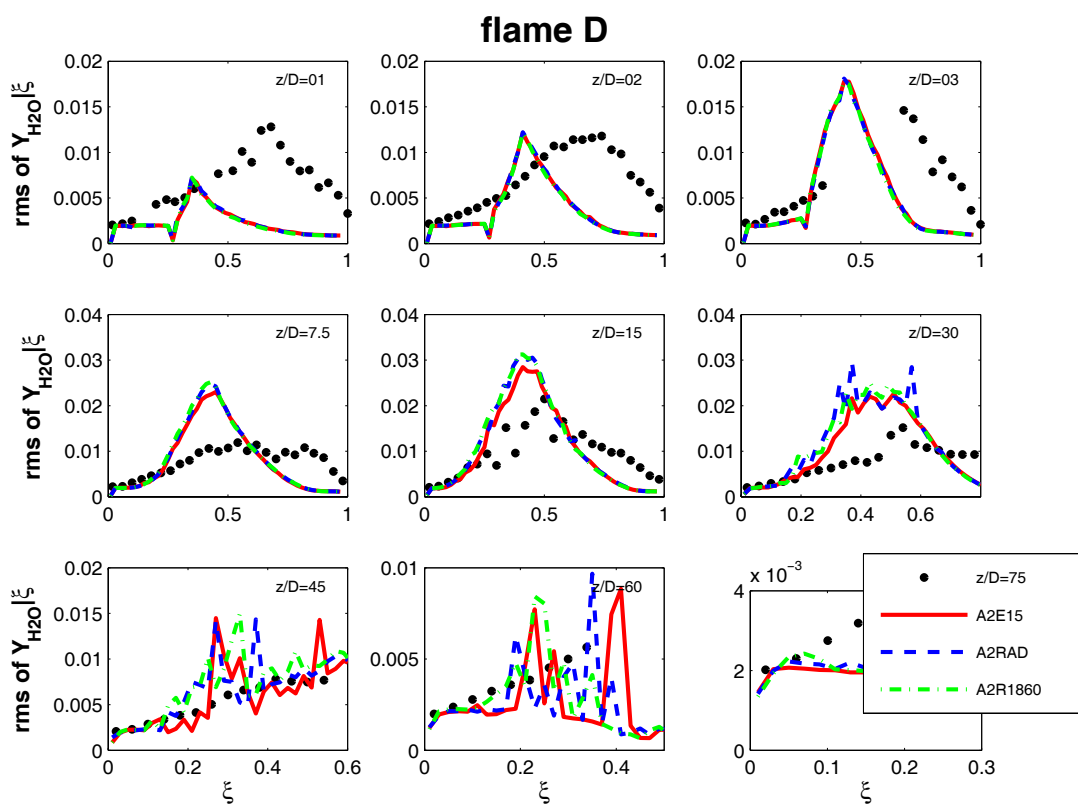
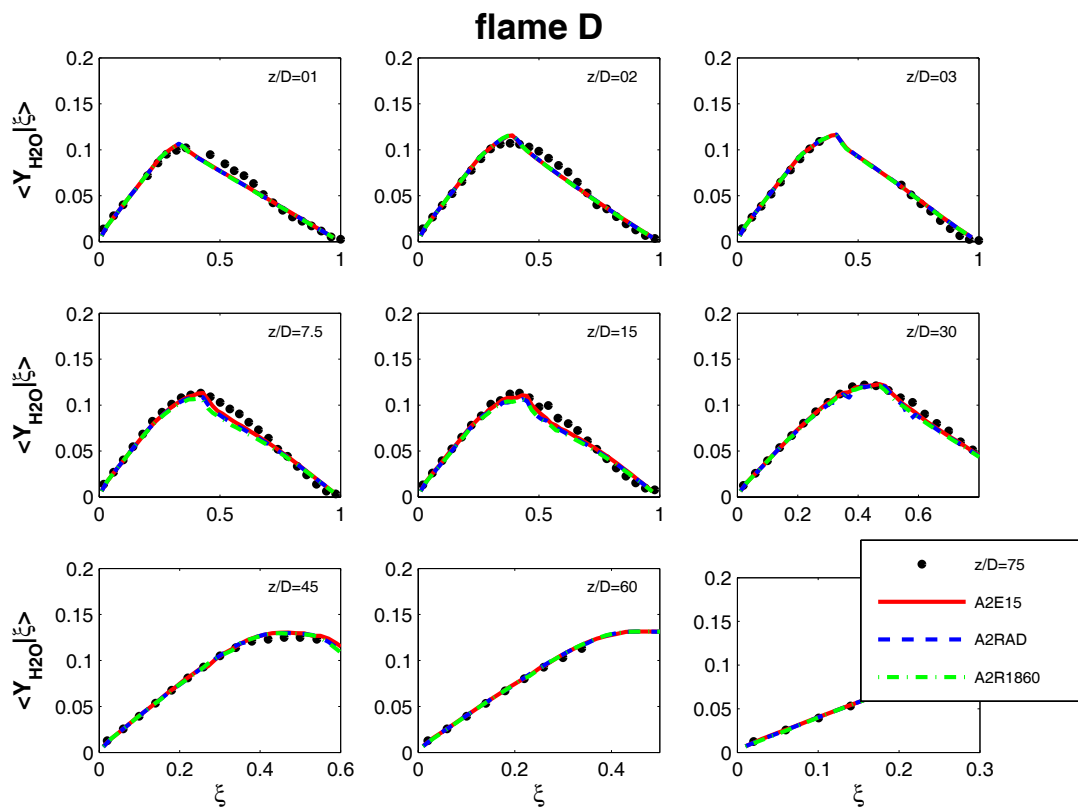


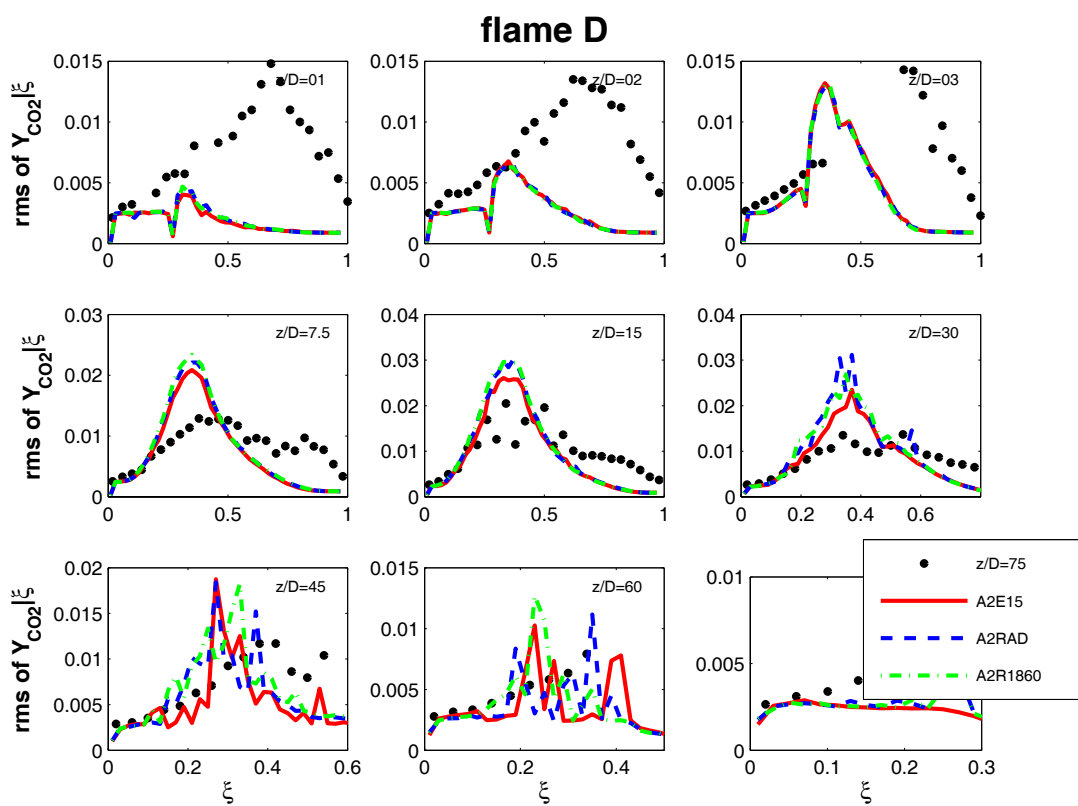
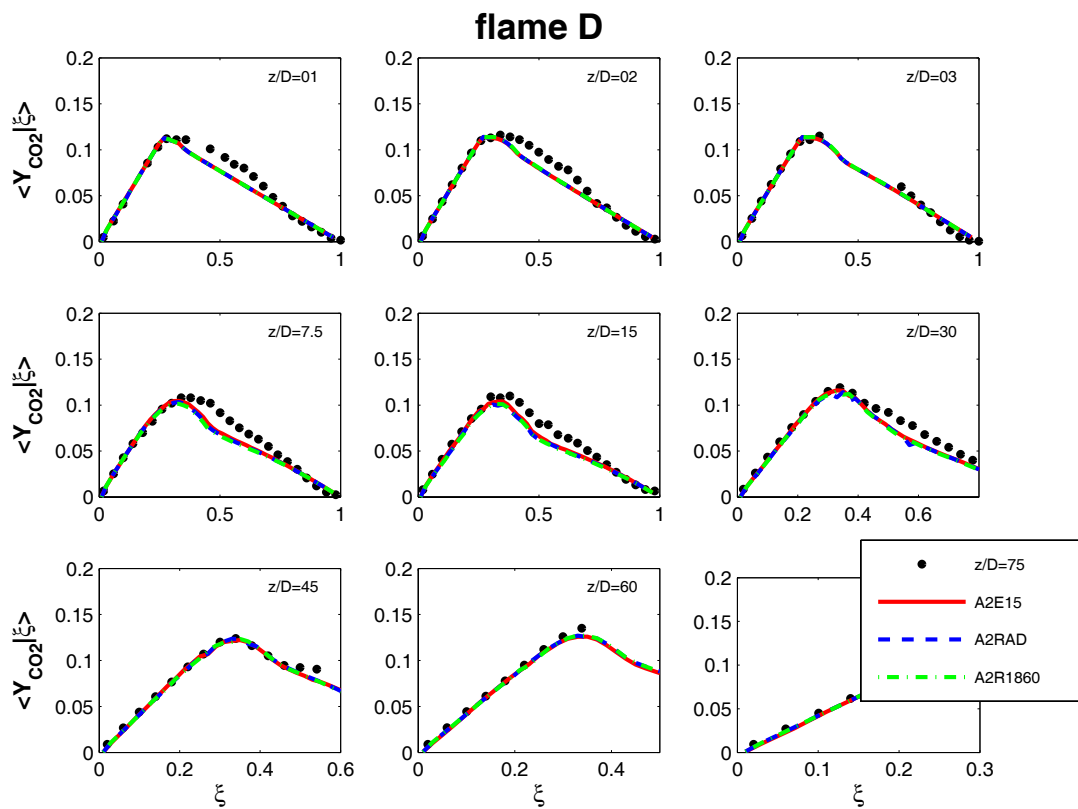


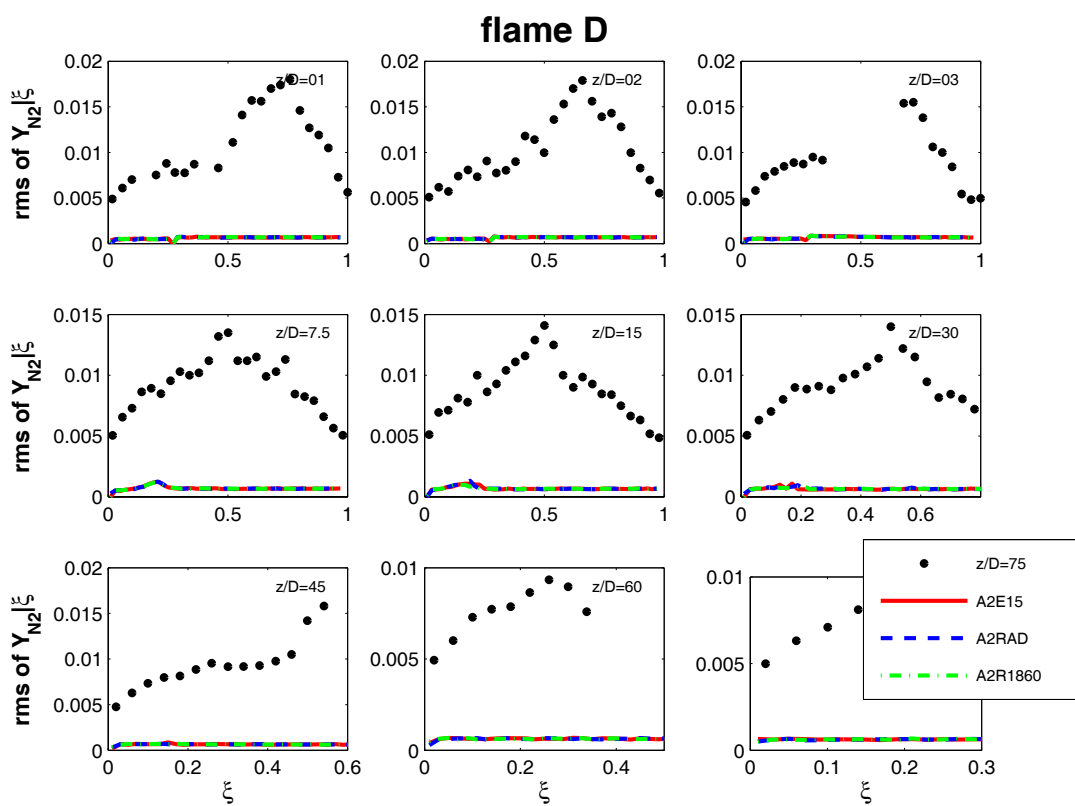
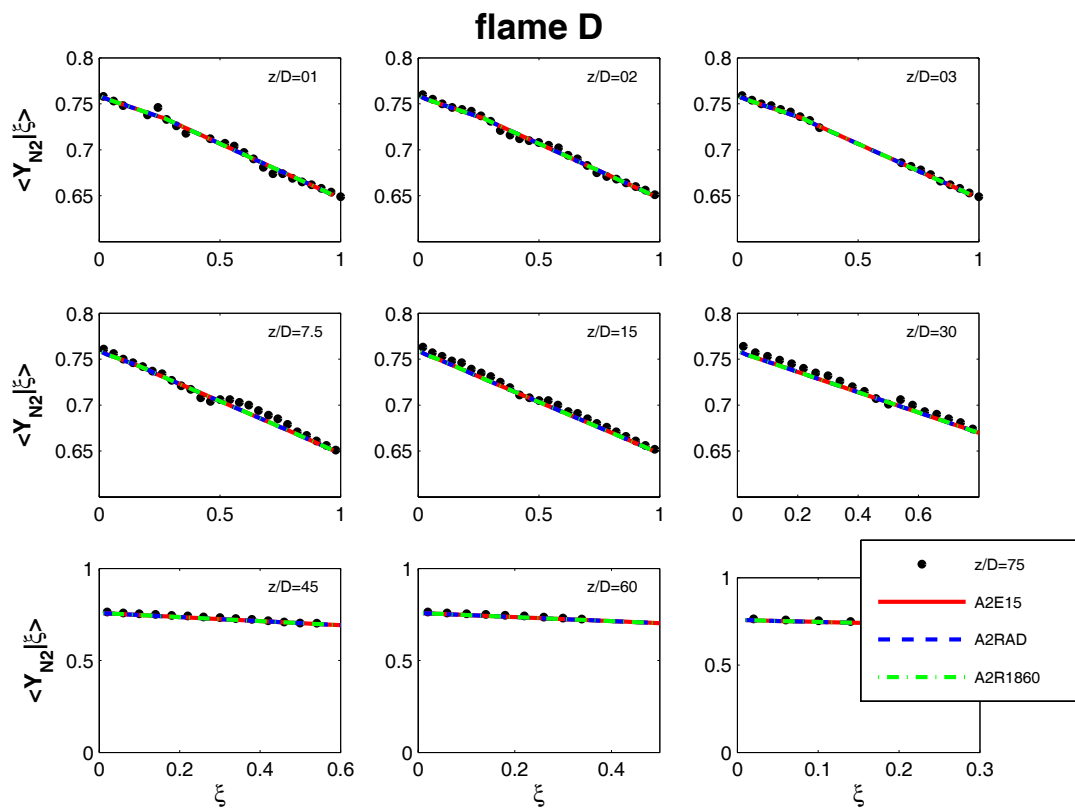


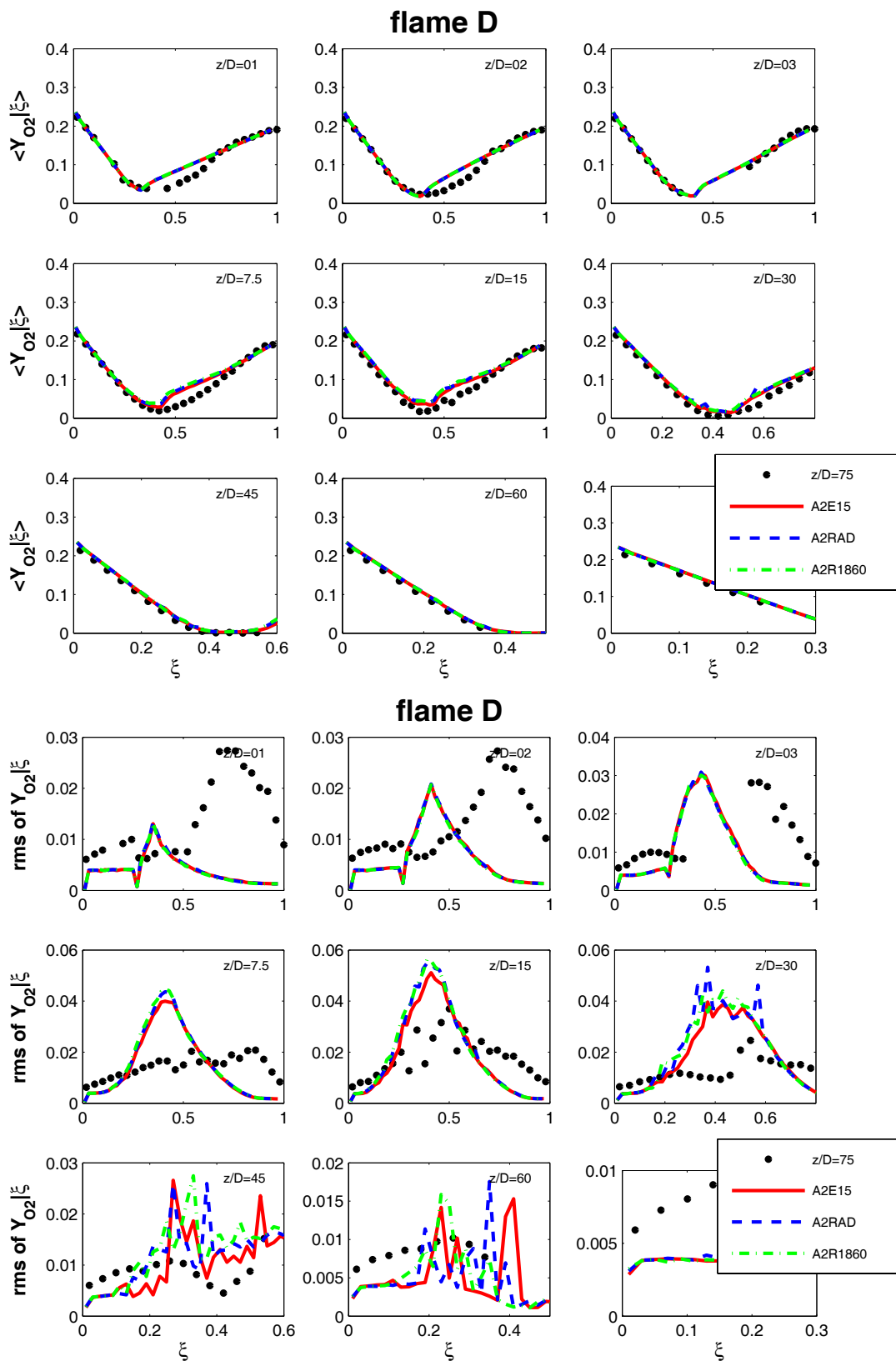
(2) A2E15, A2RAD, and A2R1860

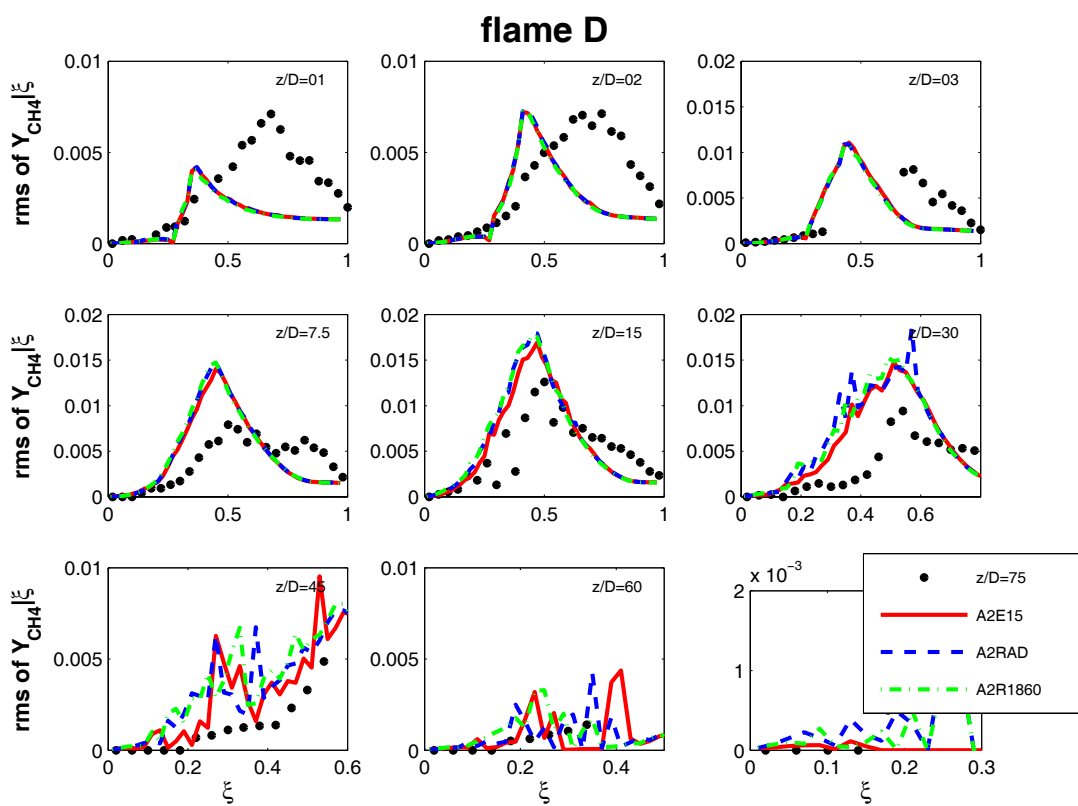
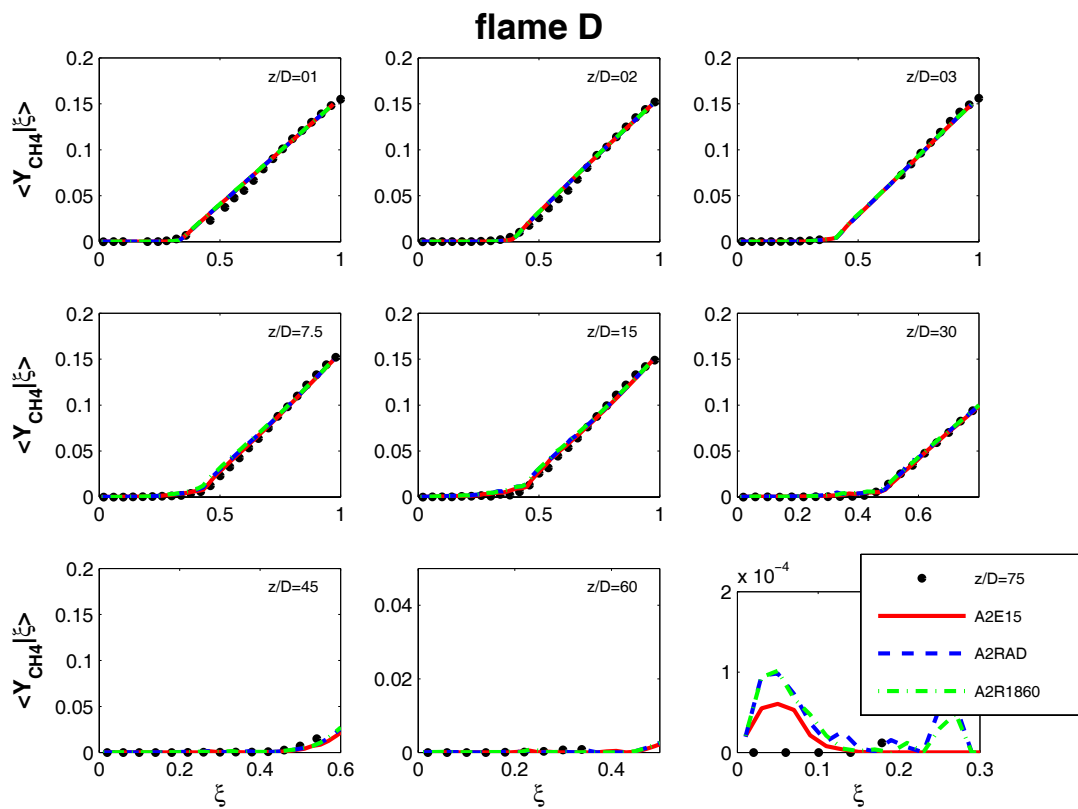


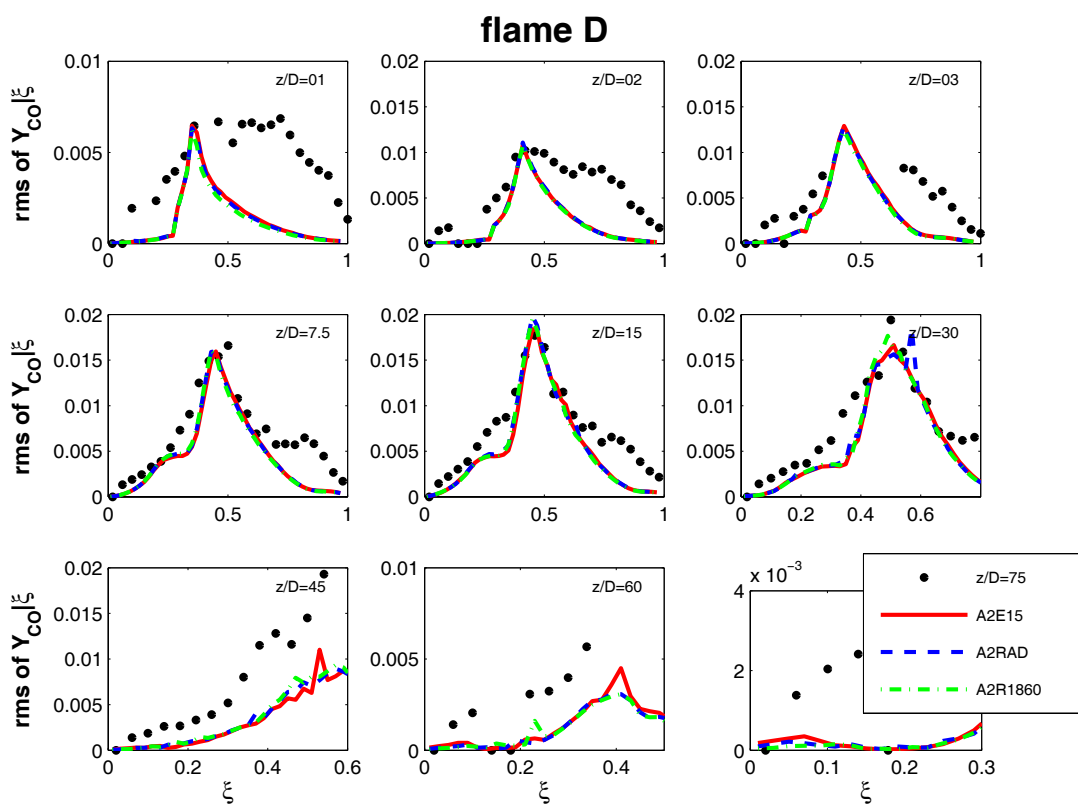
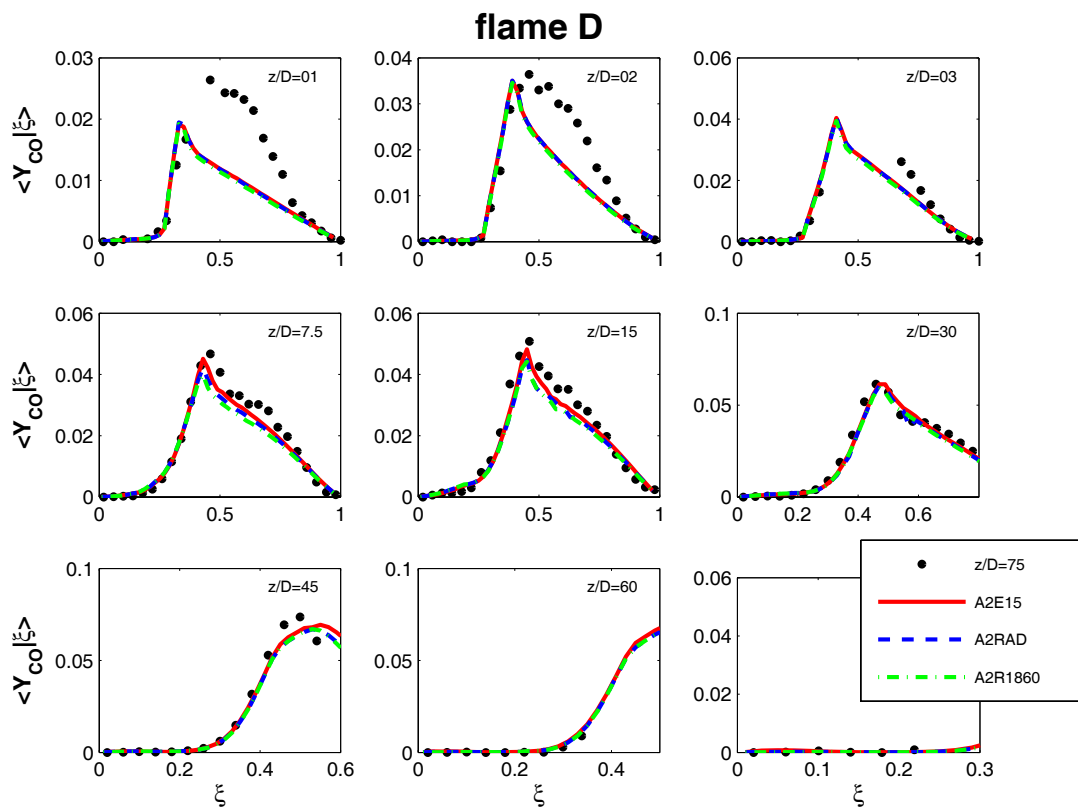


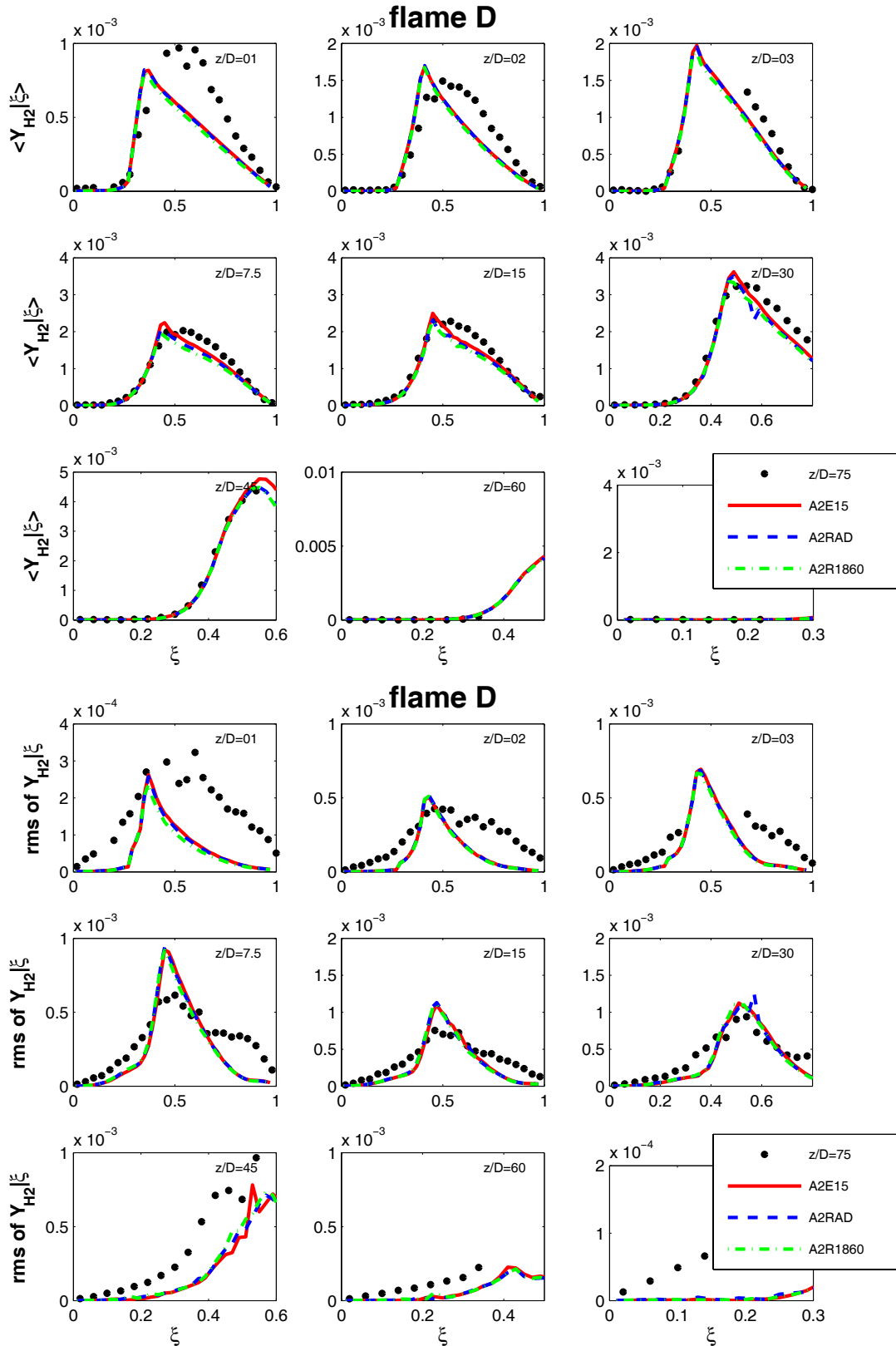


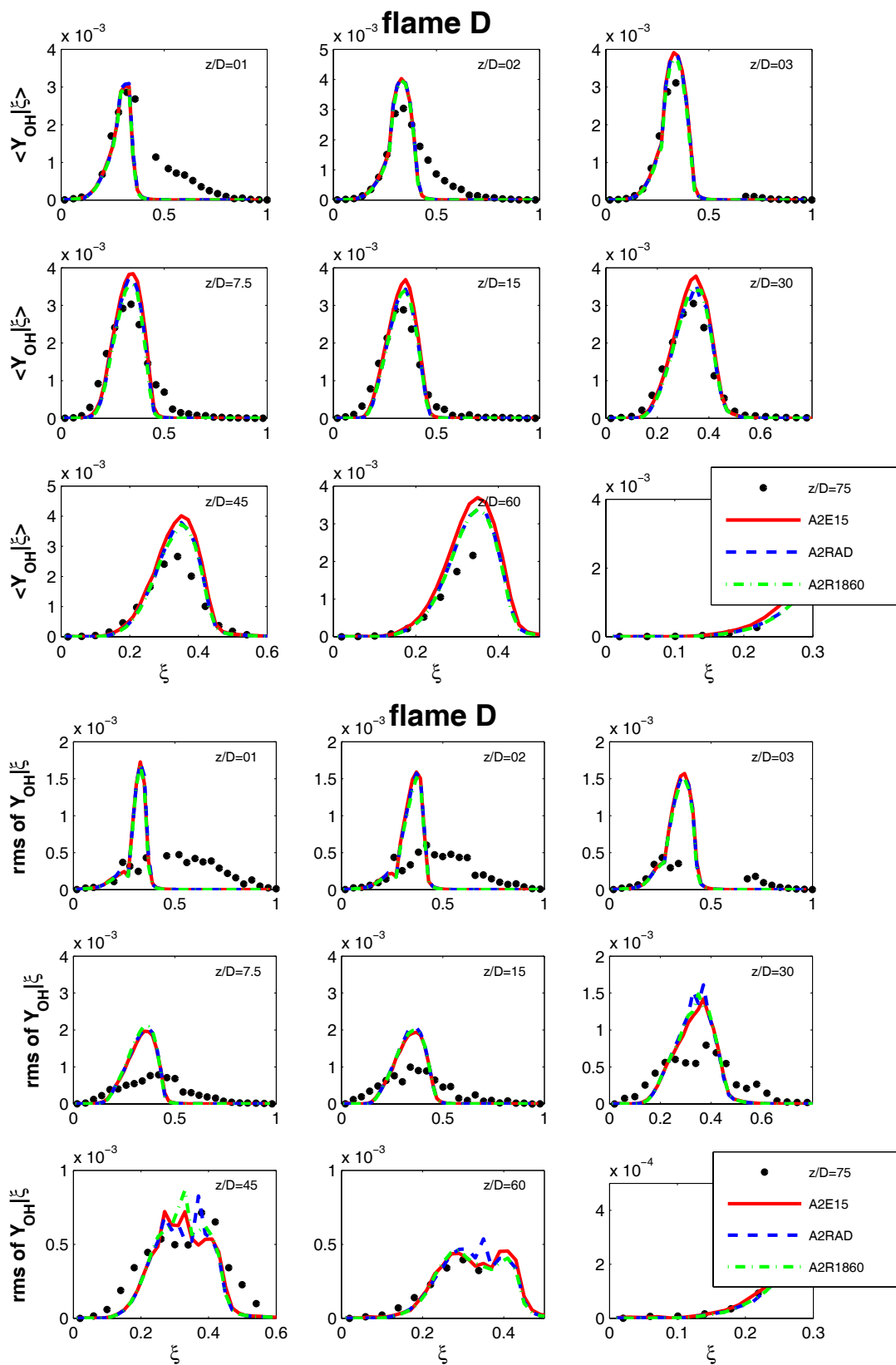


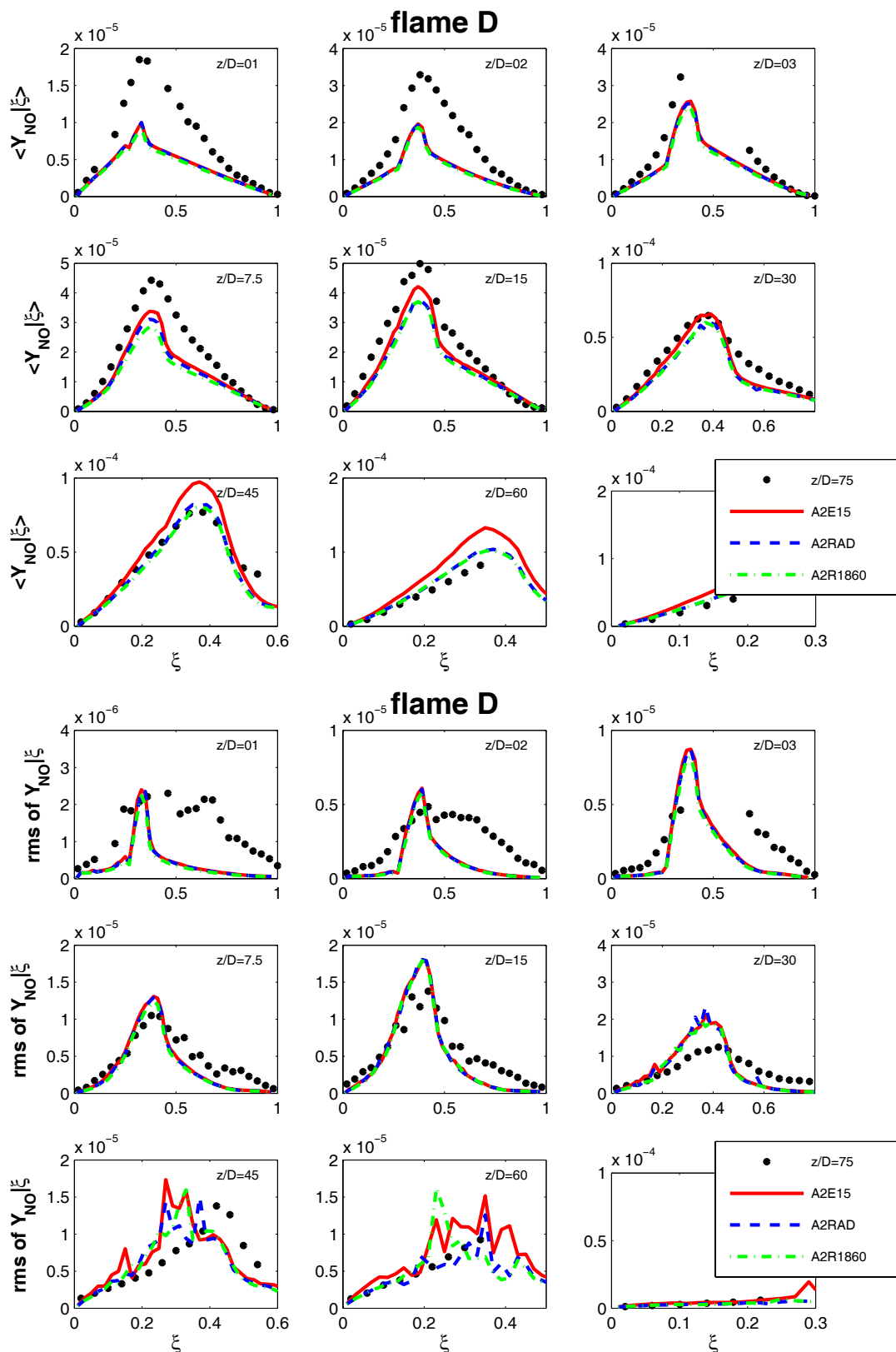




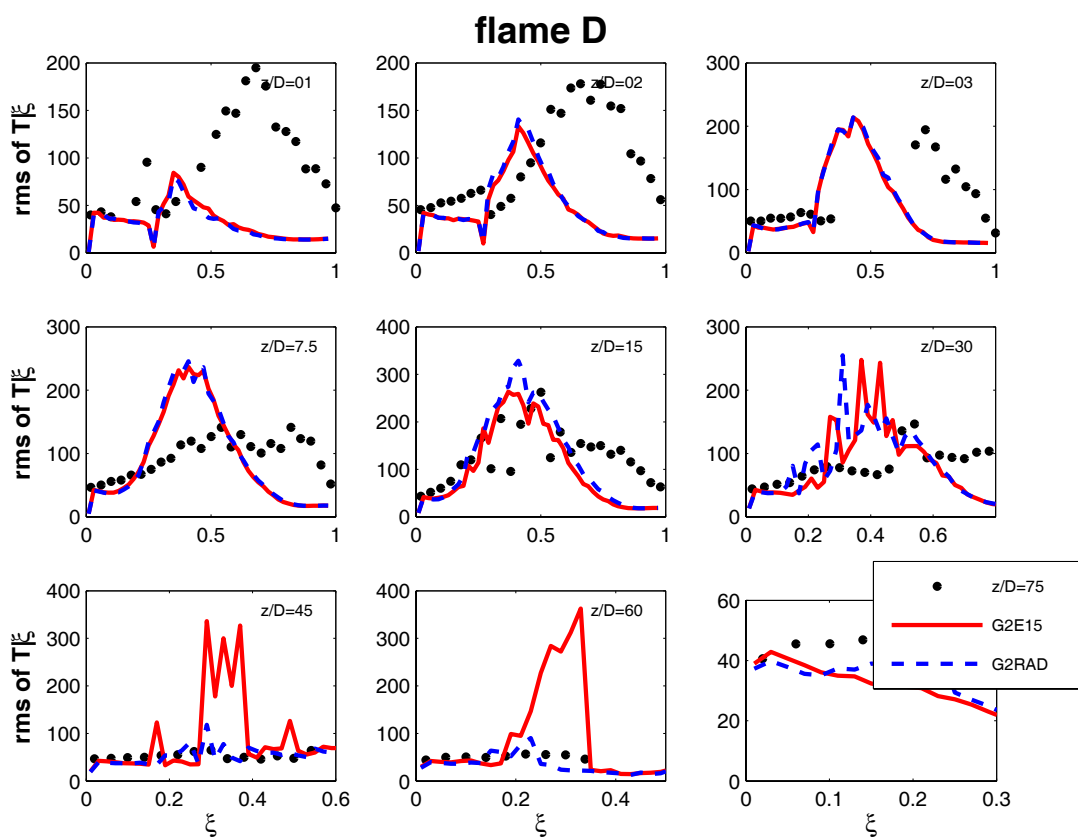
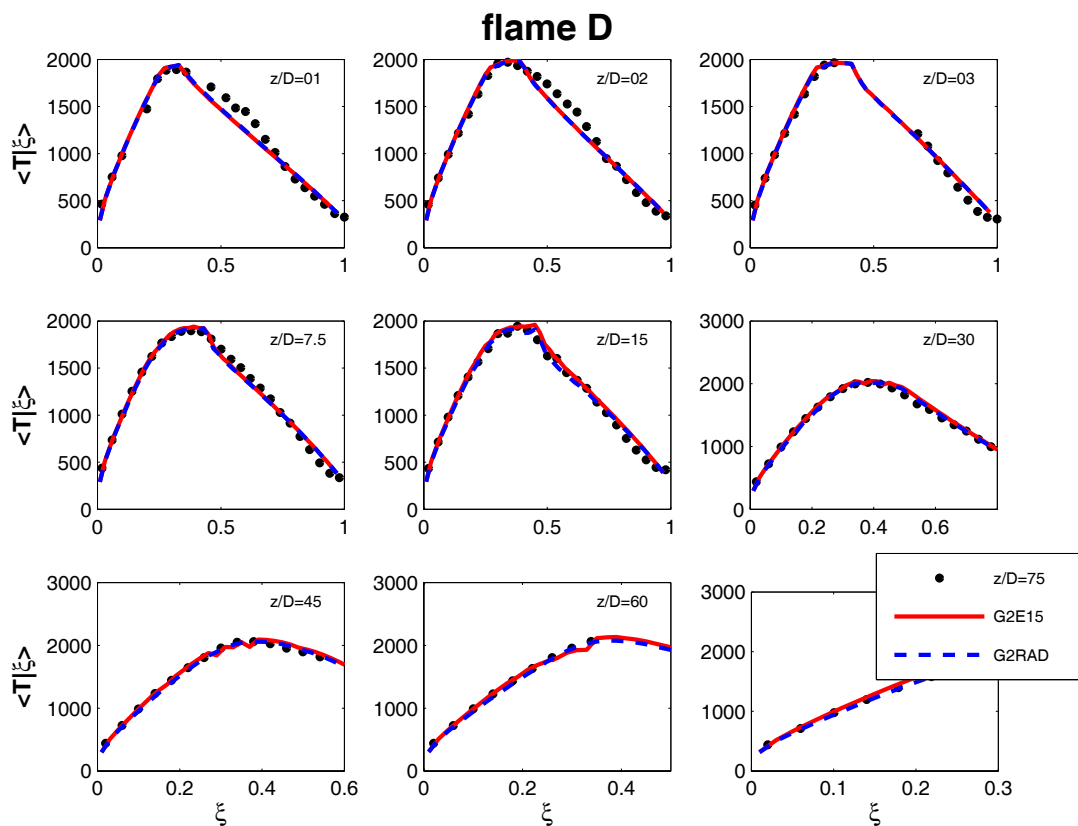


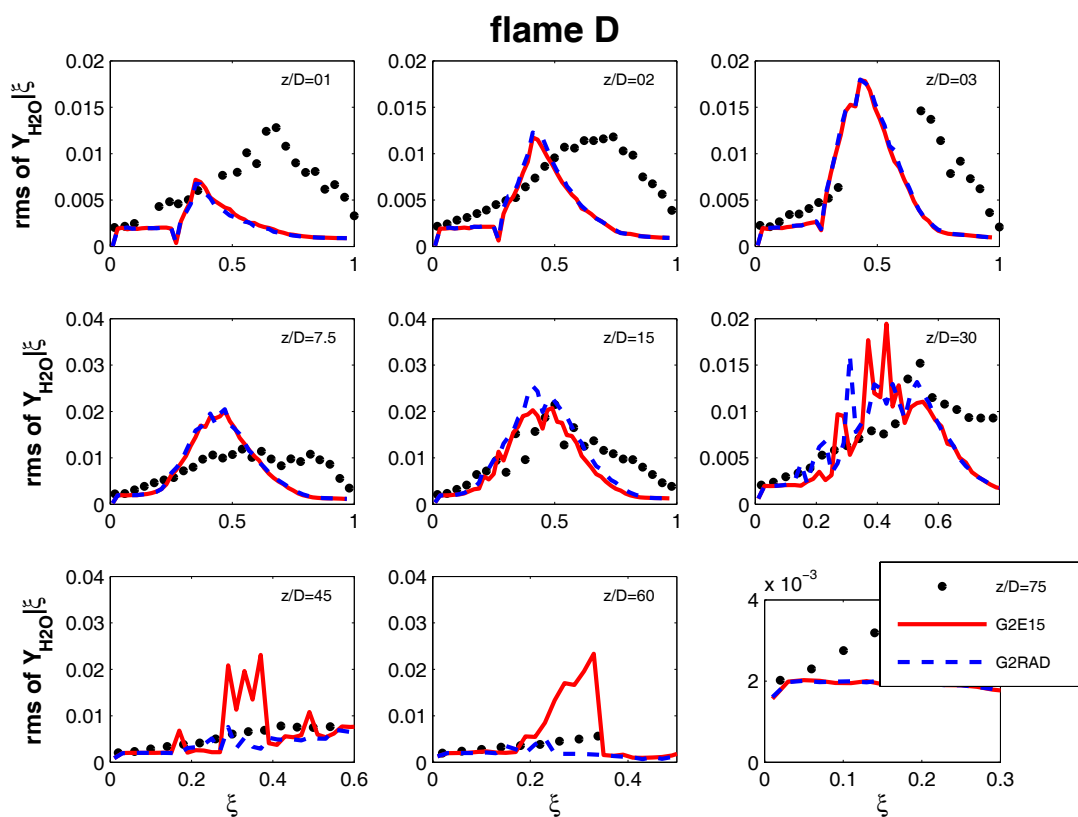
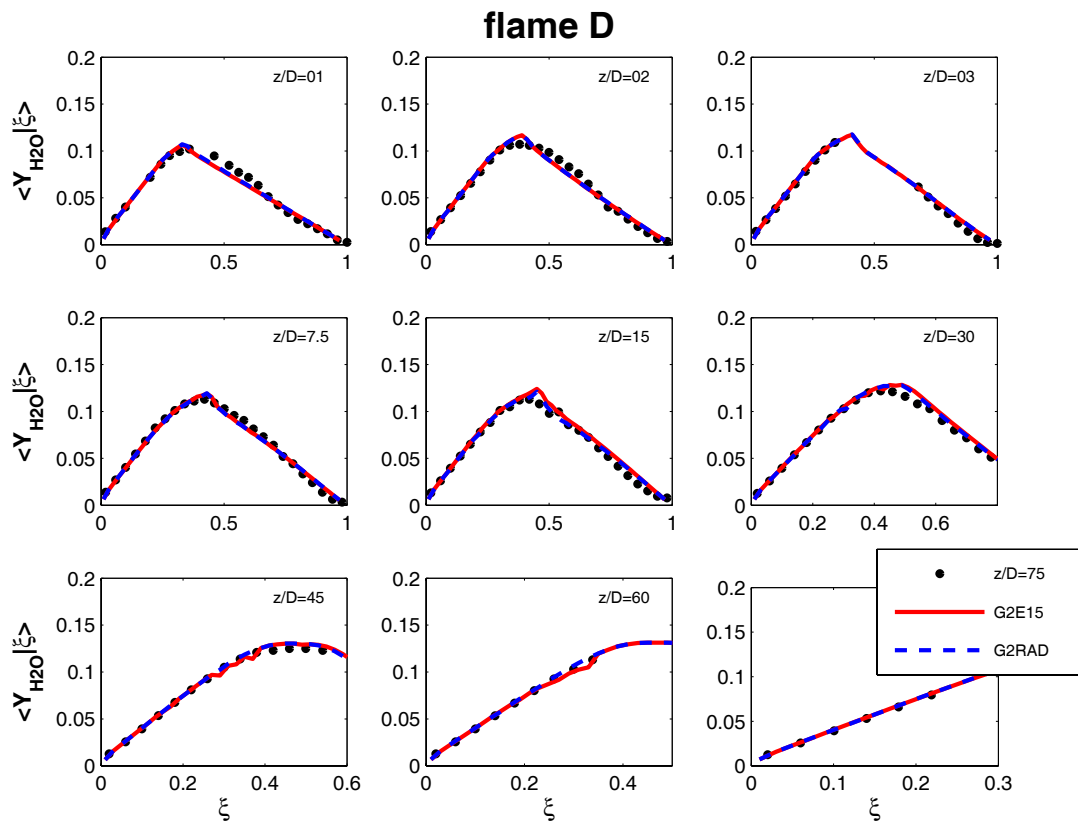


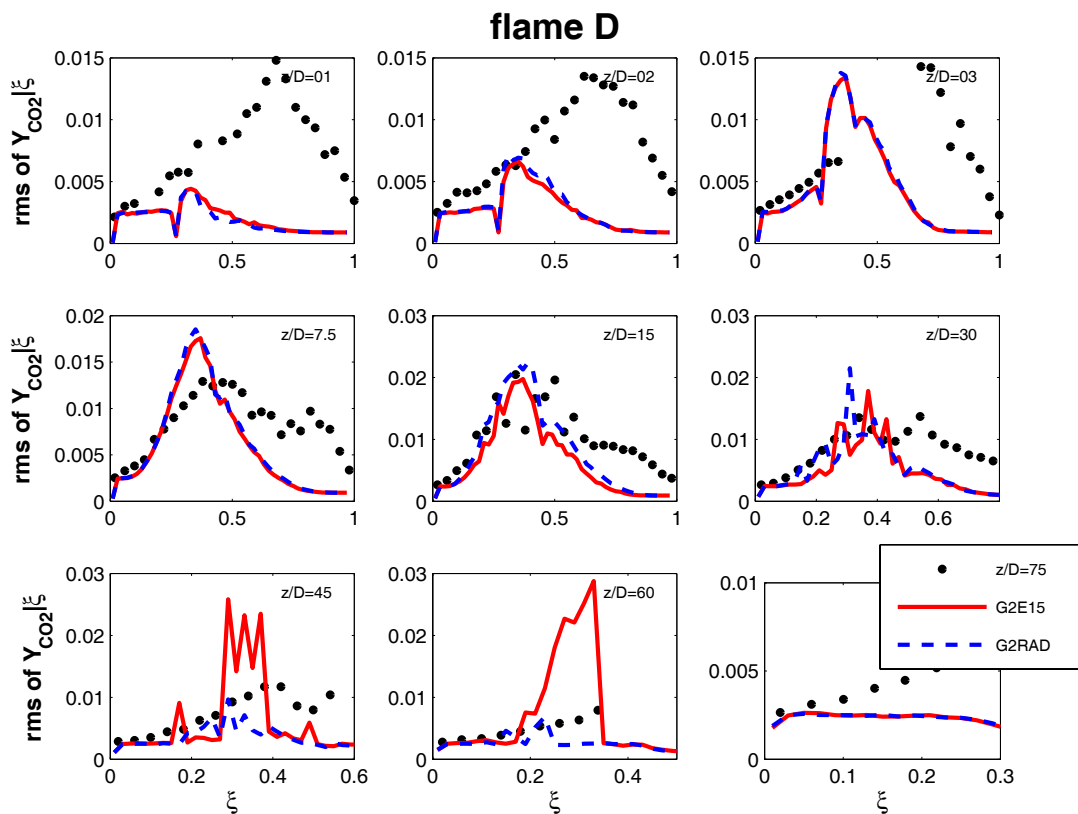
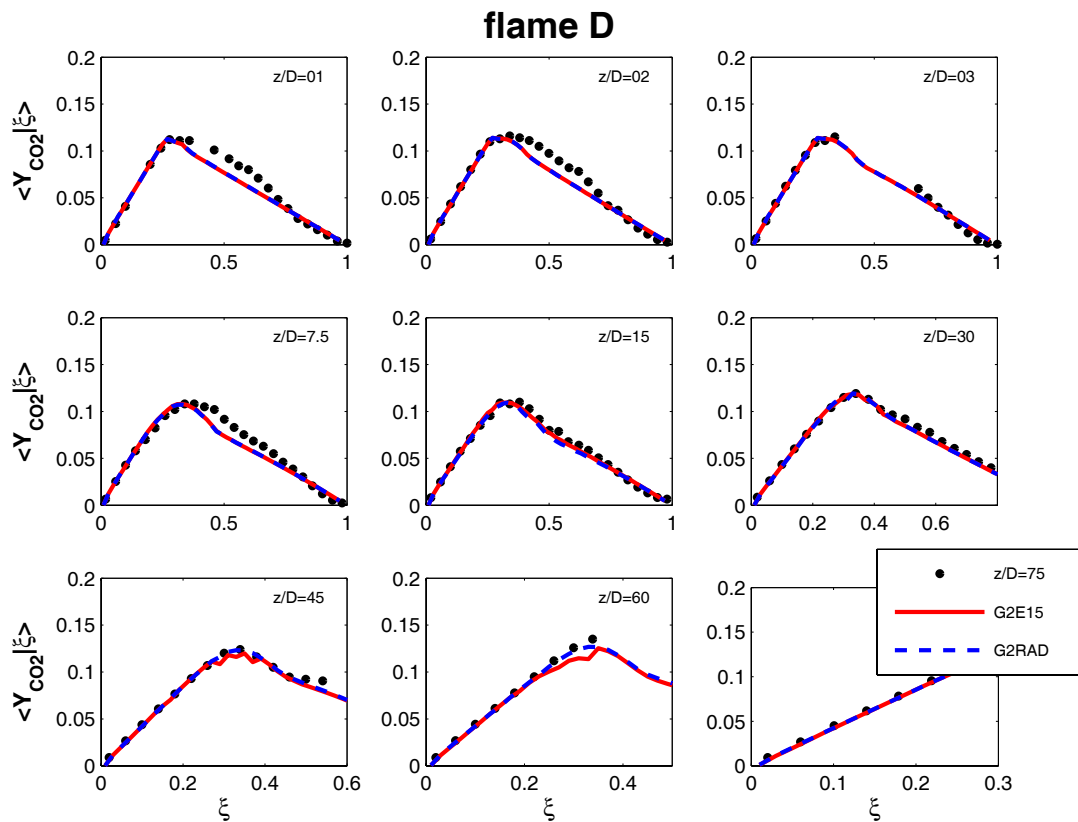


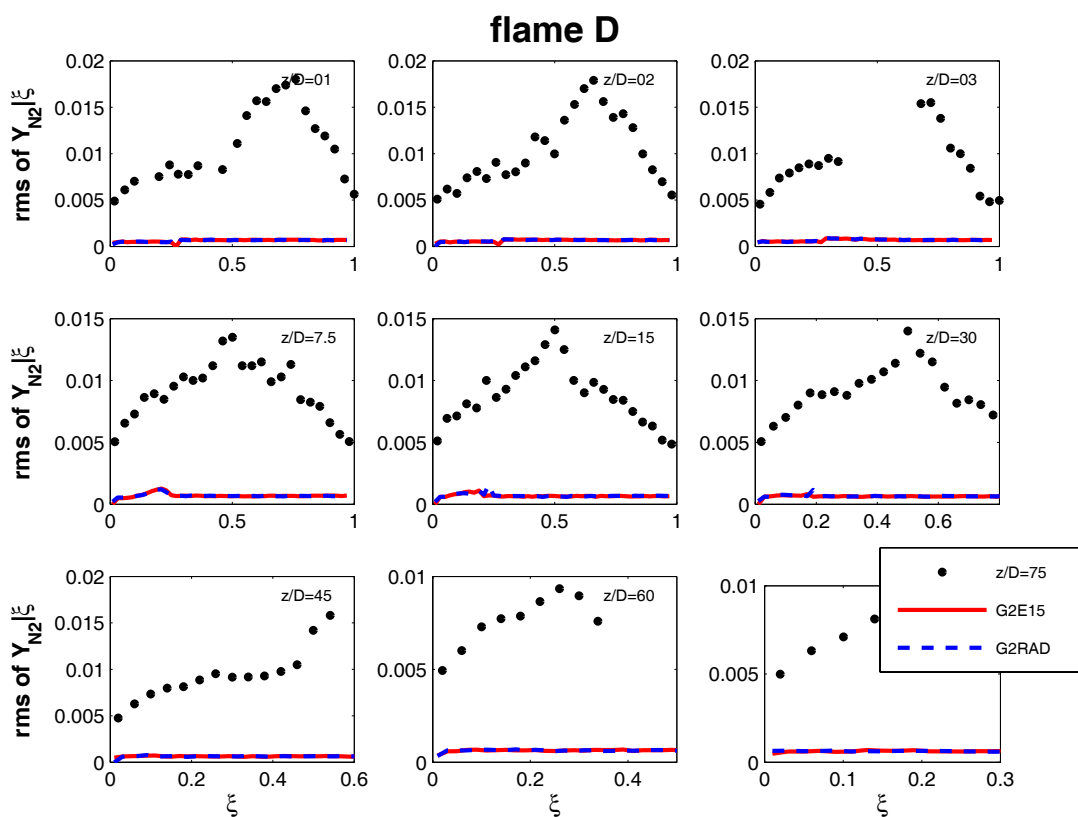
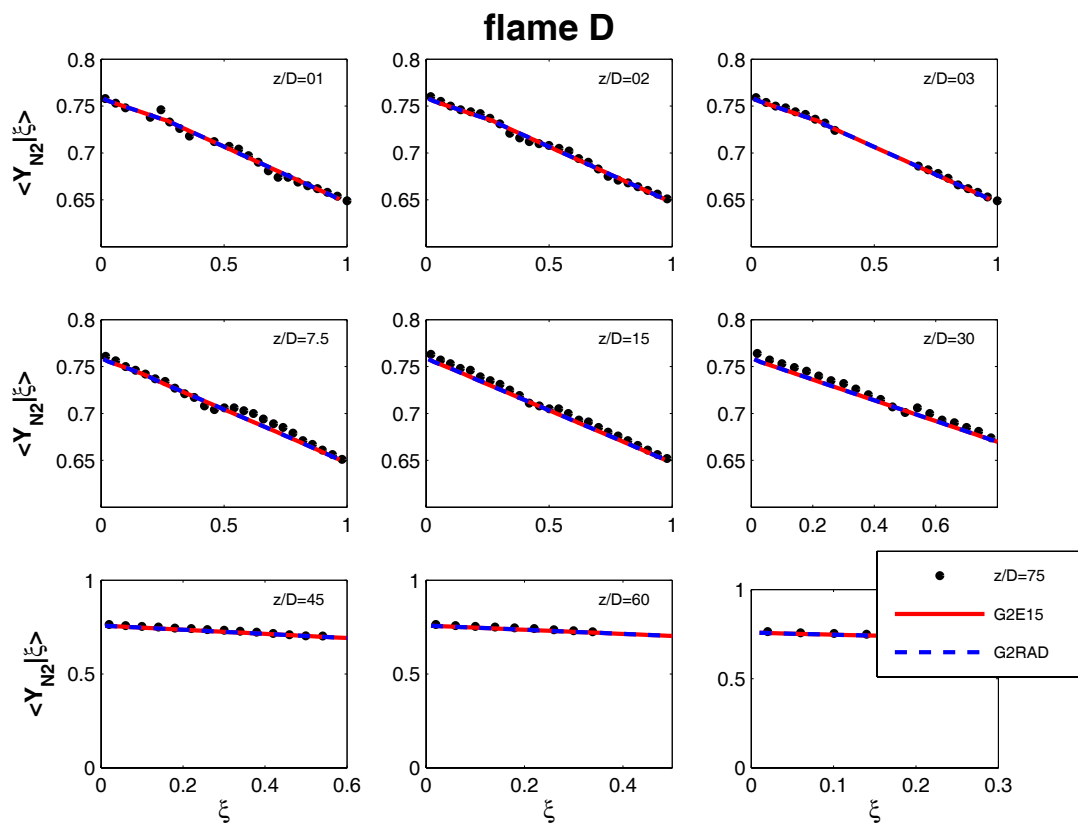


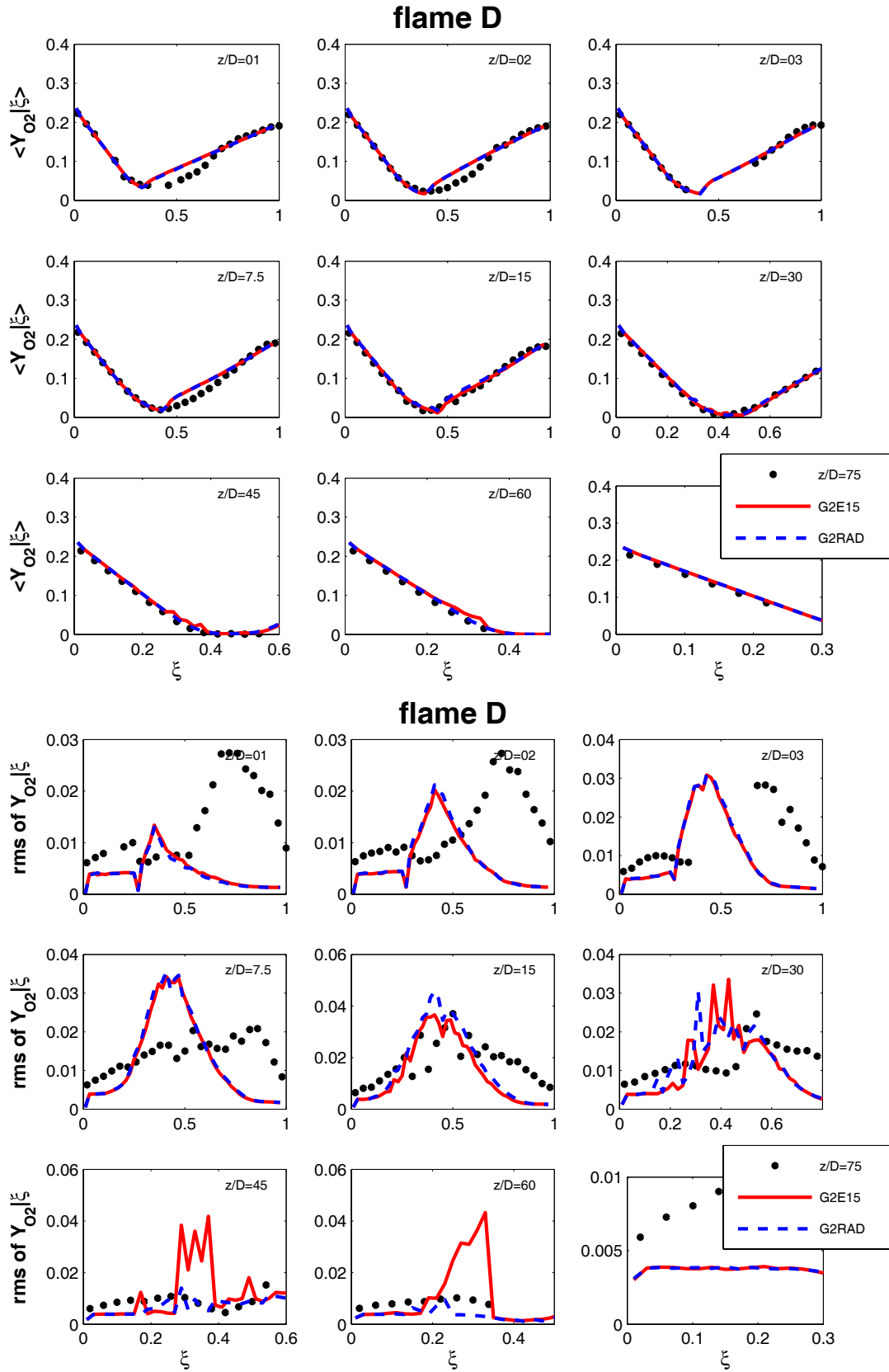
(3) G2E15 and G2RAD

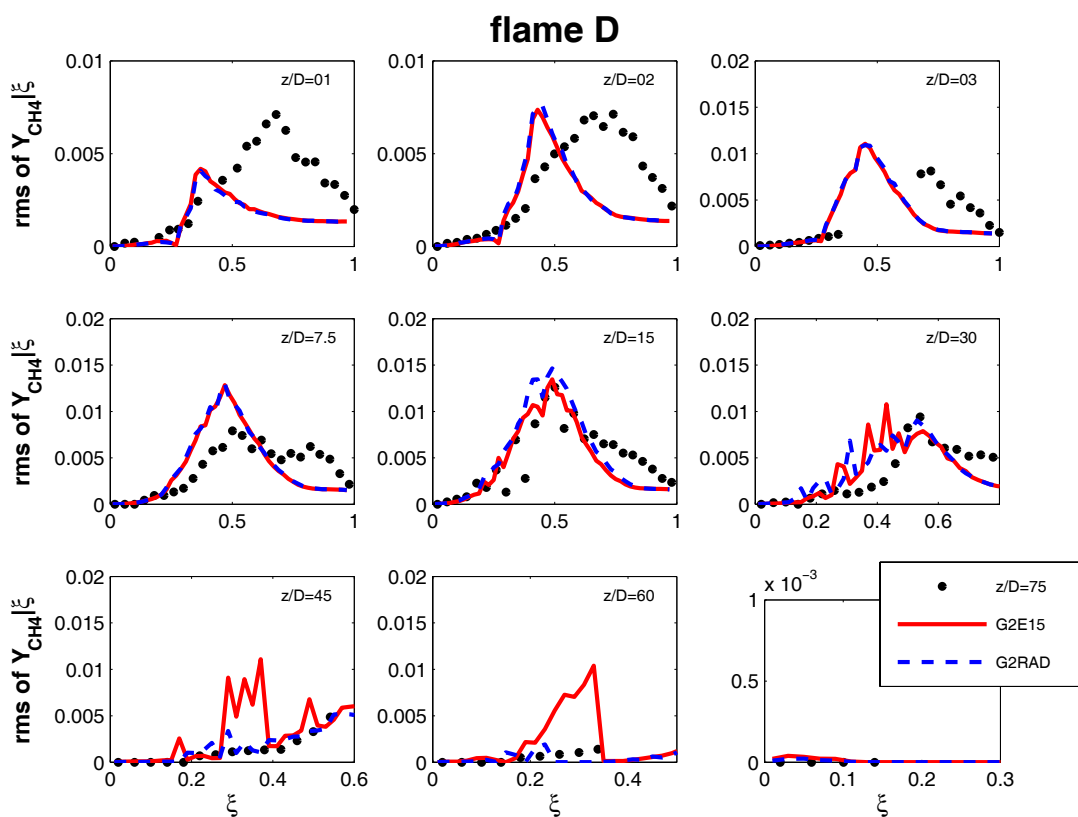
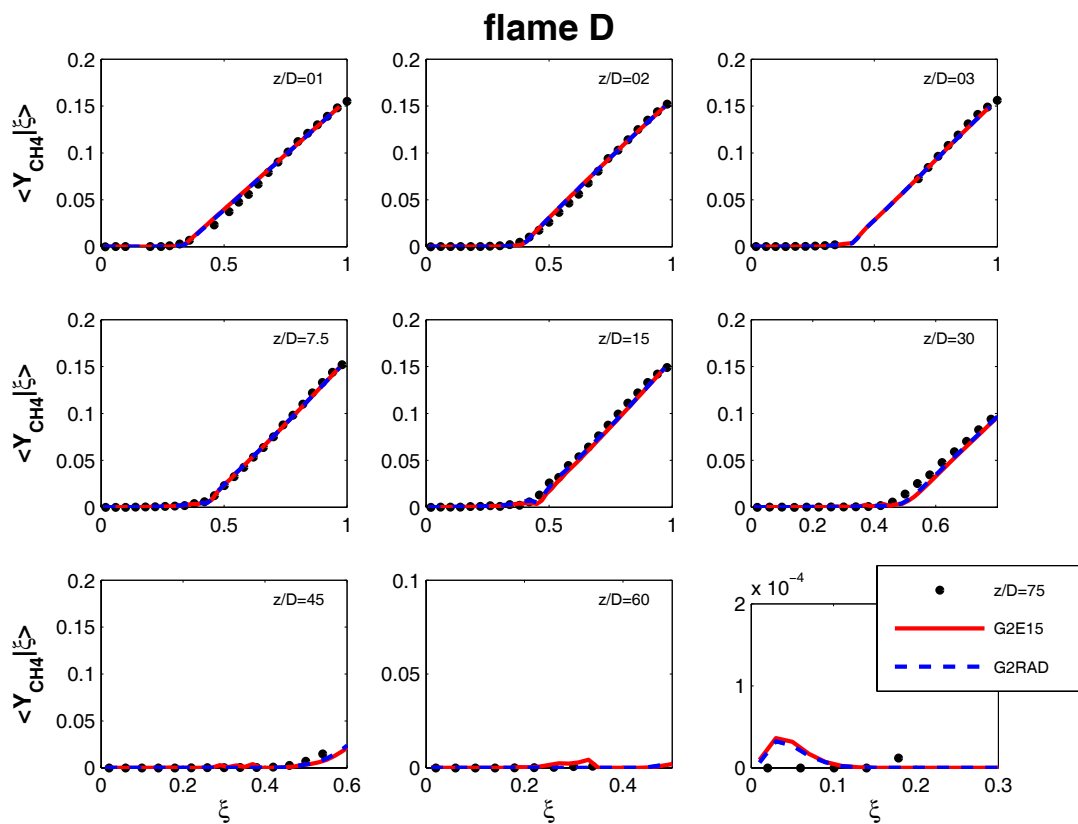


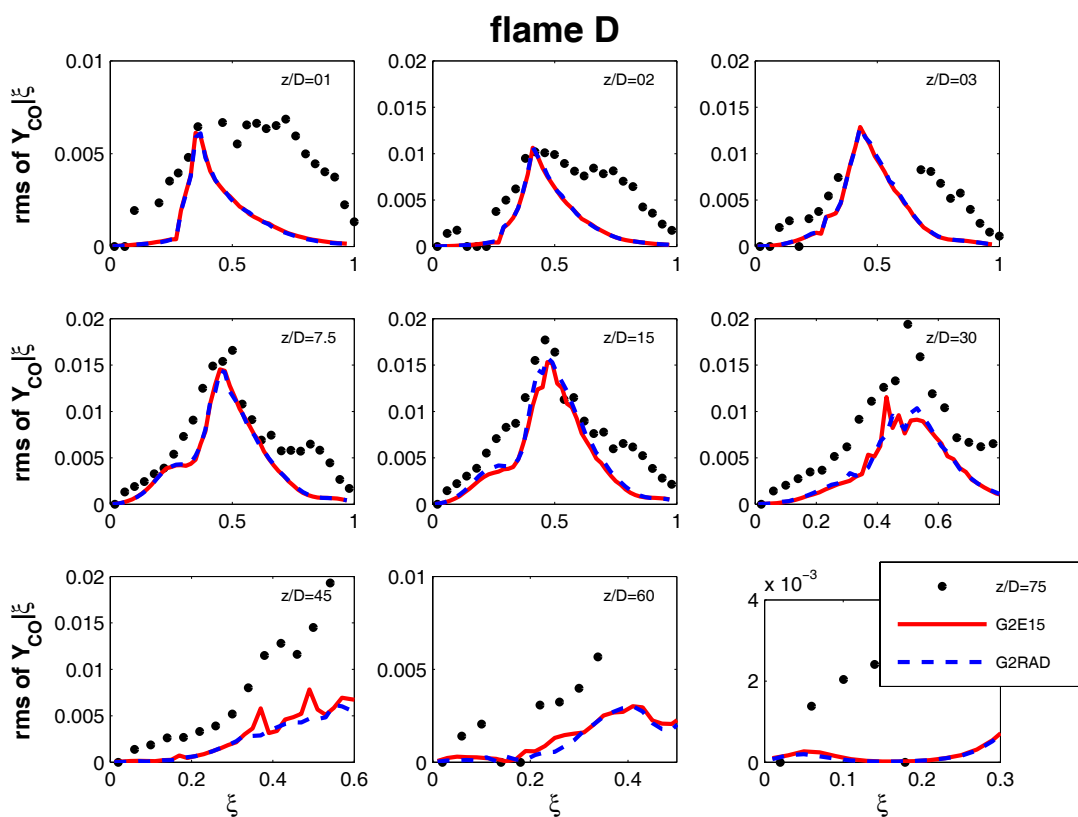
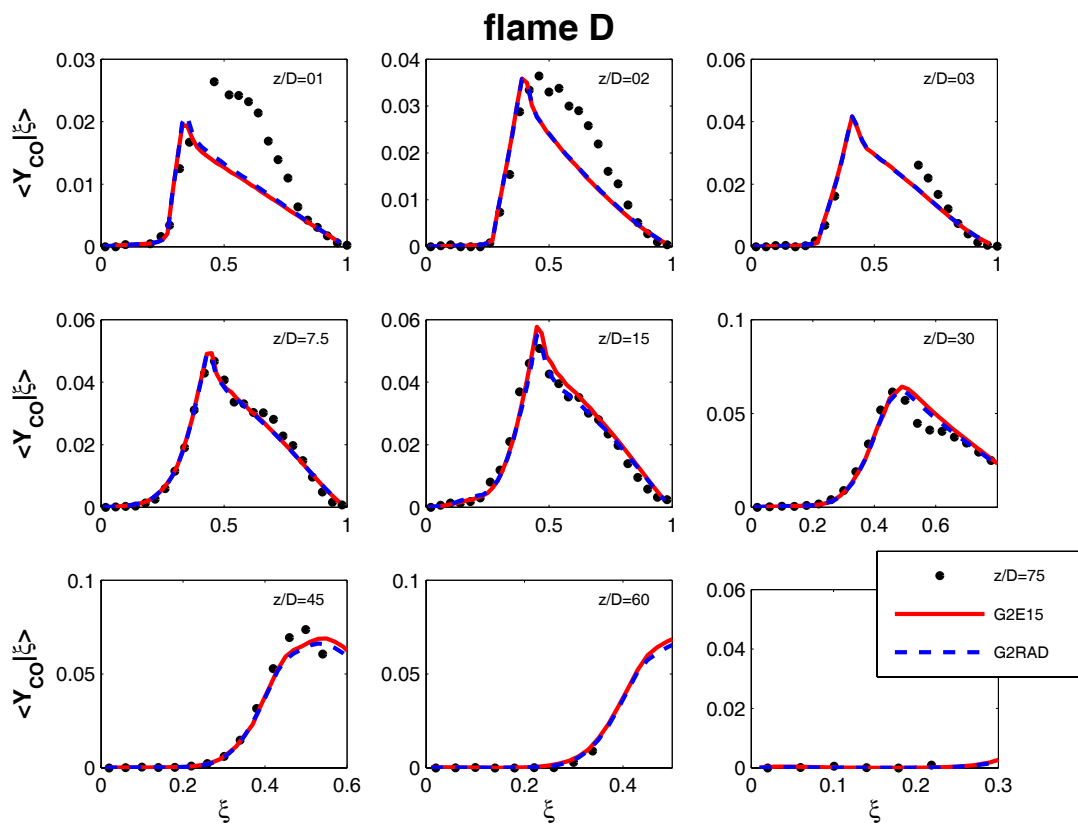


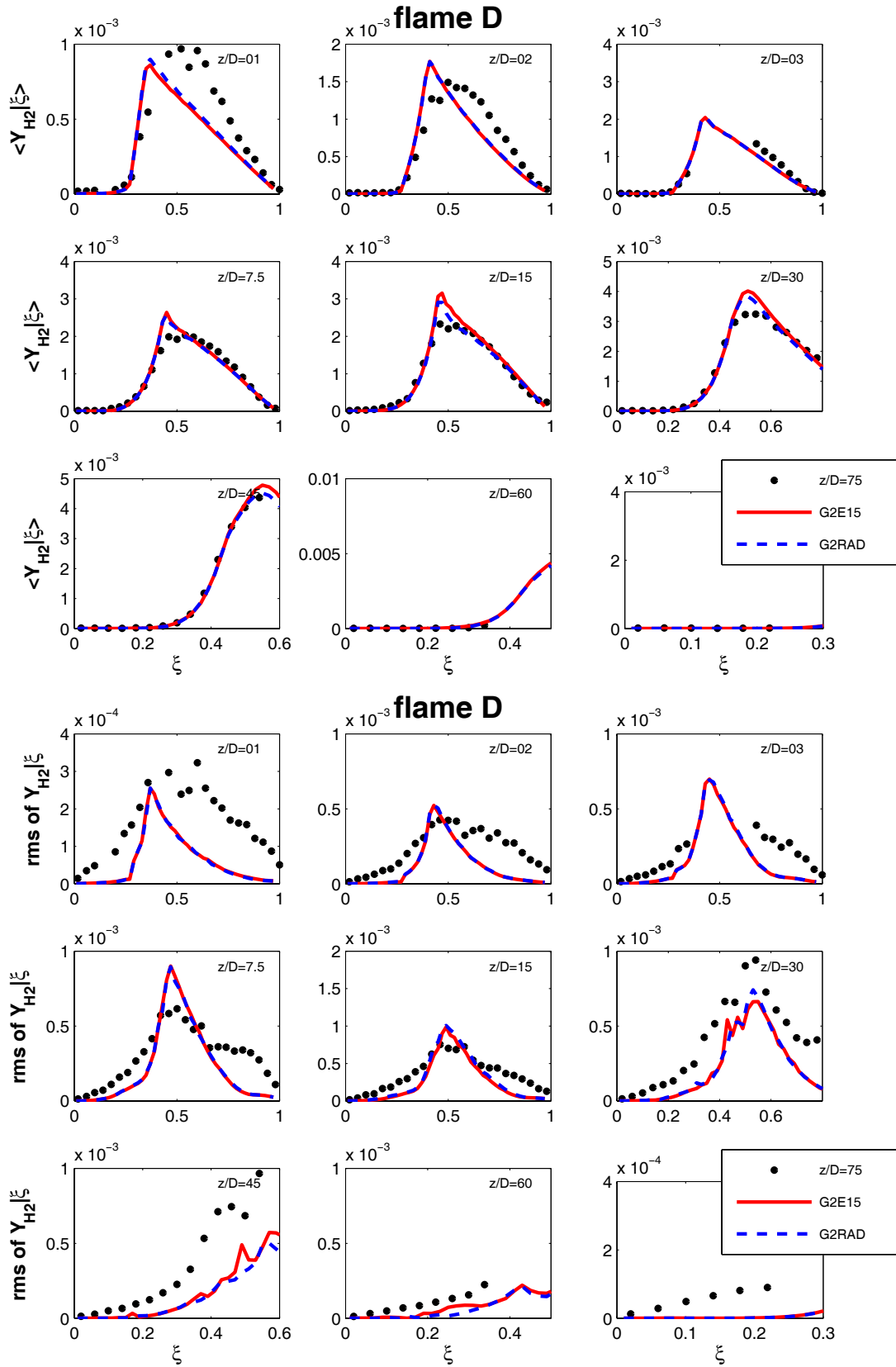


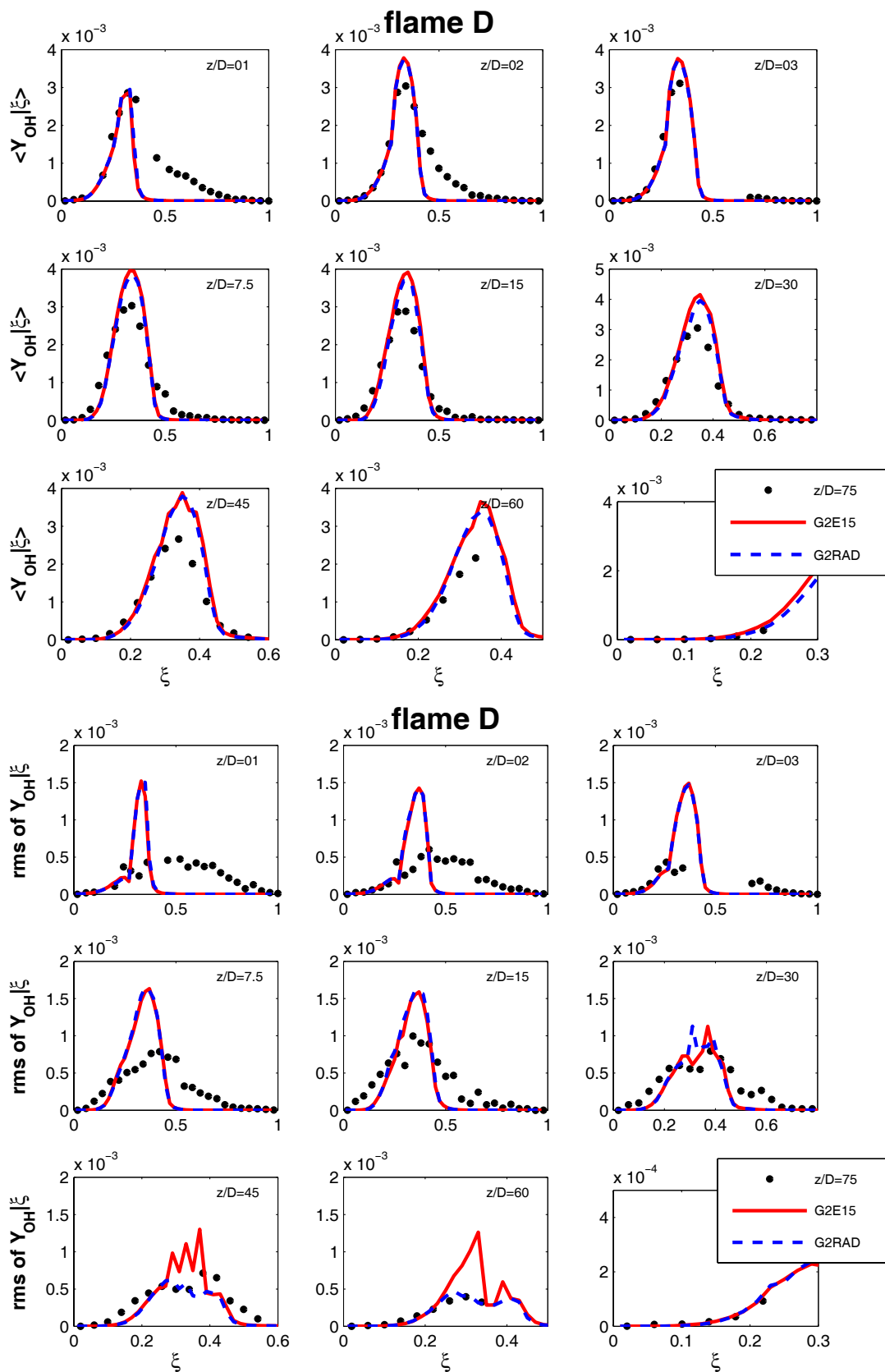


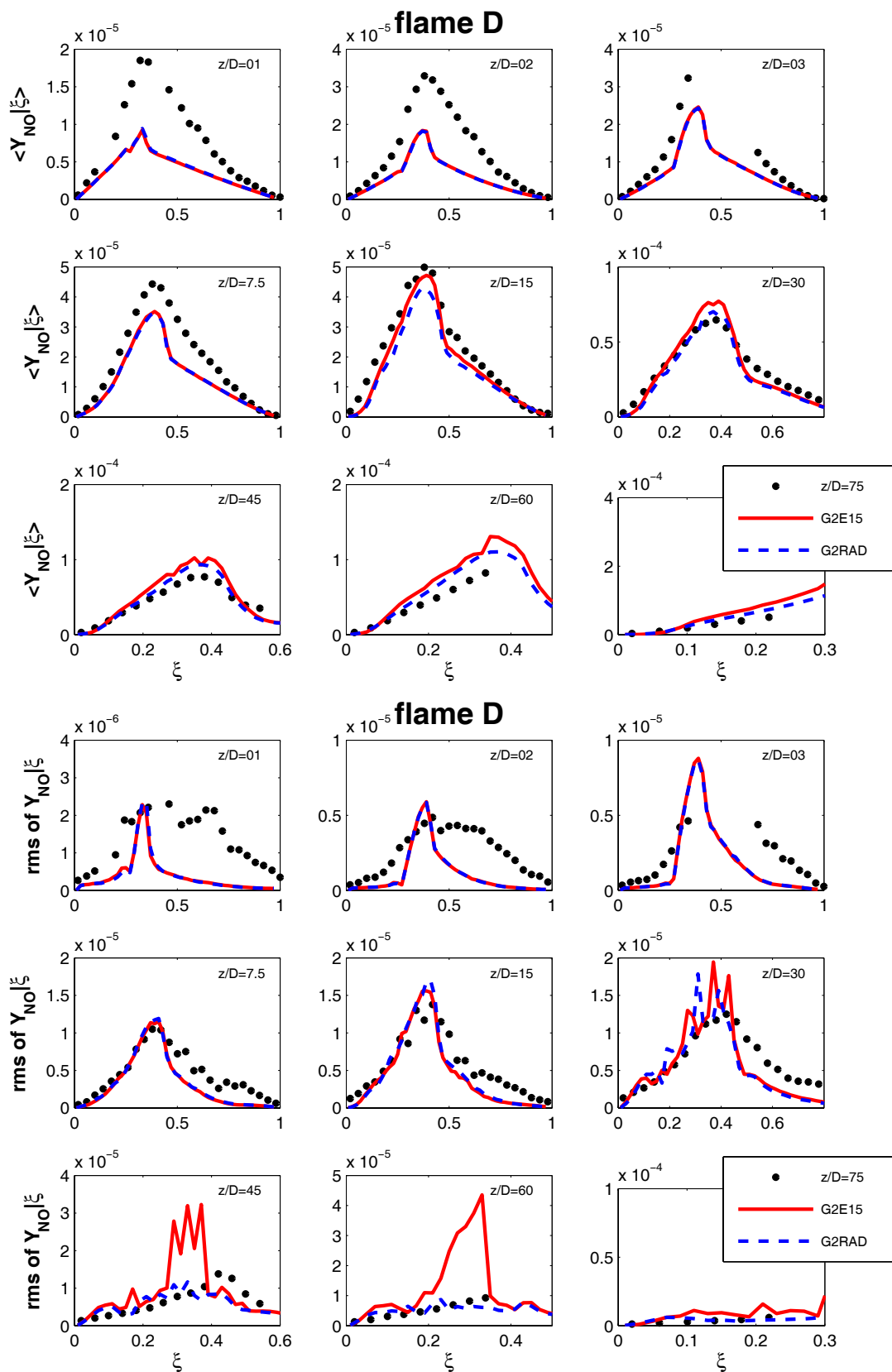




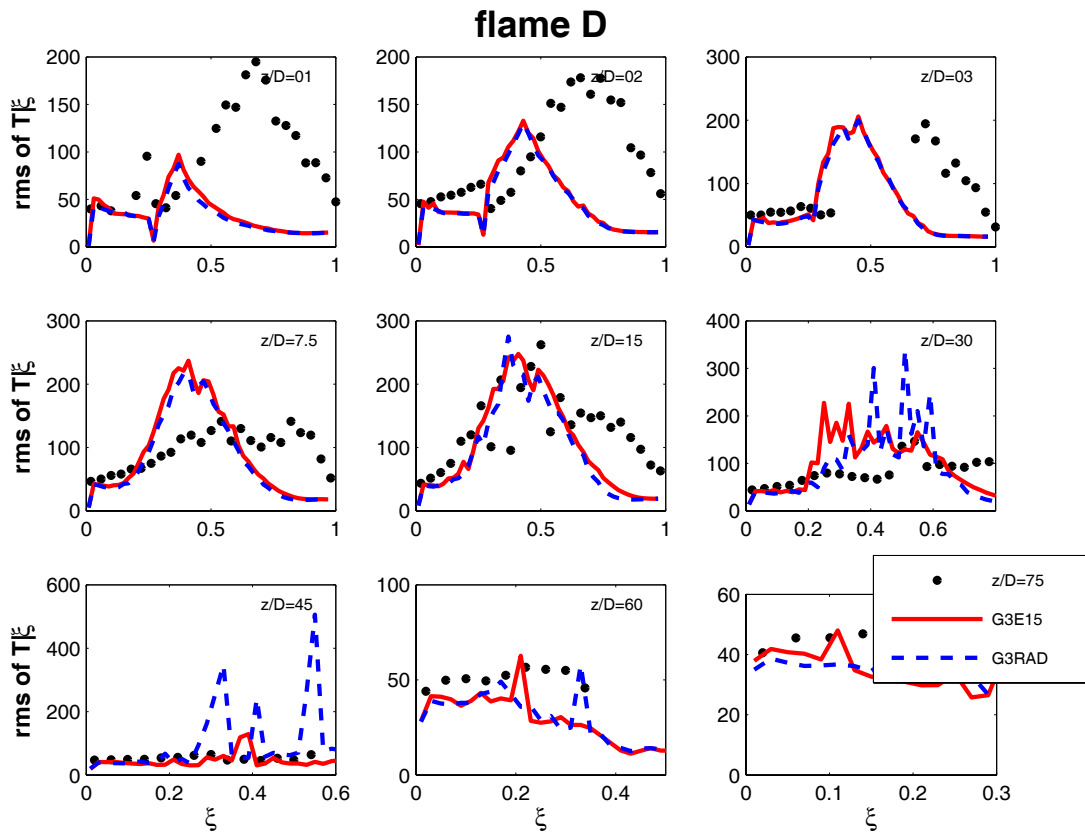
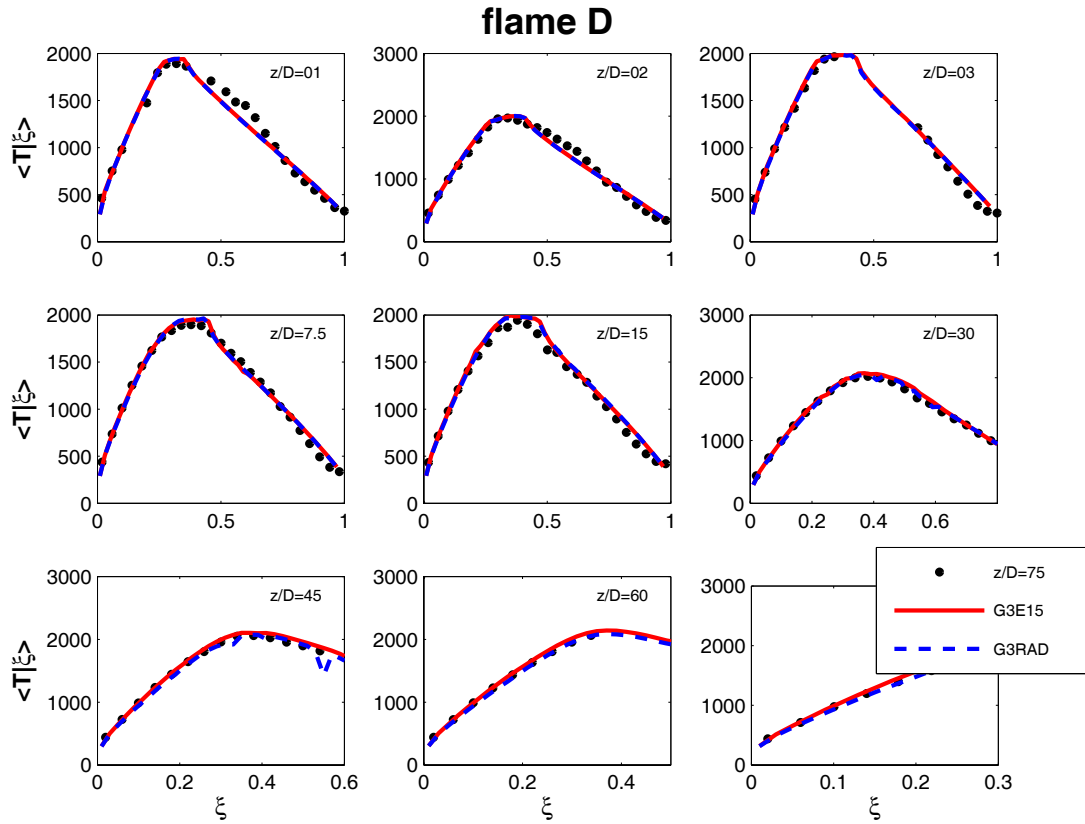


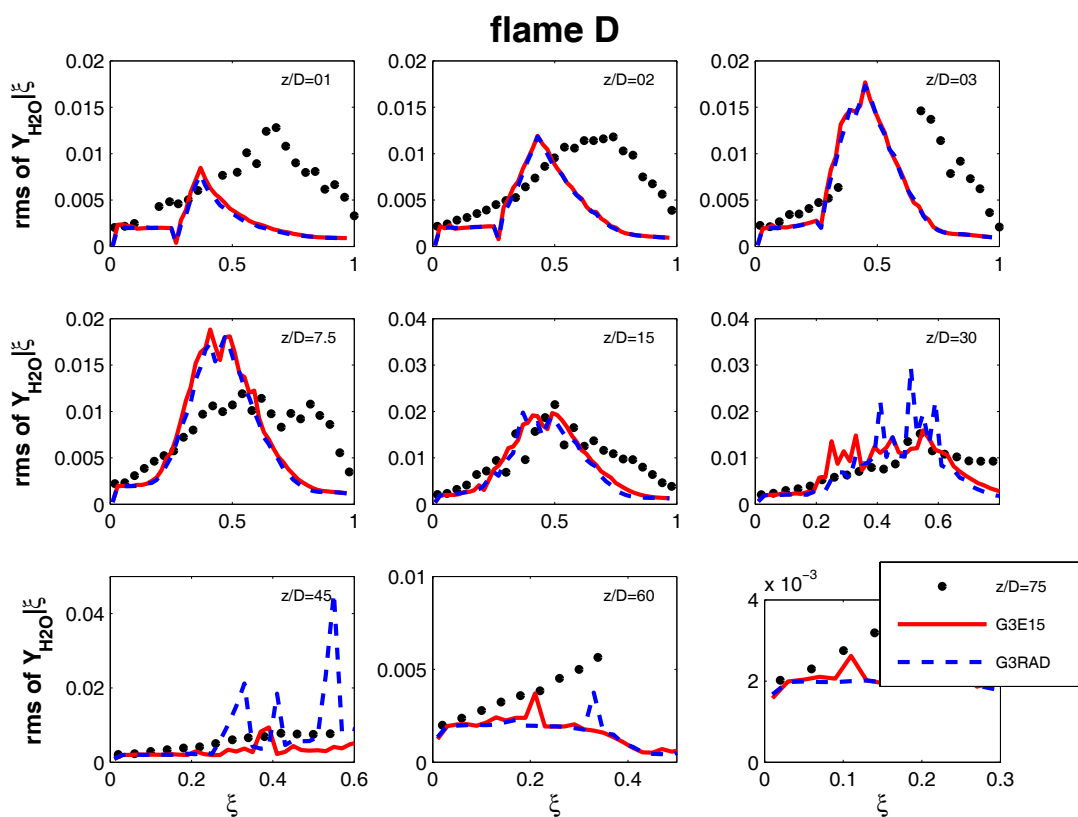
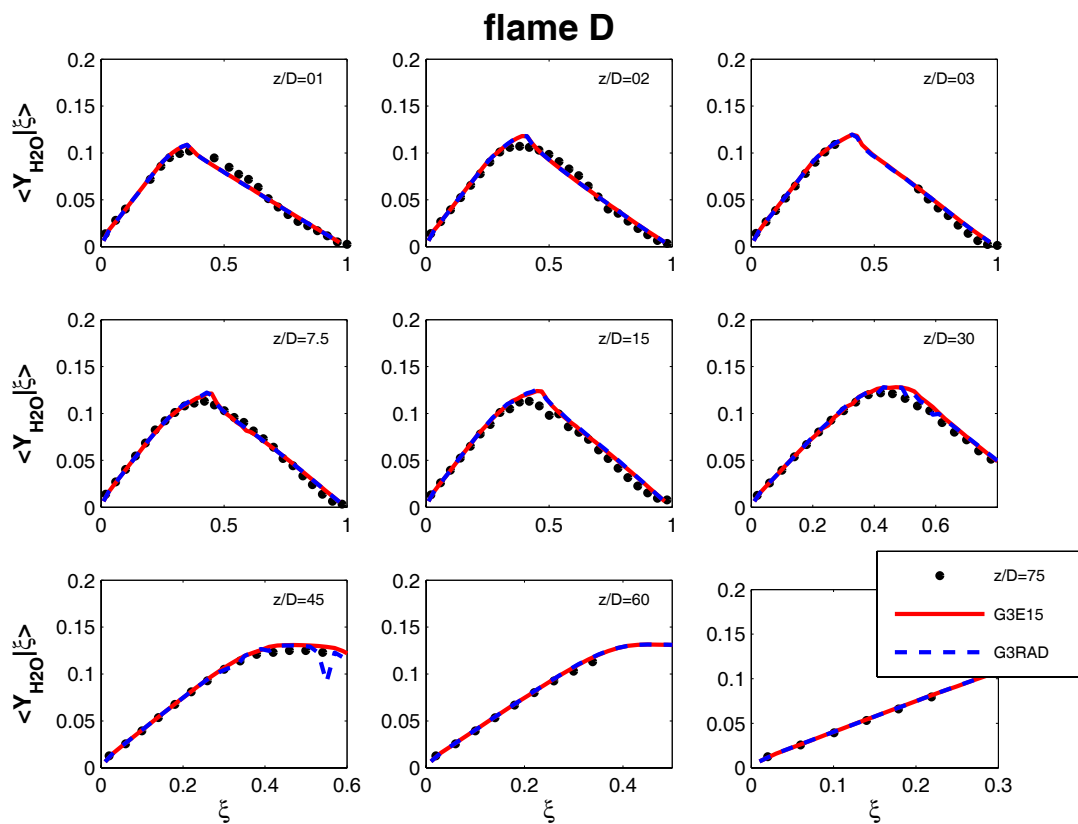


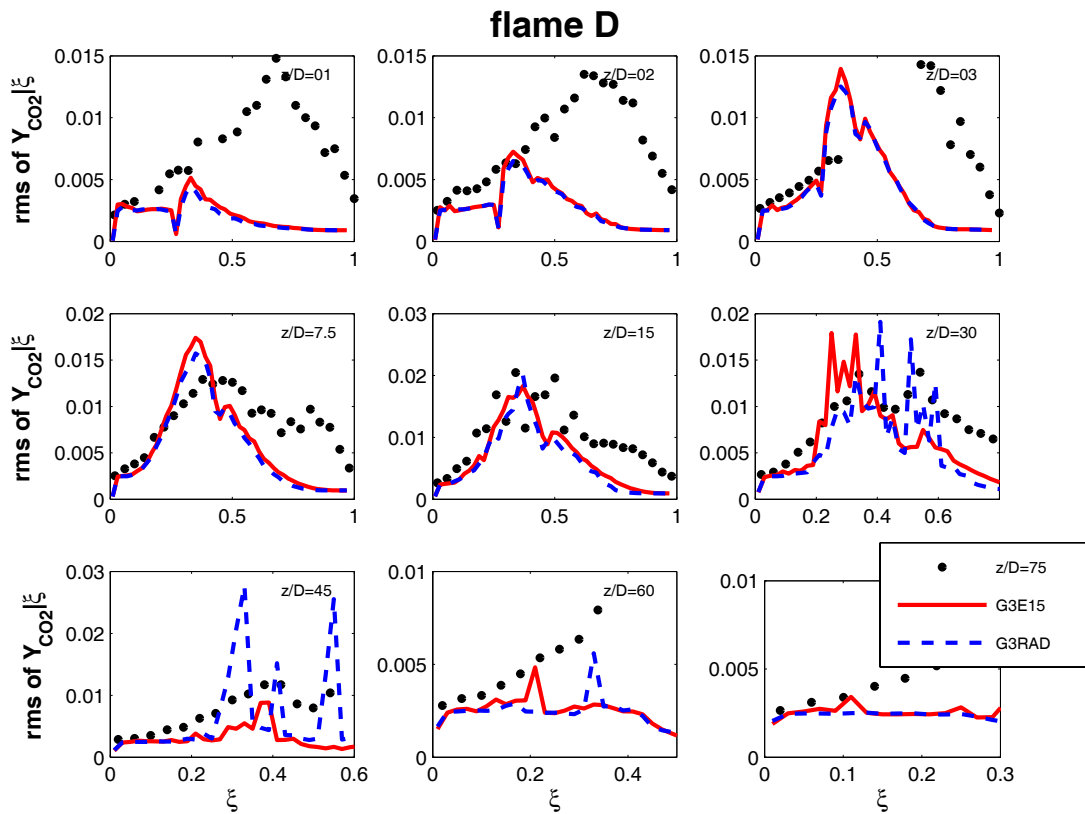
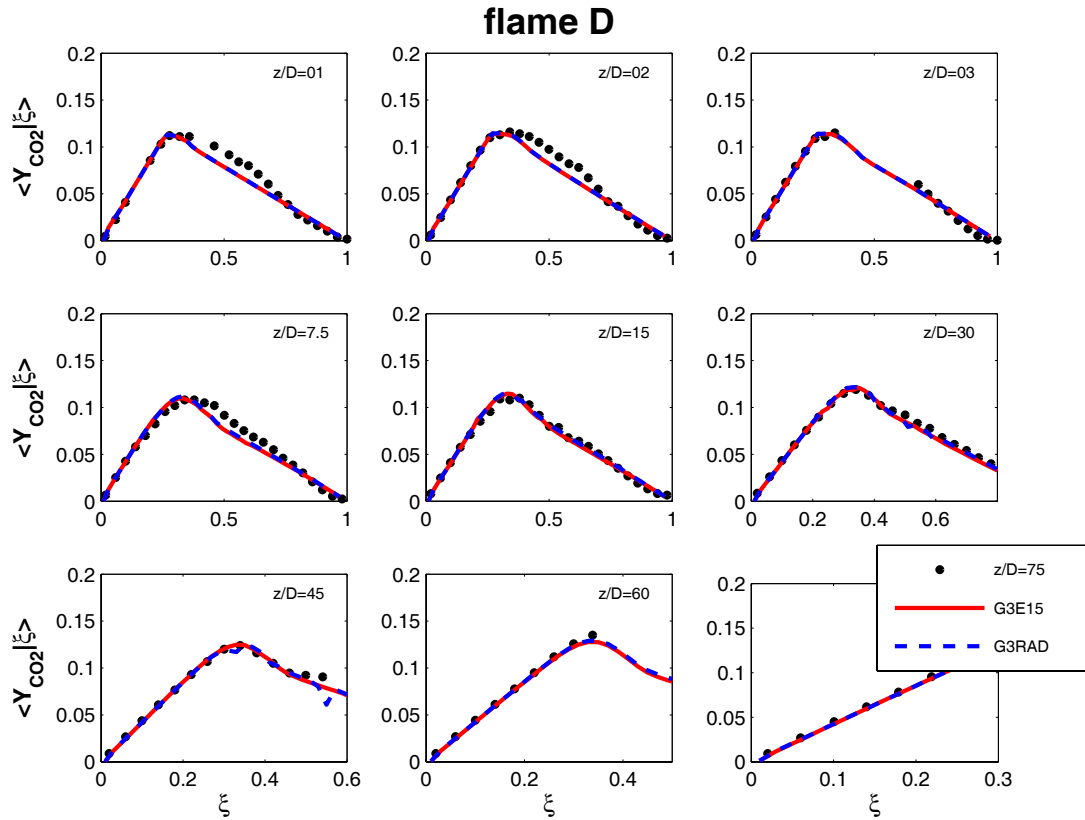


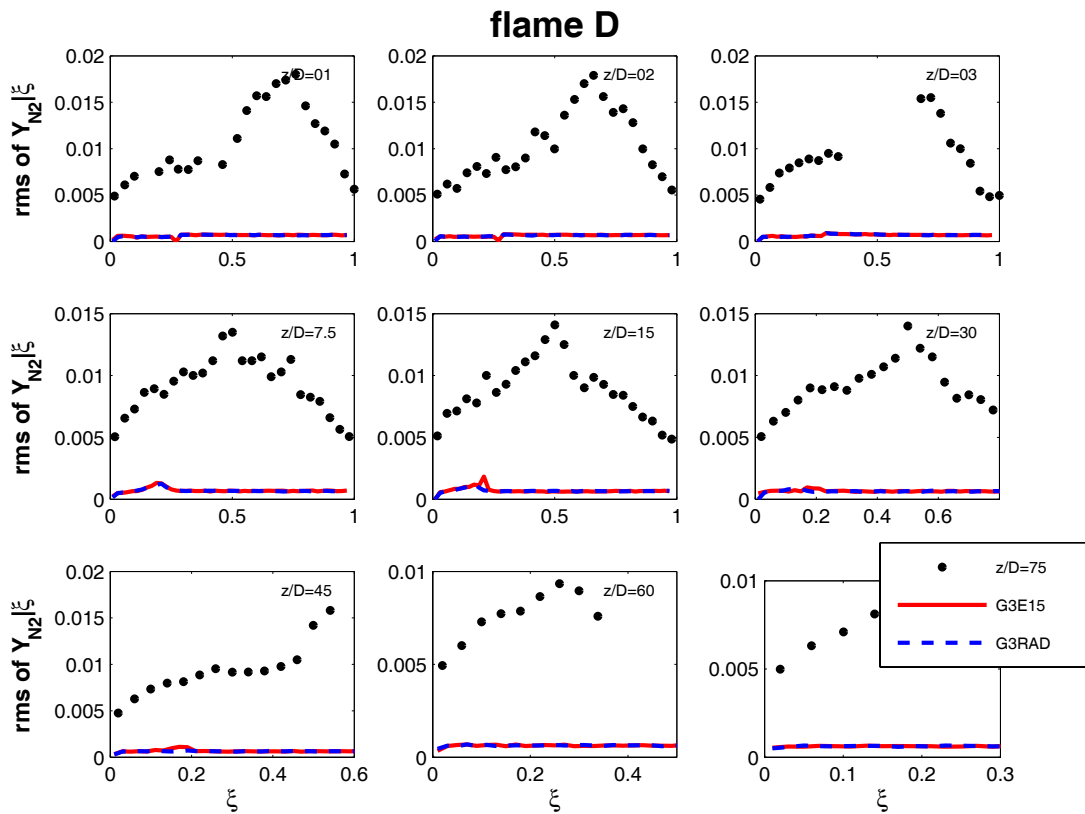
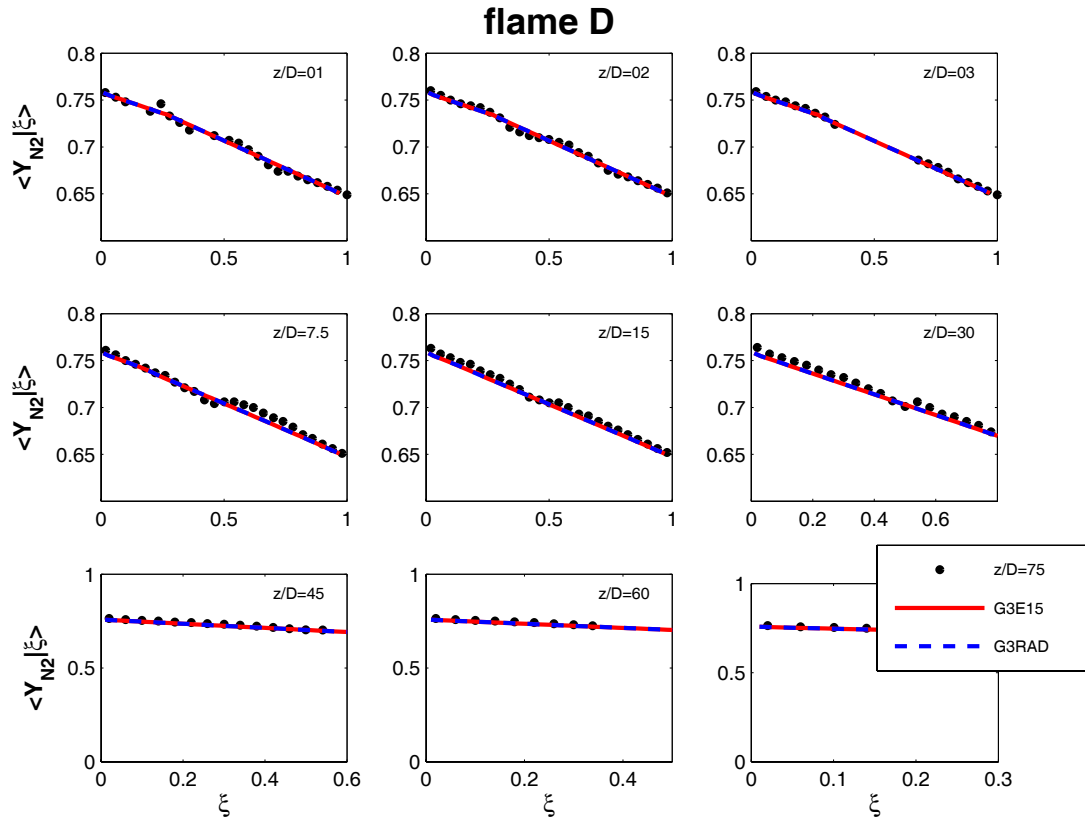


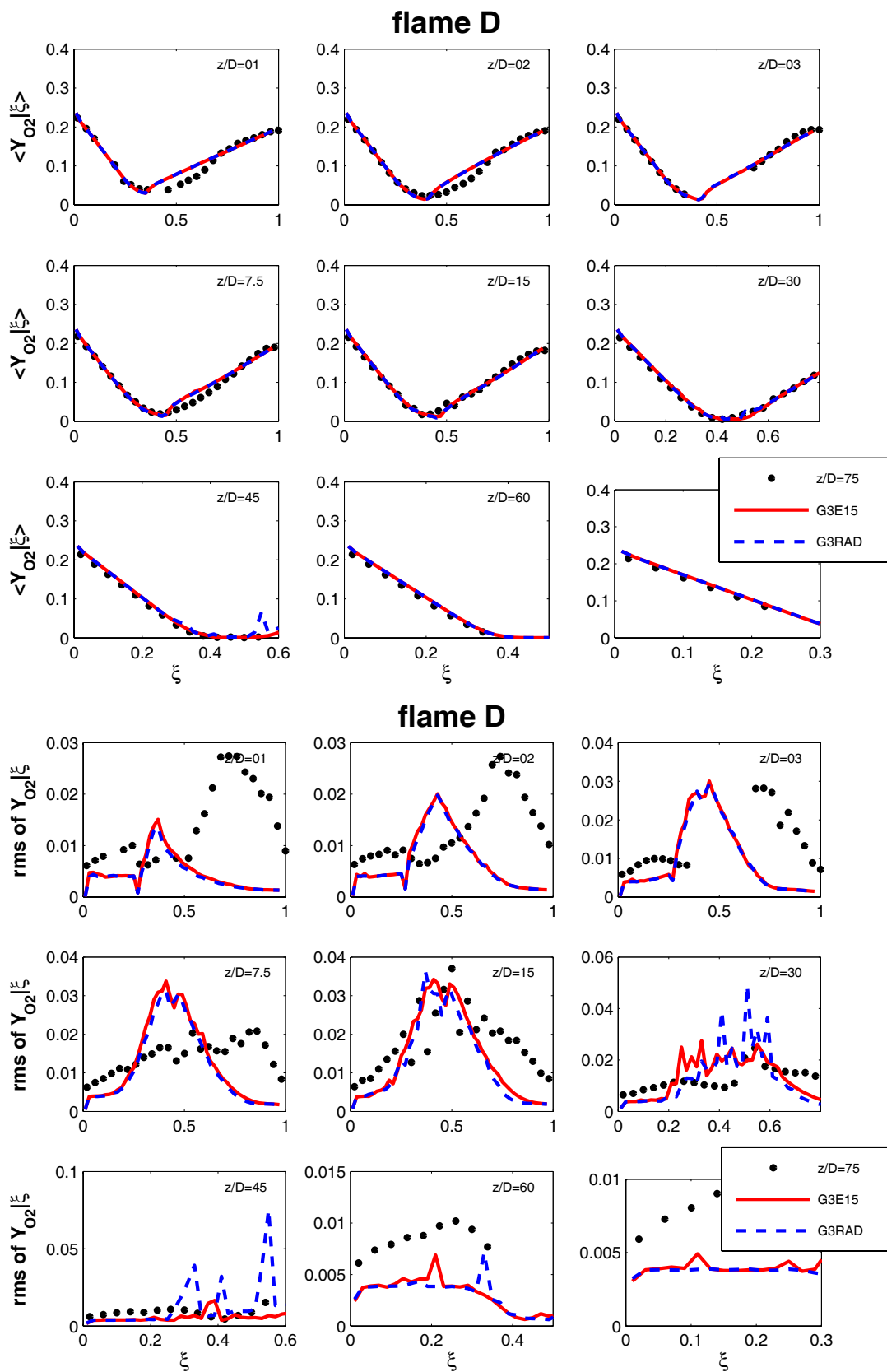
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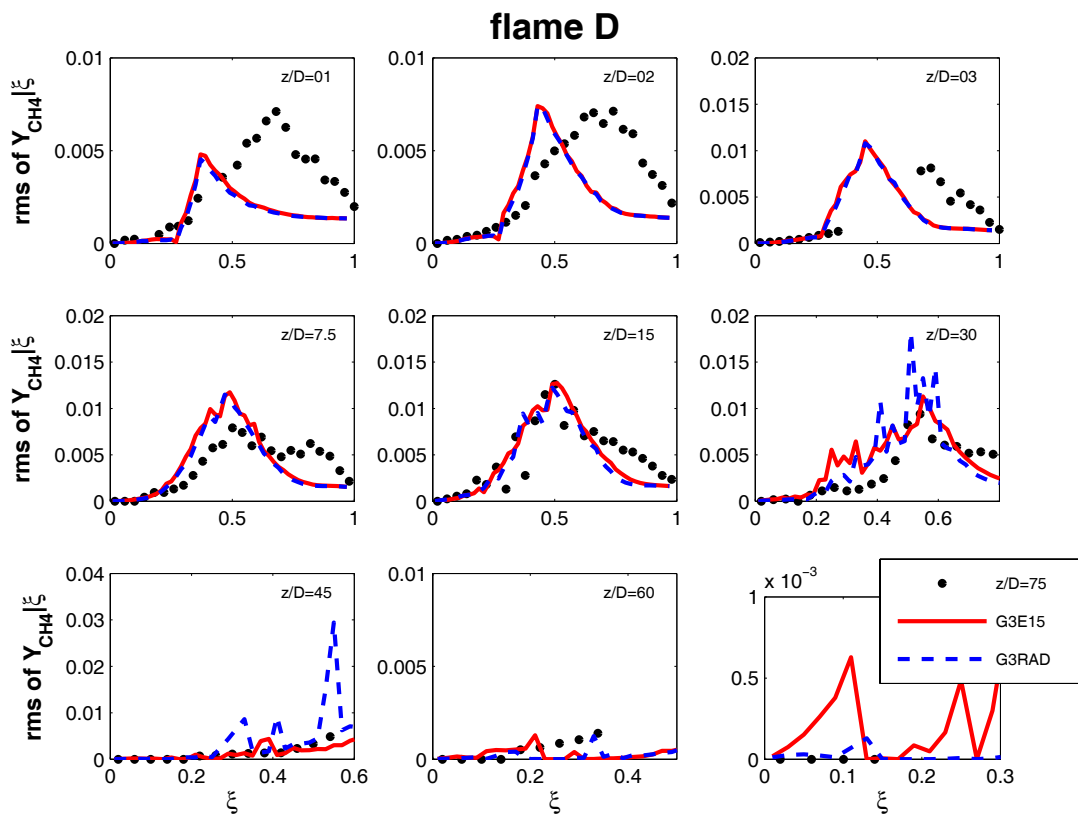
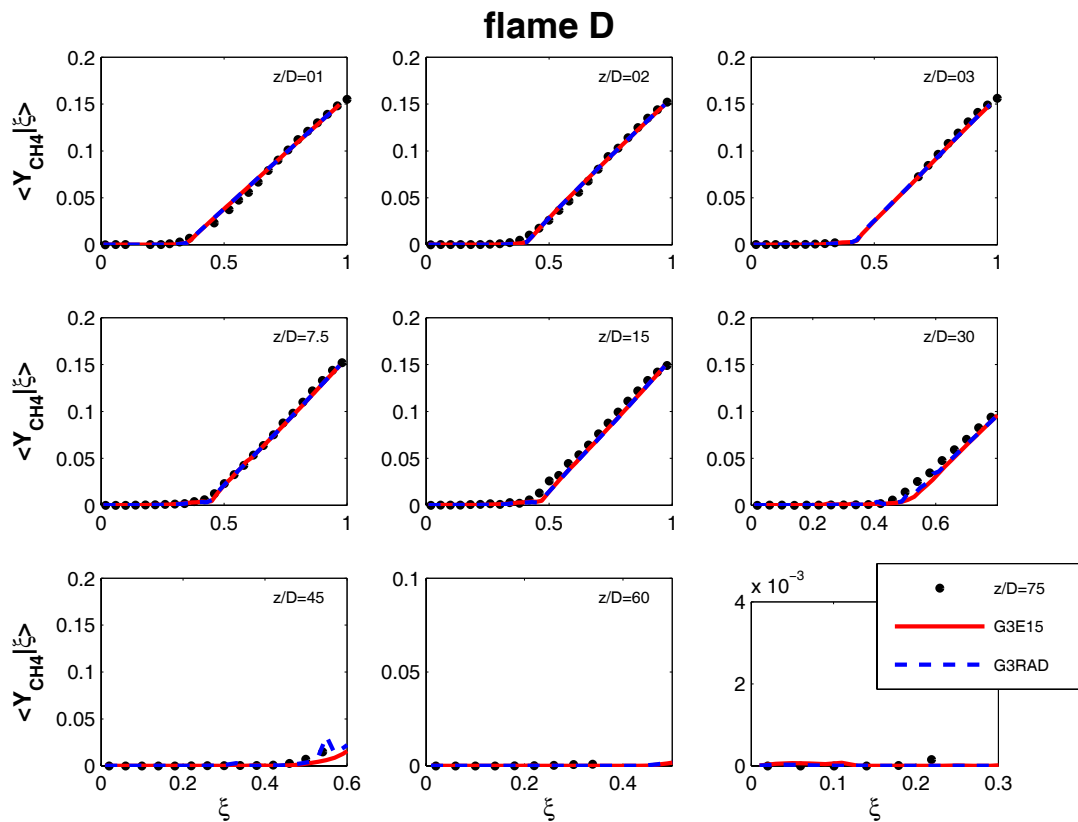


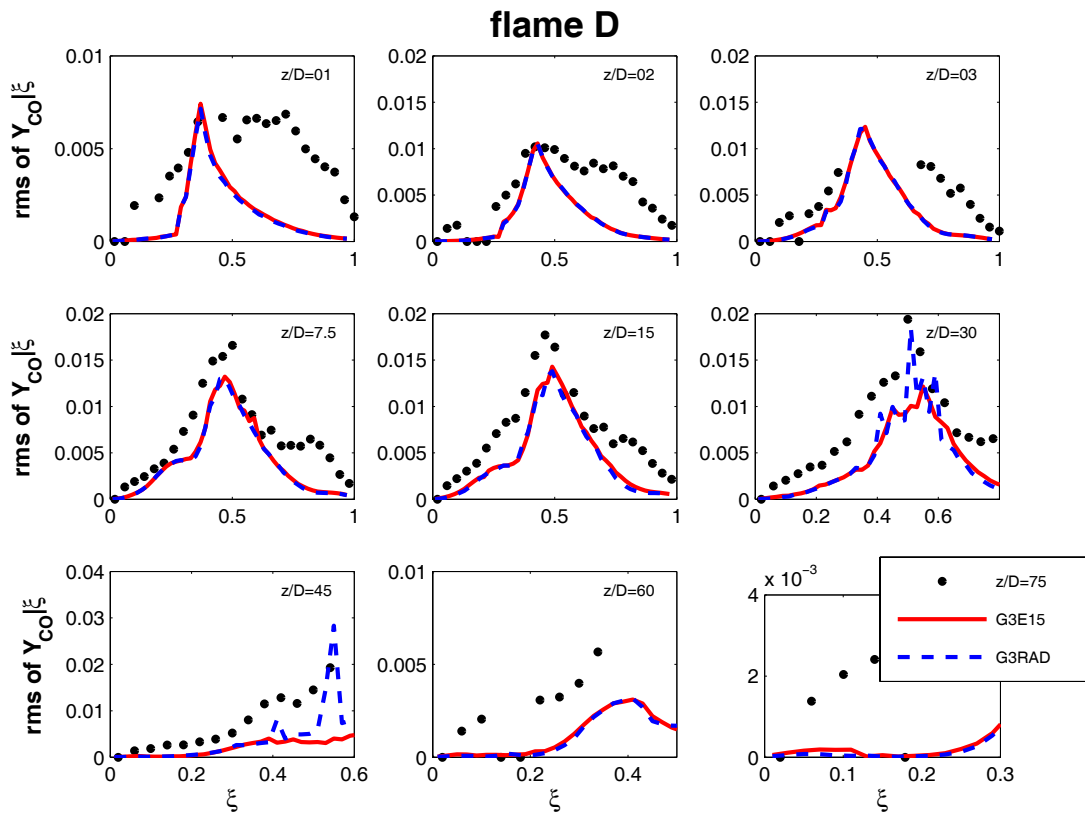
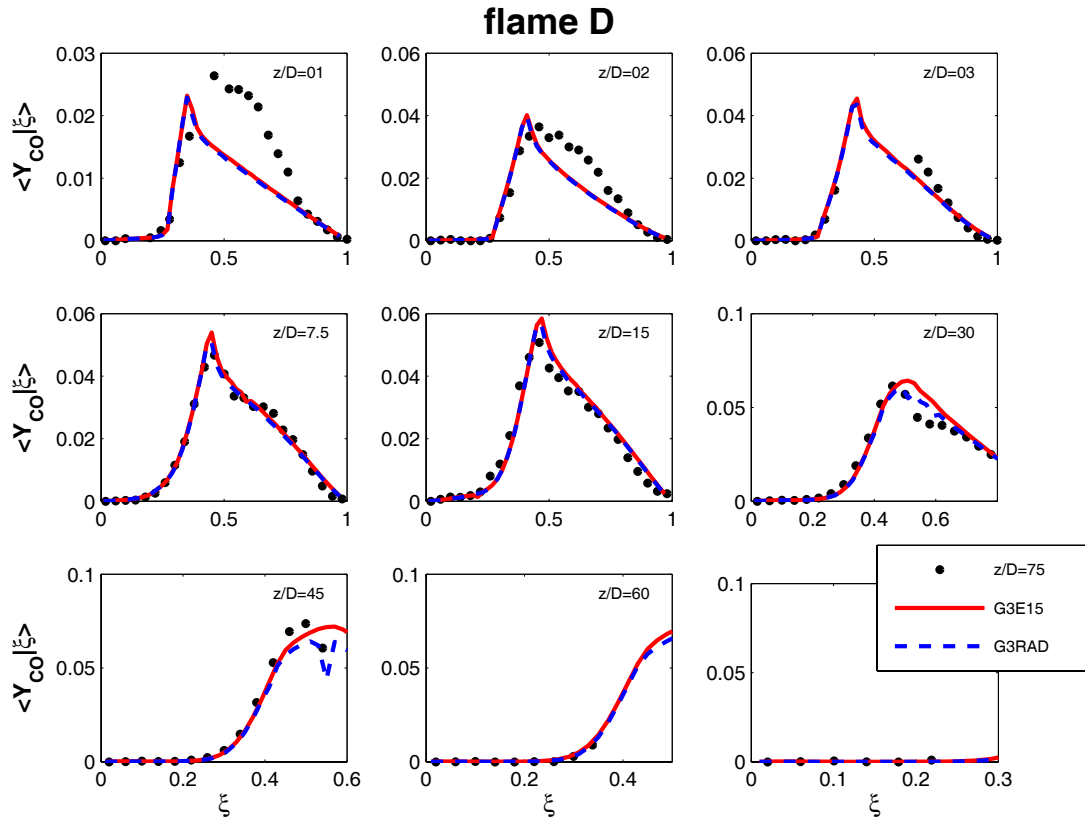


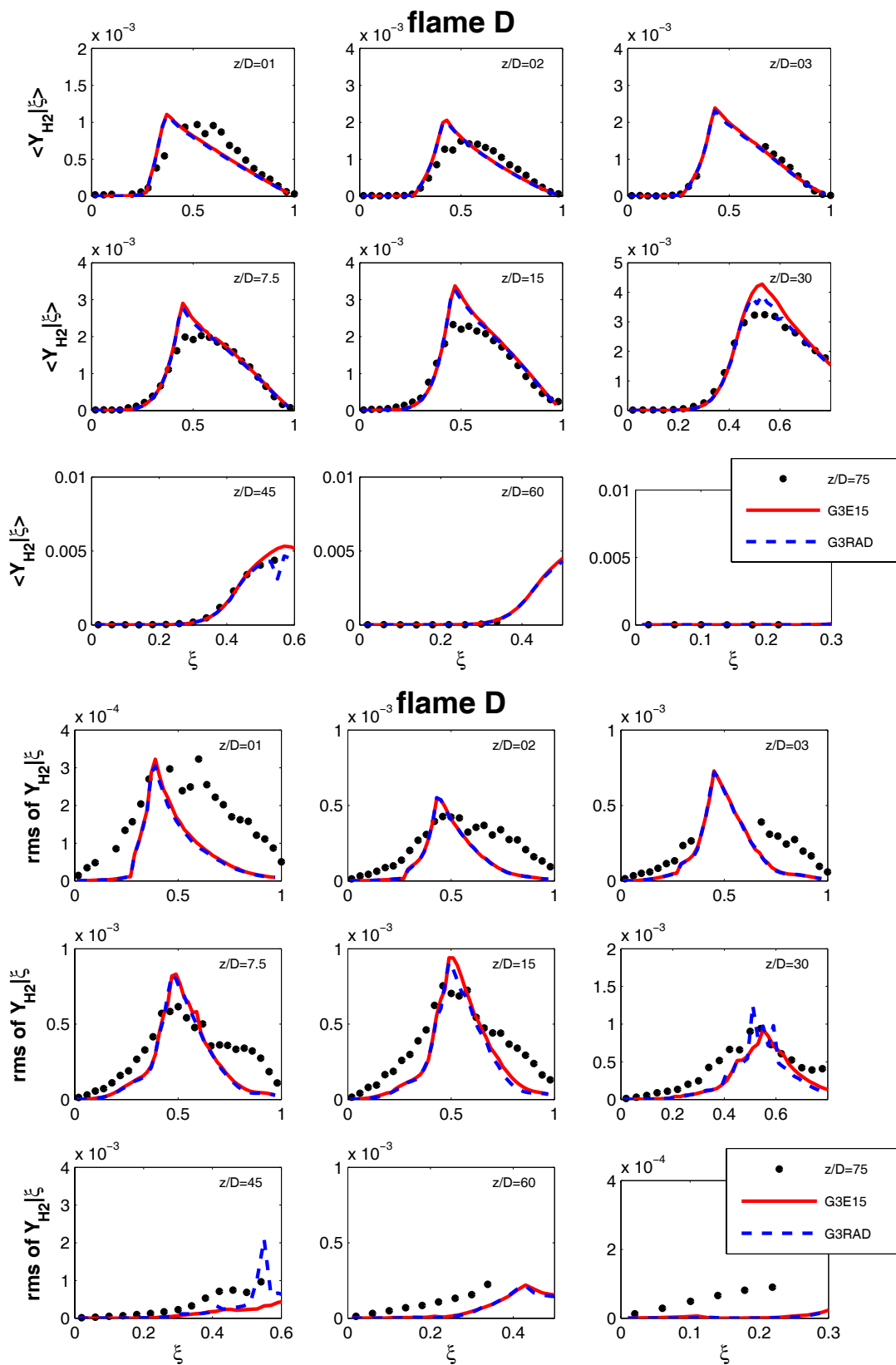


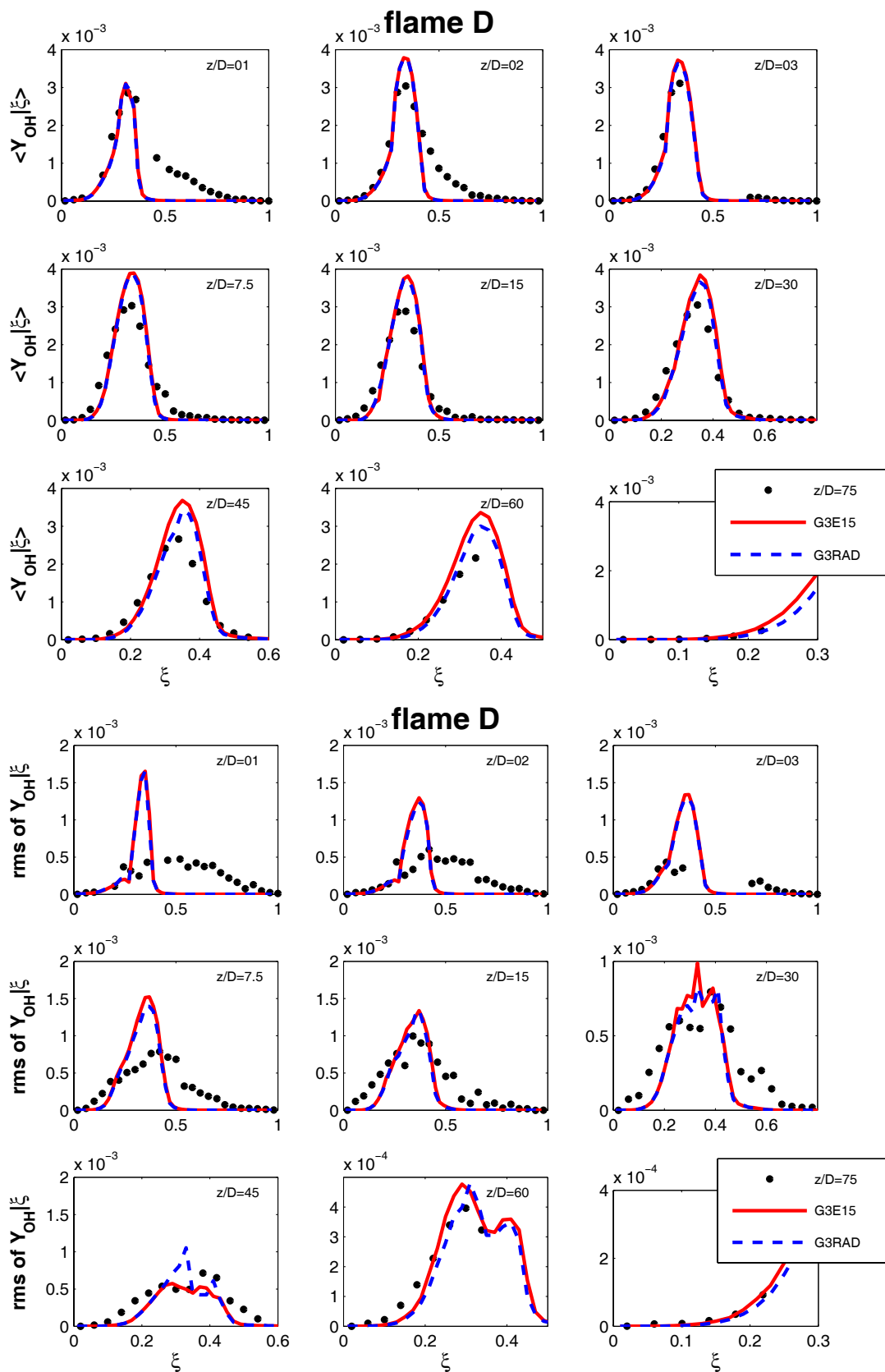


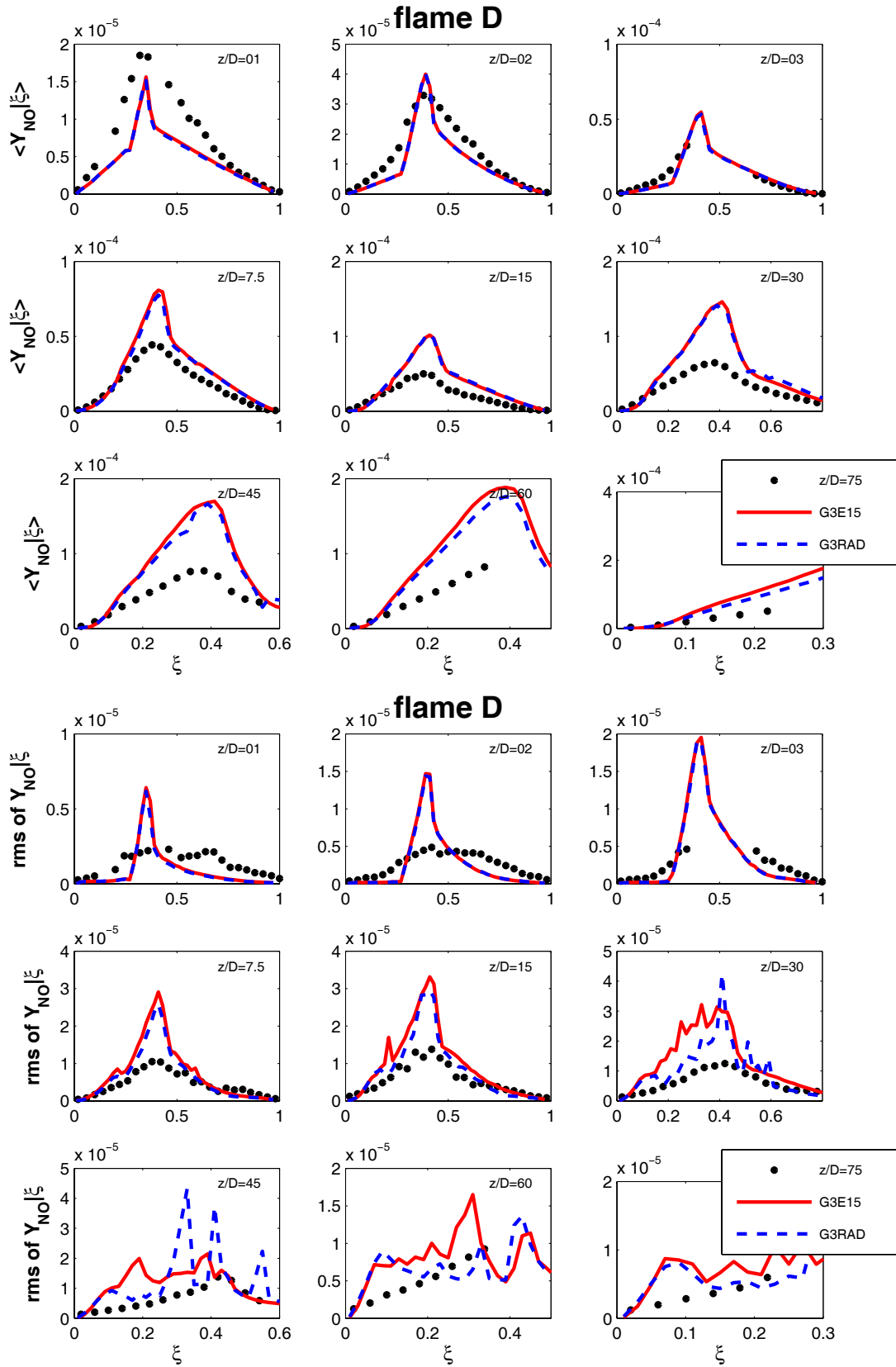




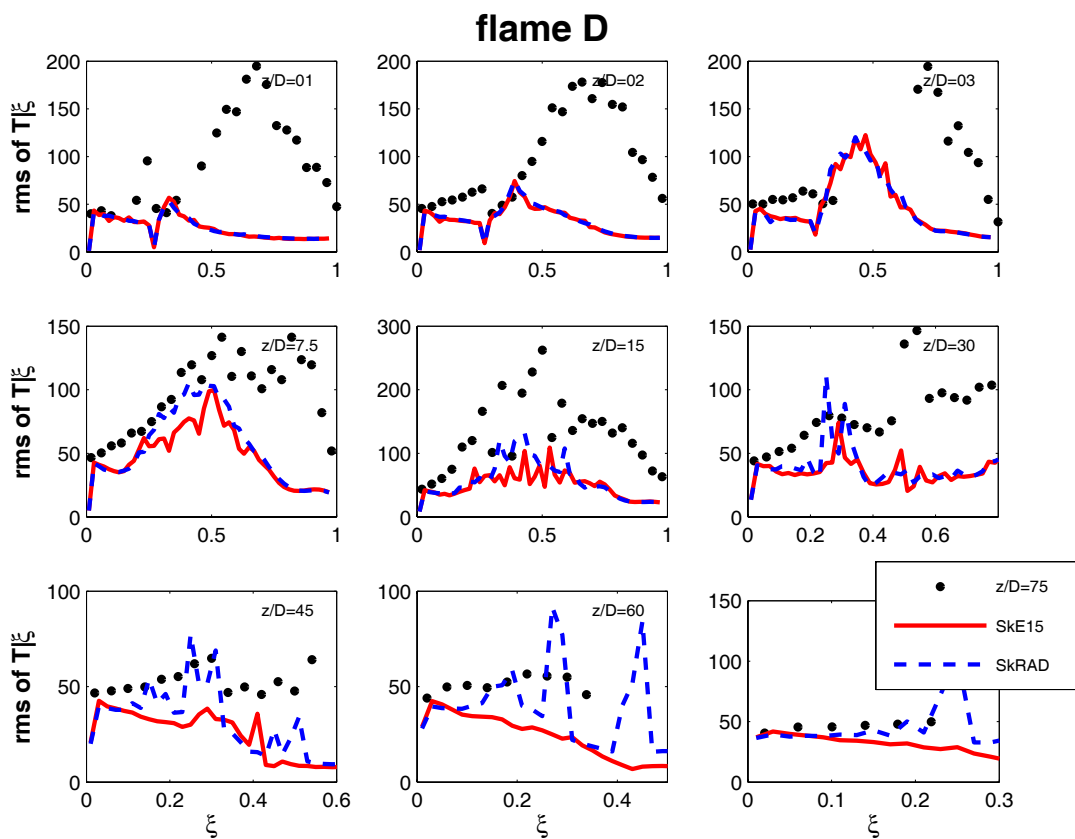
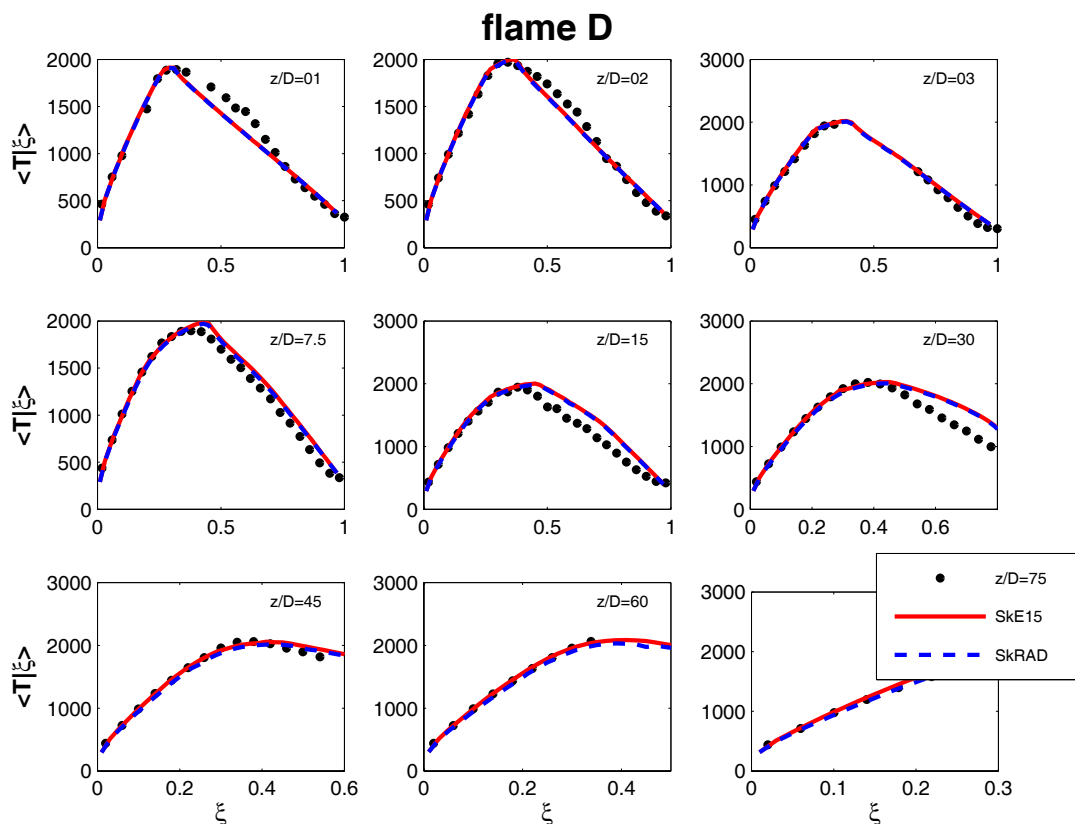


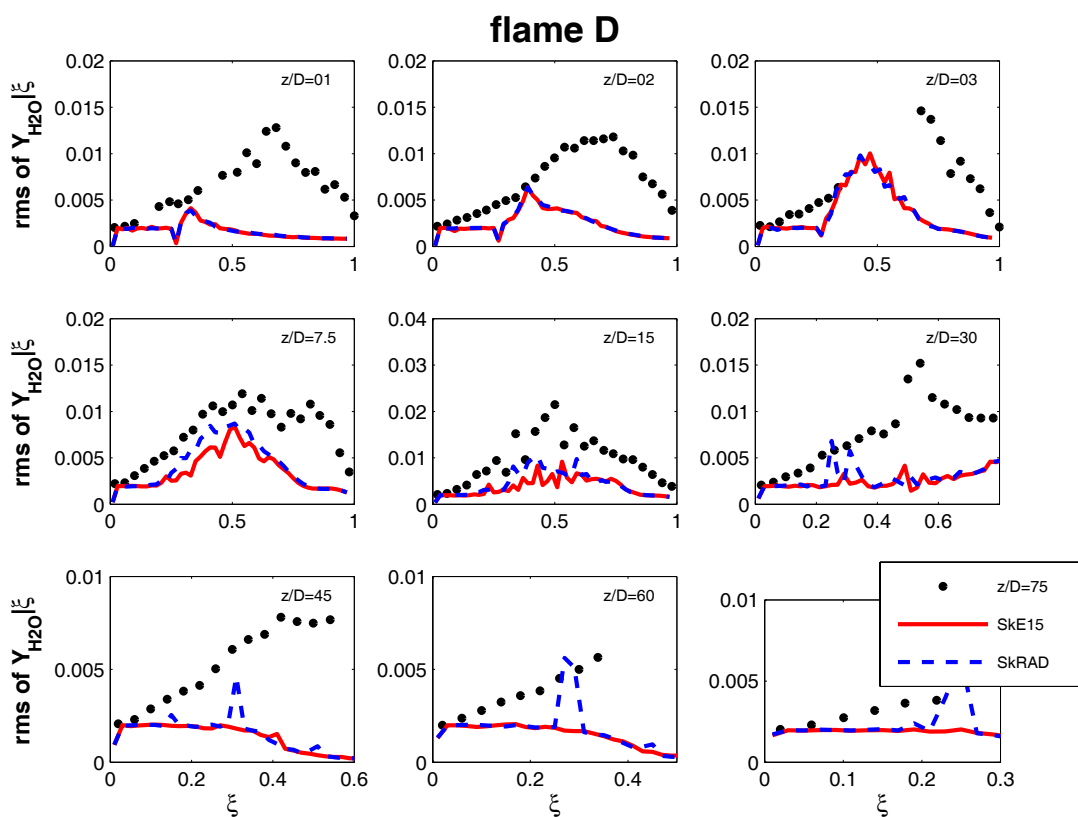
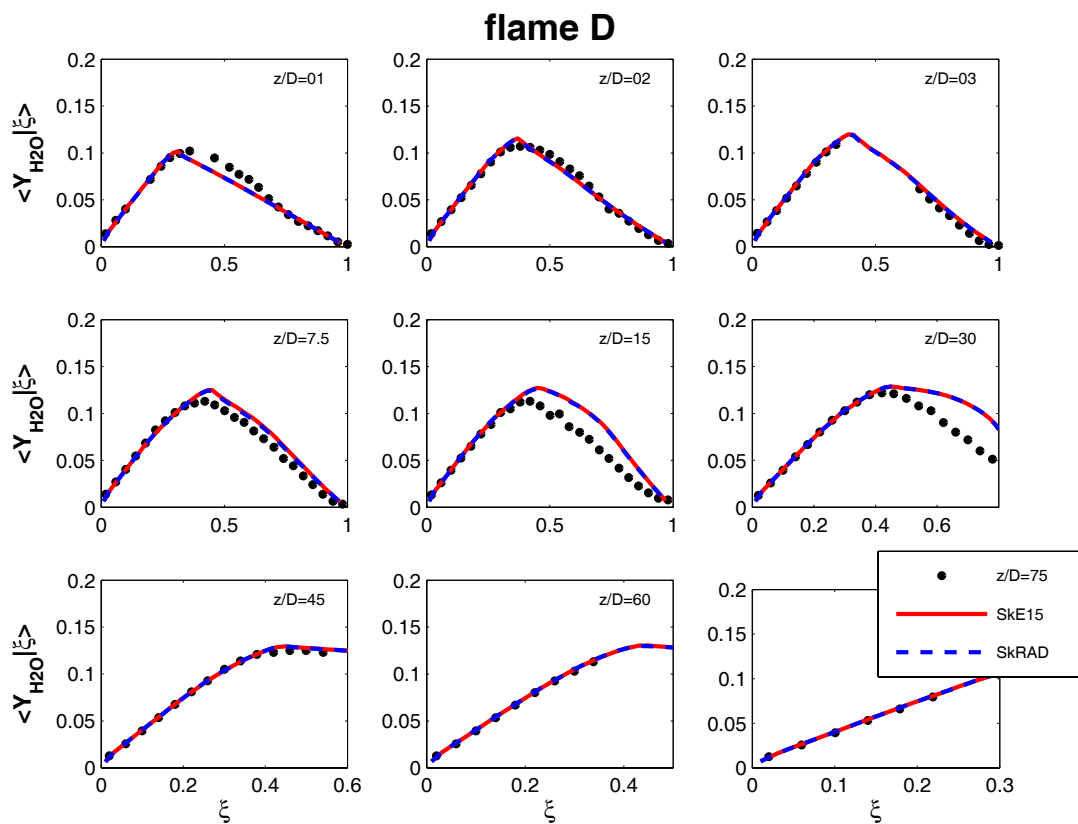


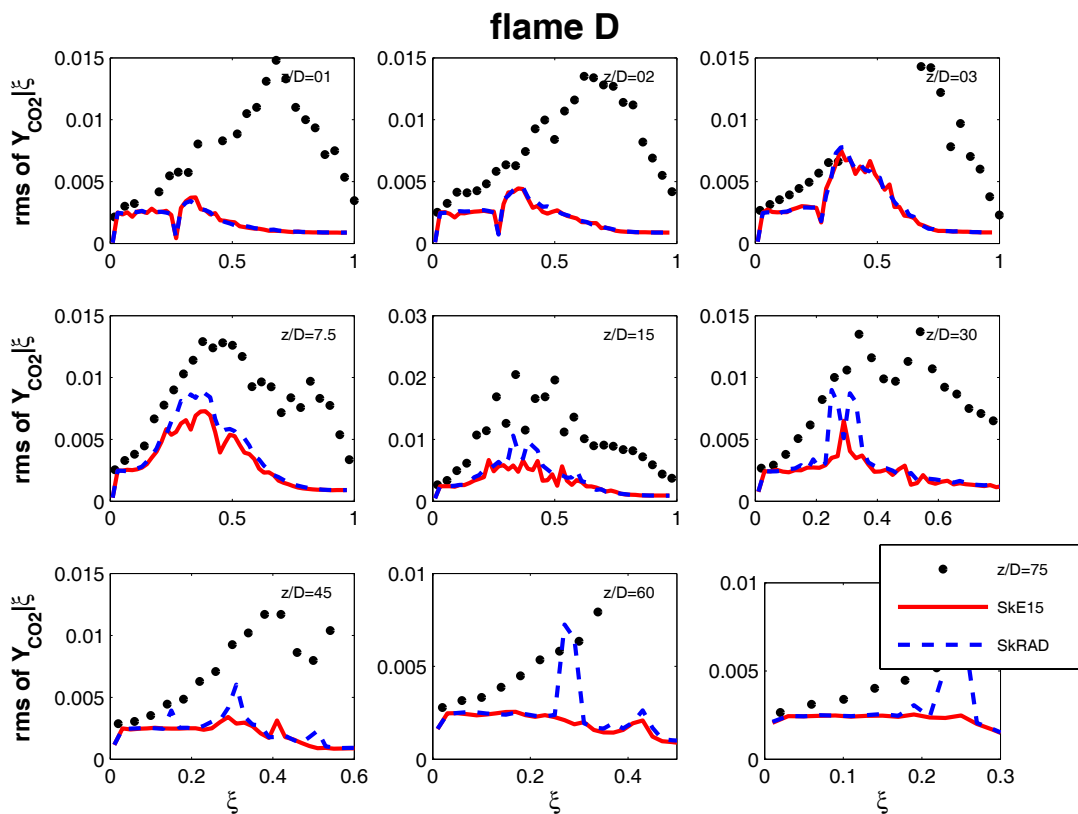
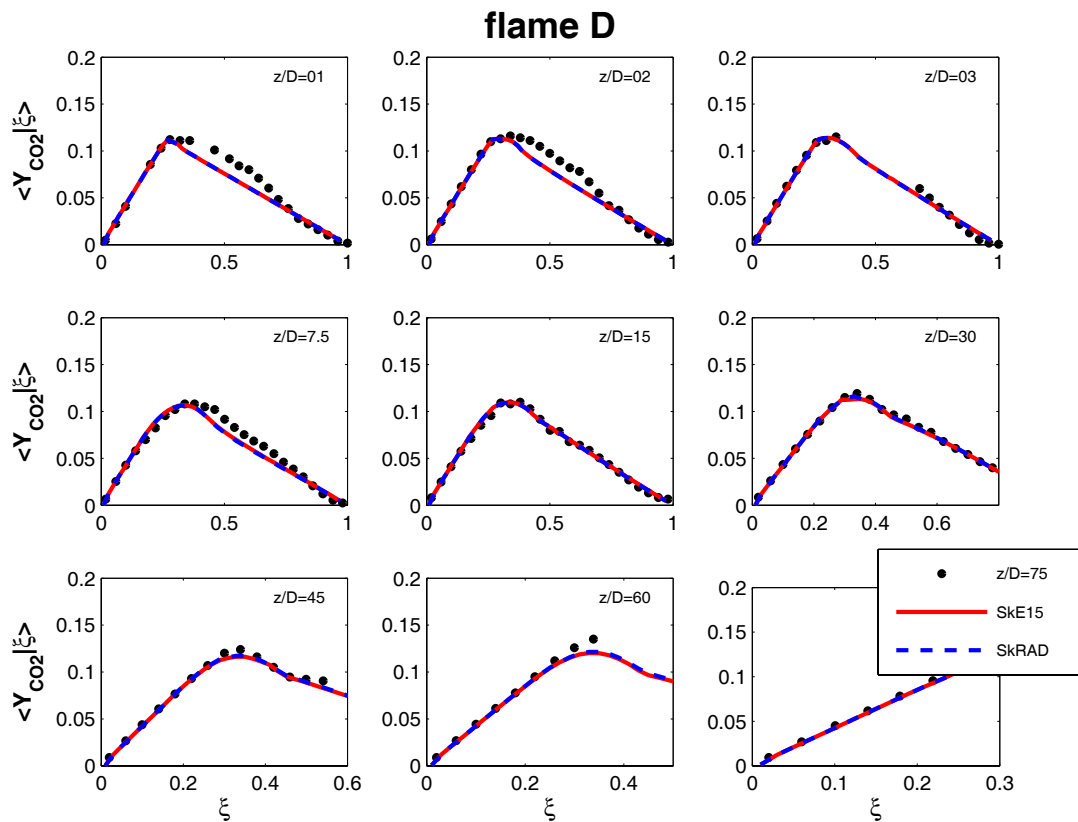


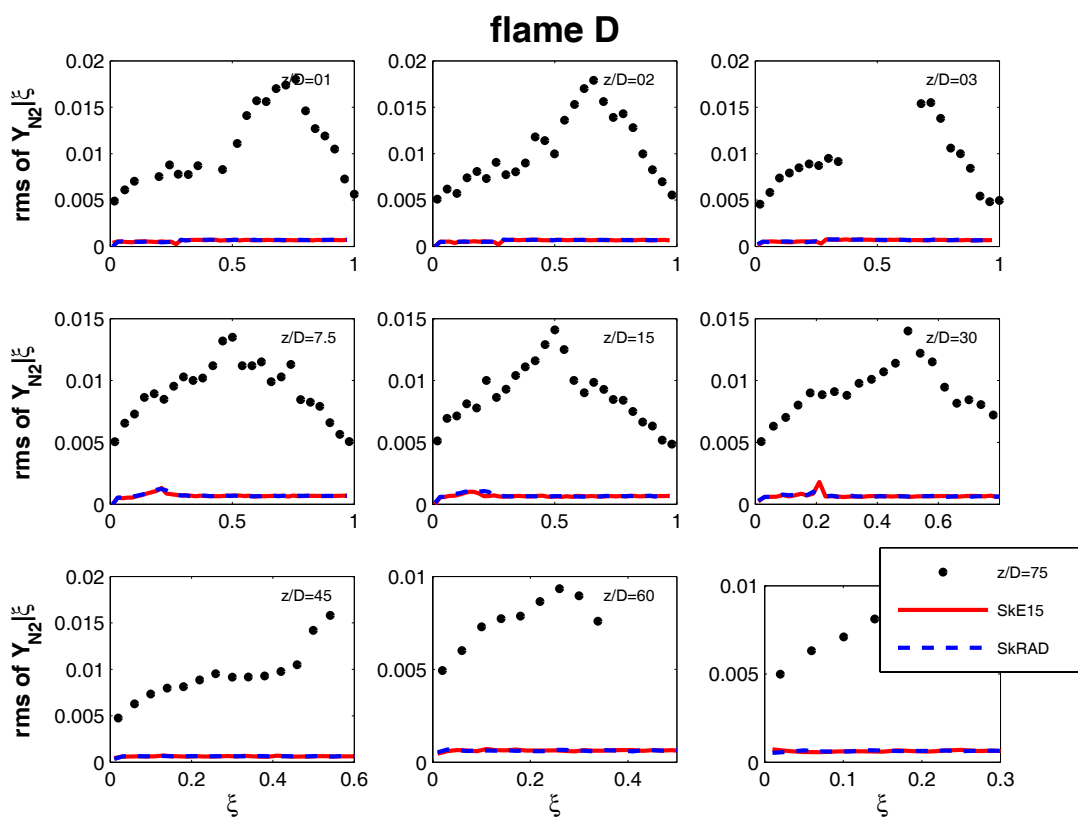
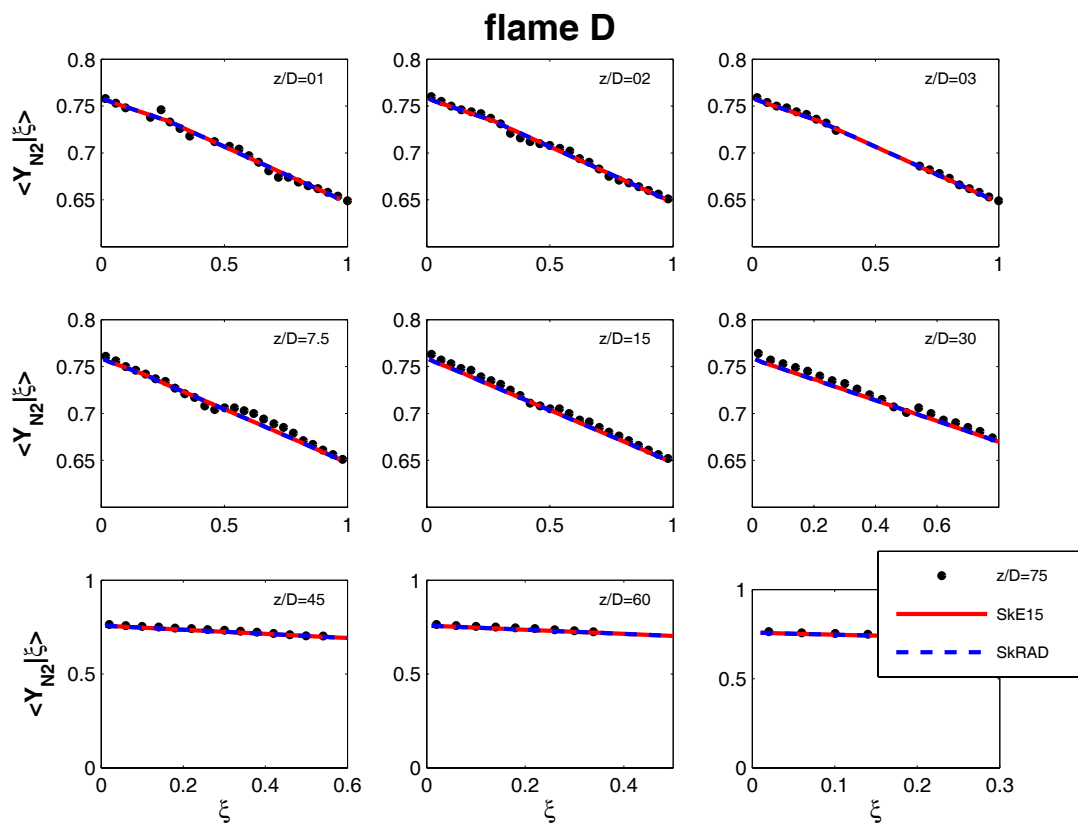


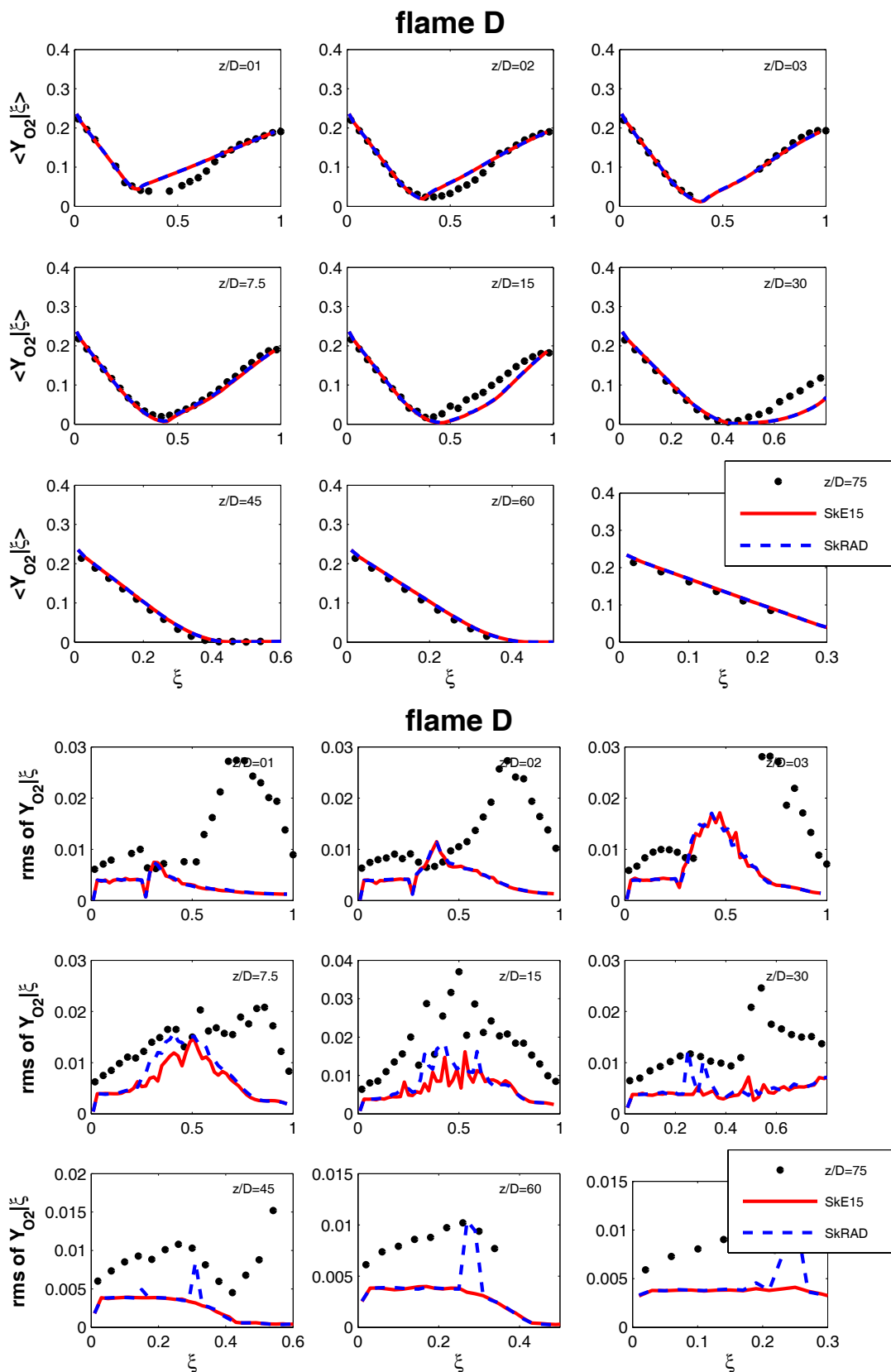
(5) SkE15 and SkRAD

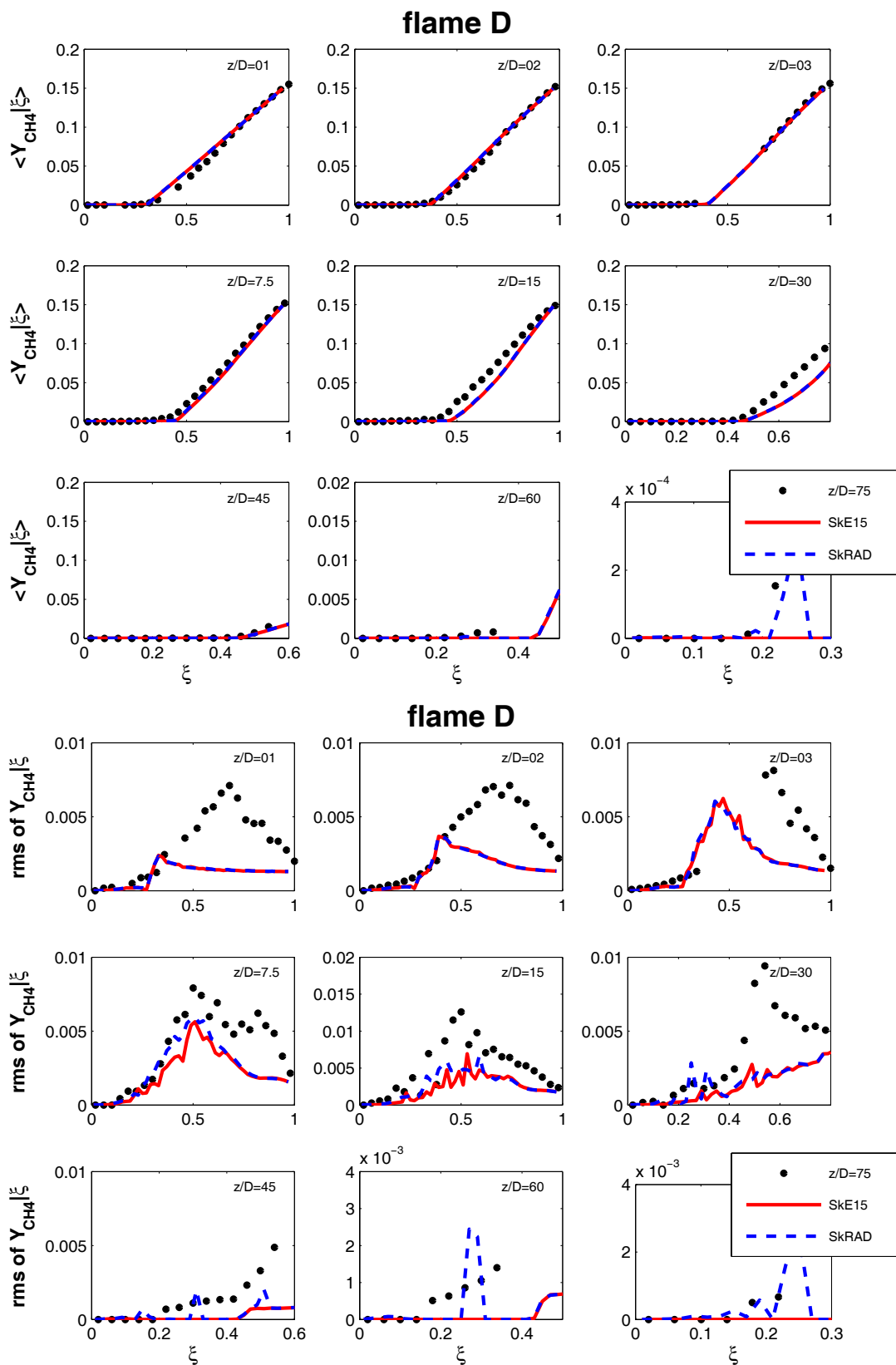


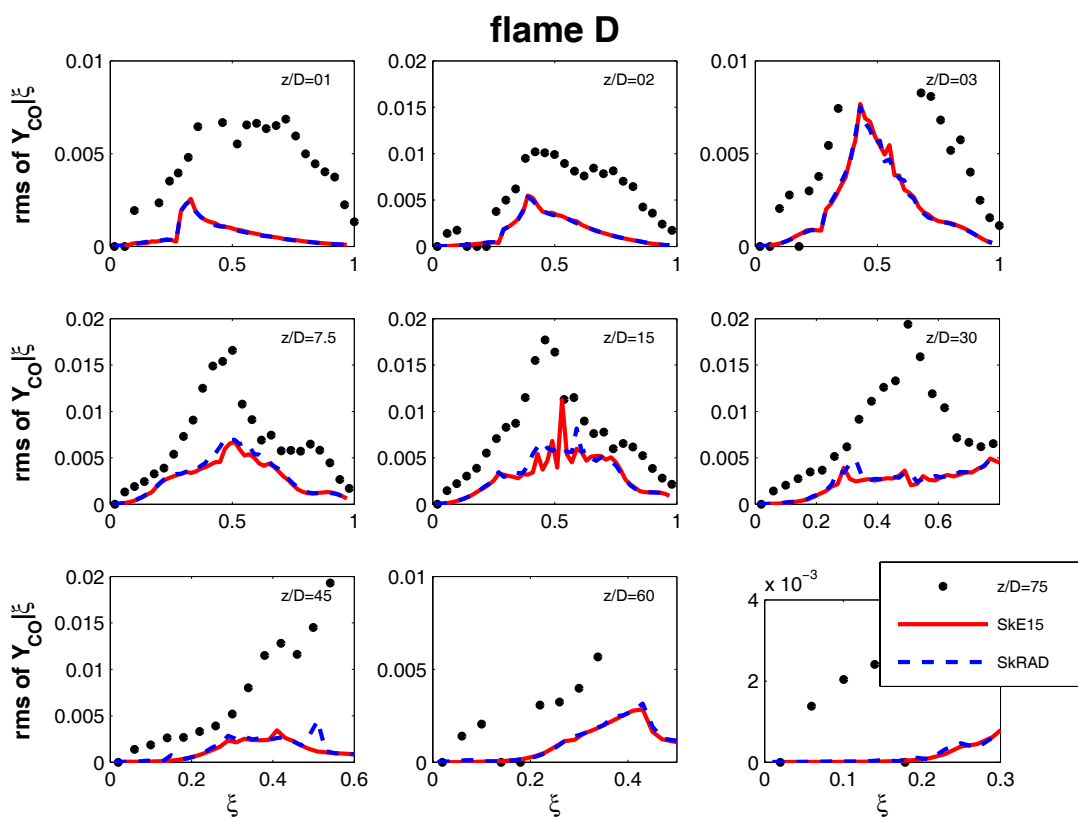
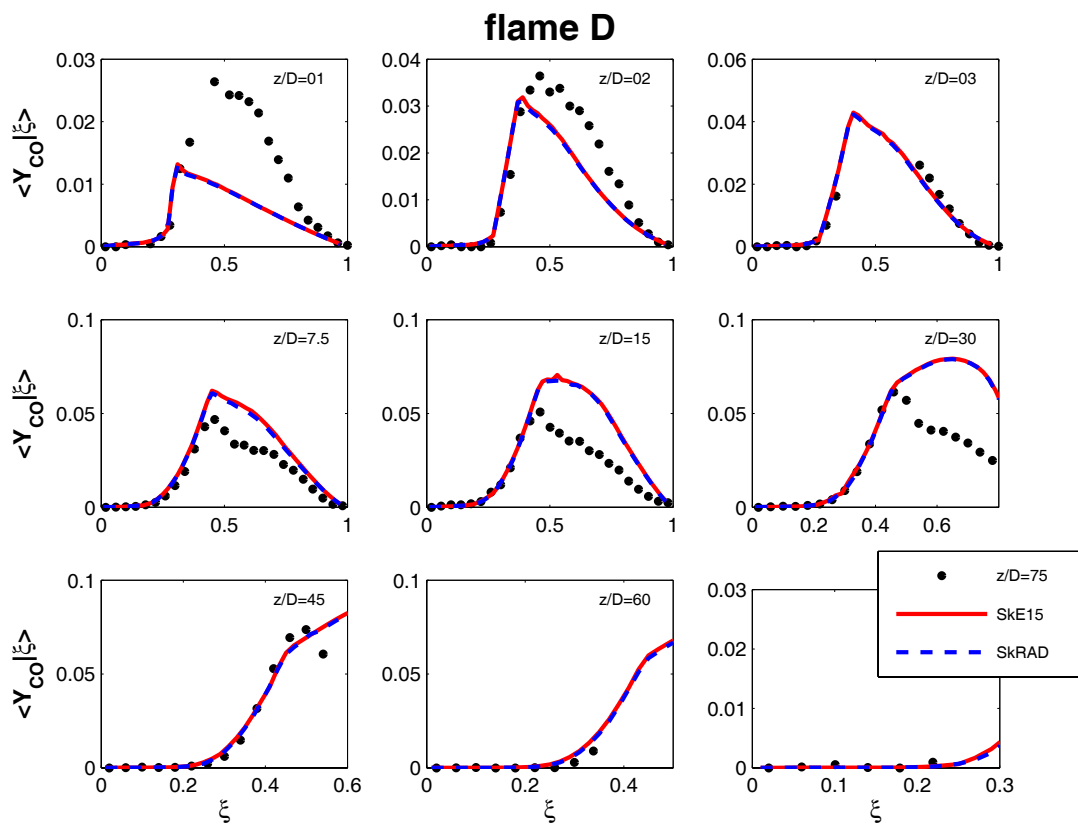


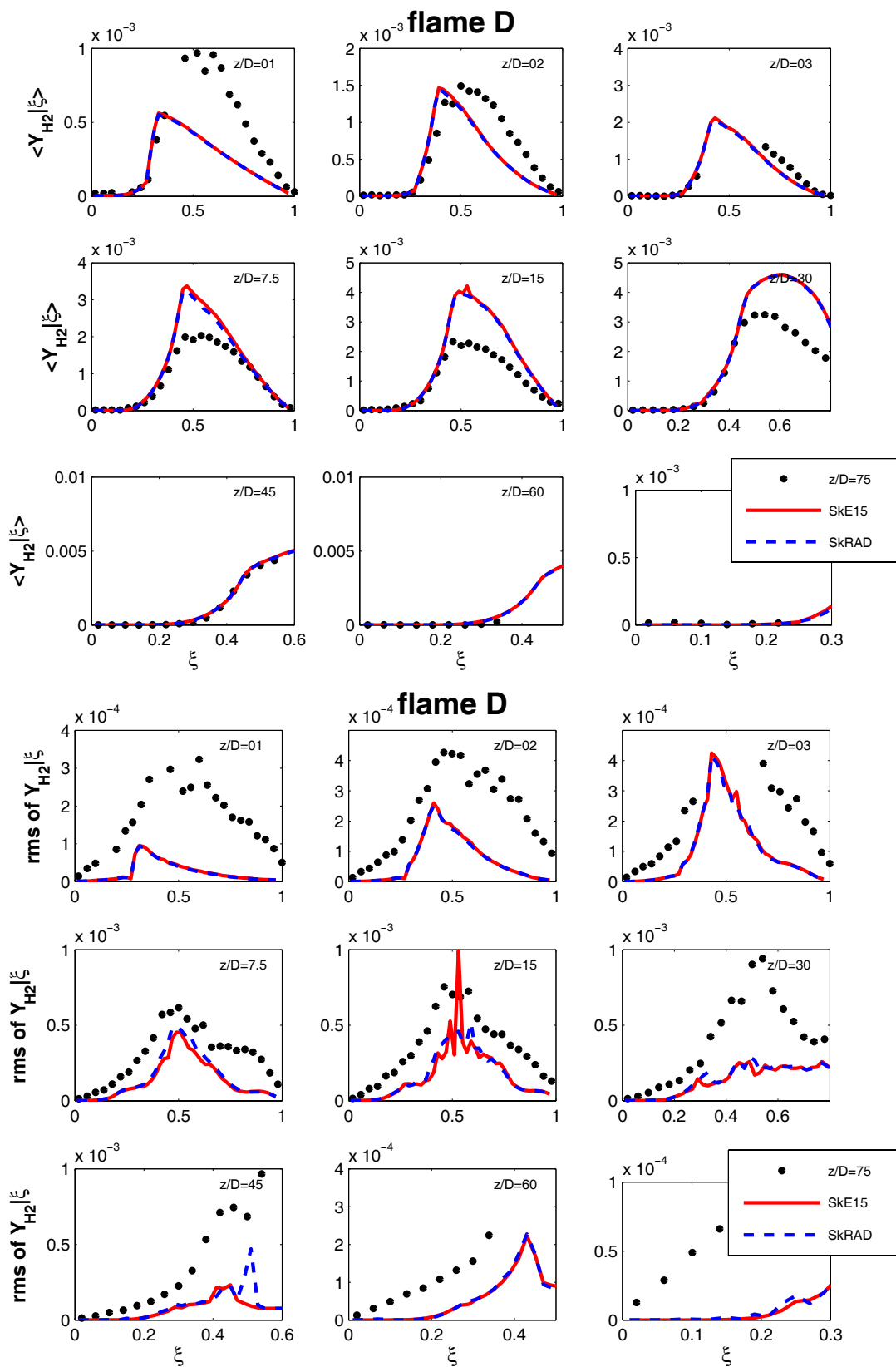


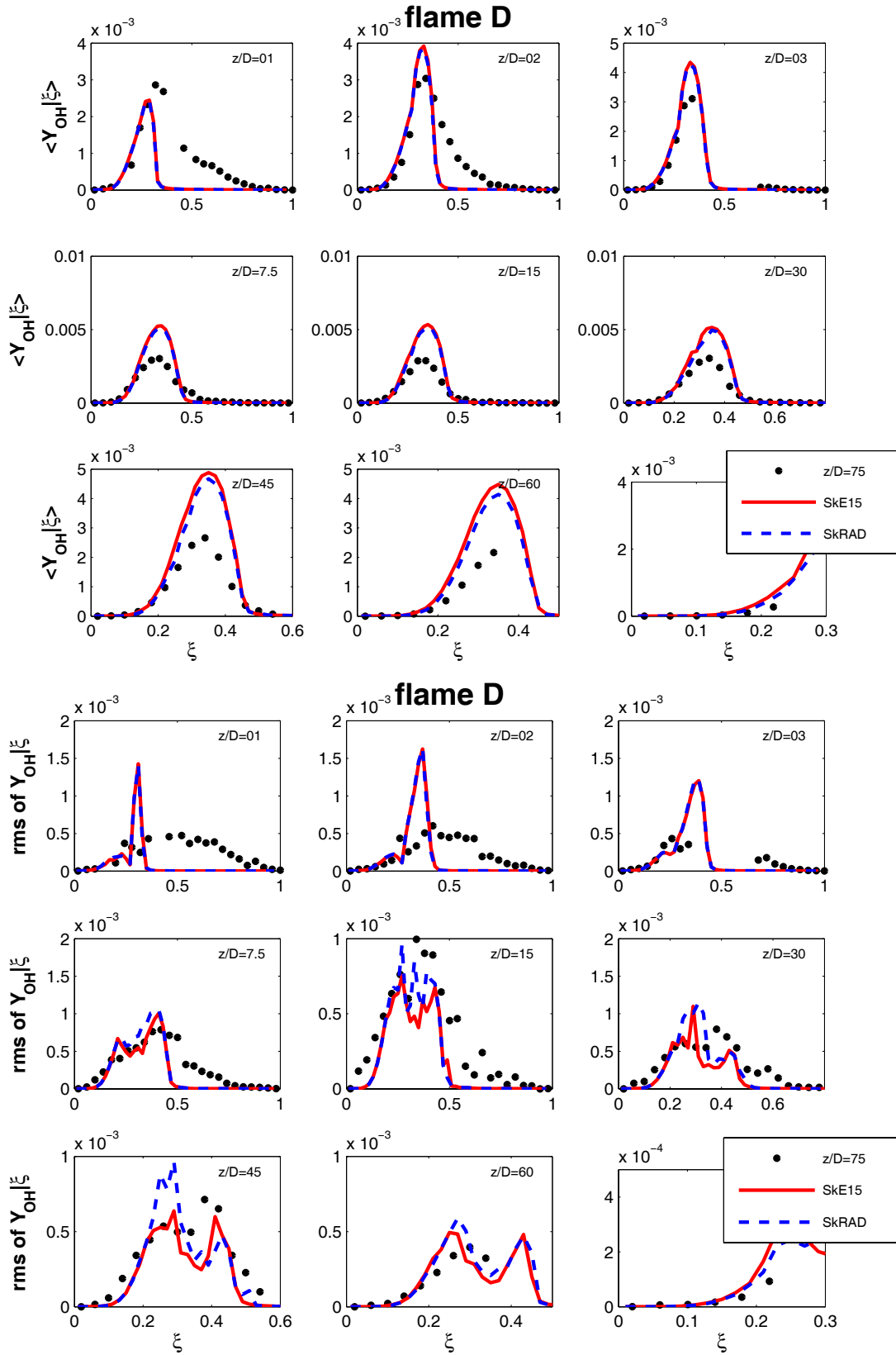




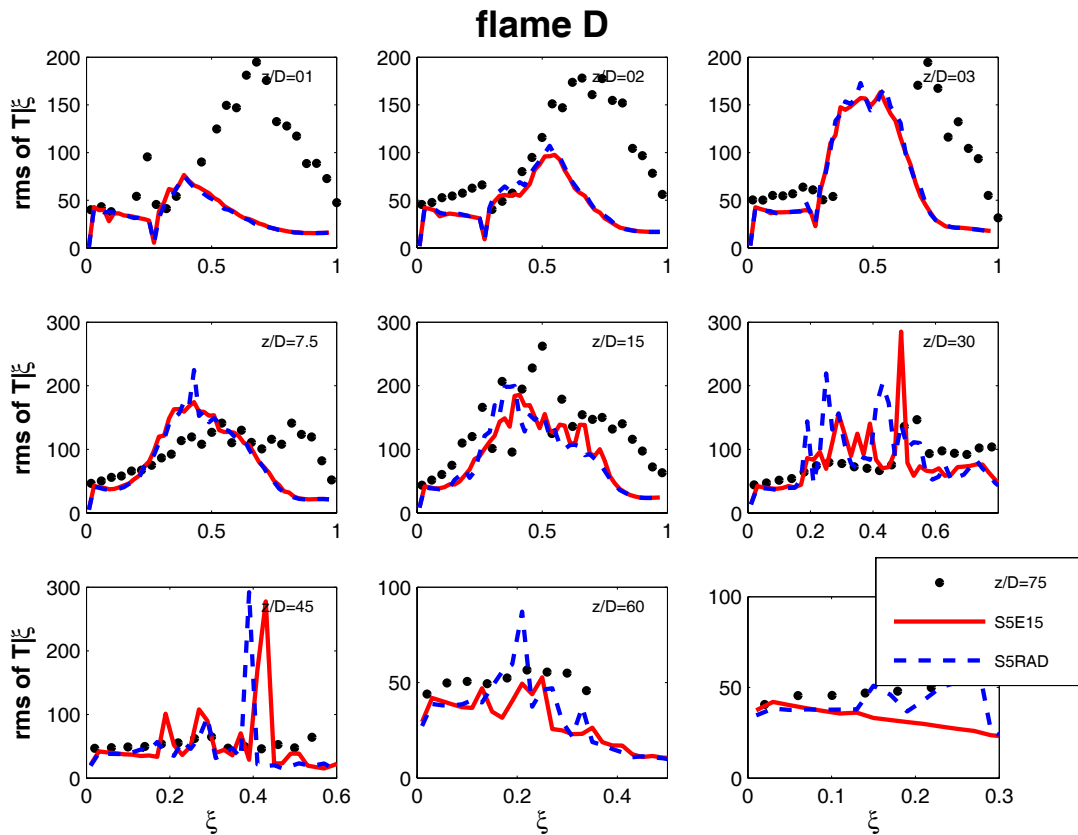
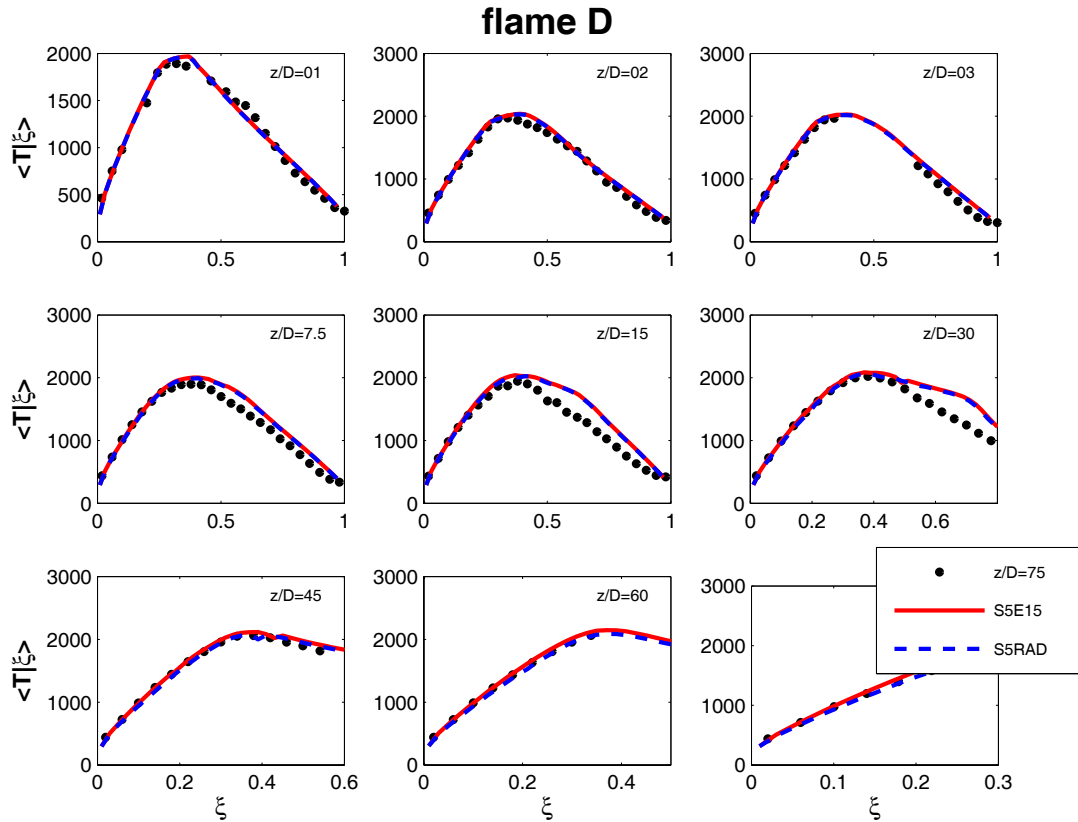


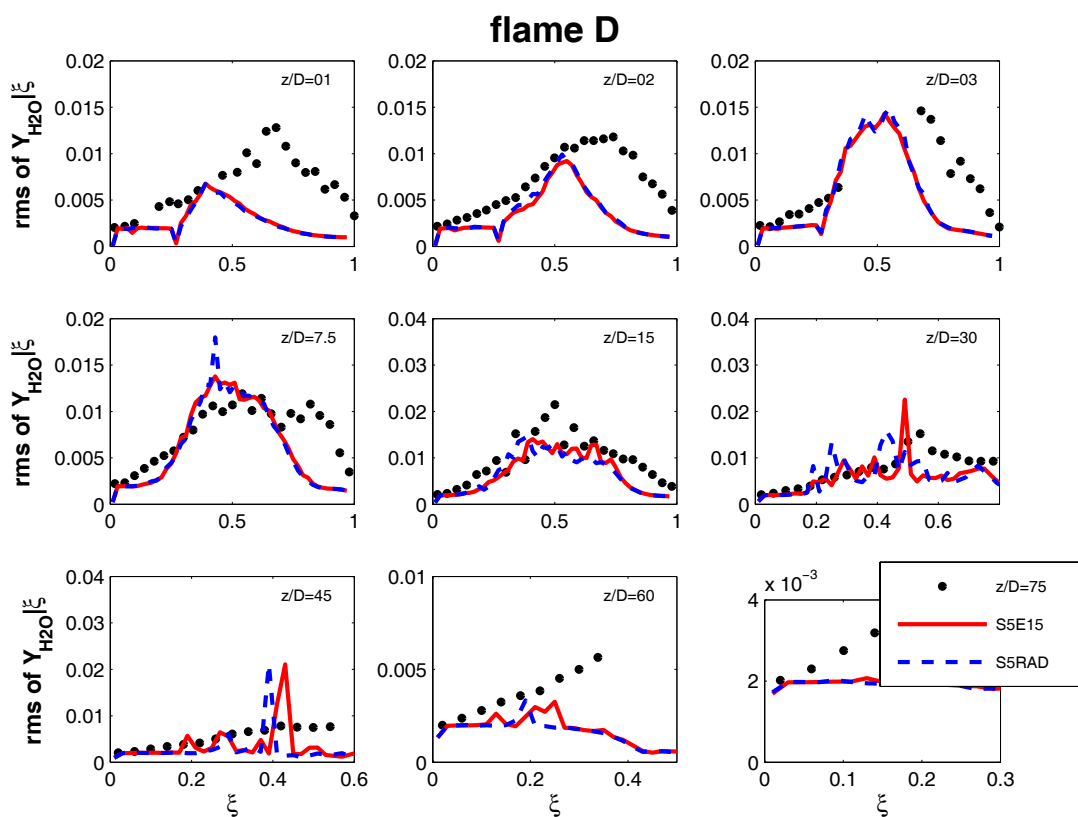
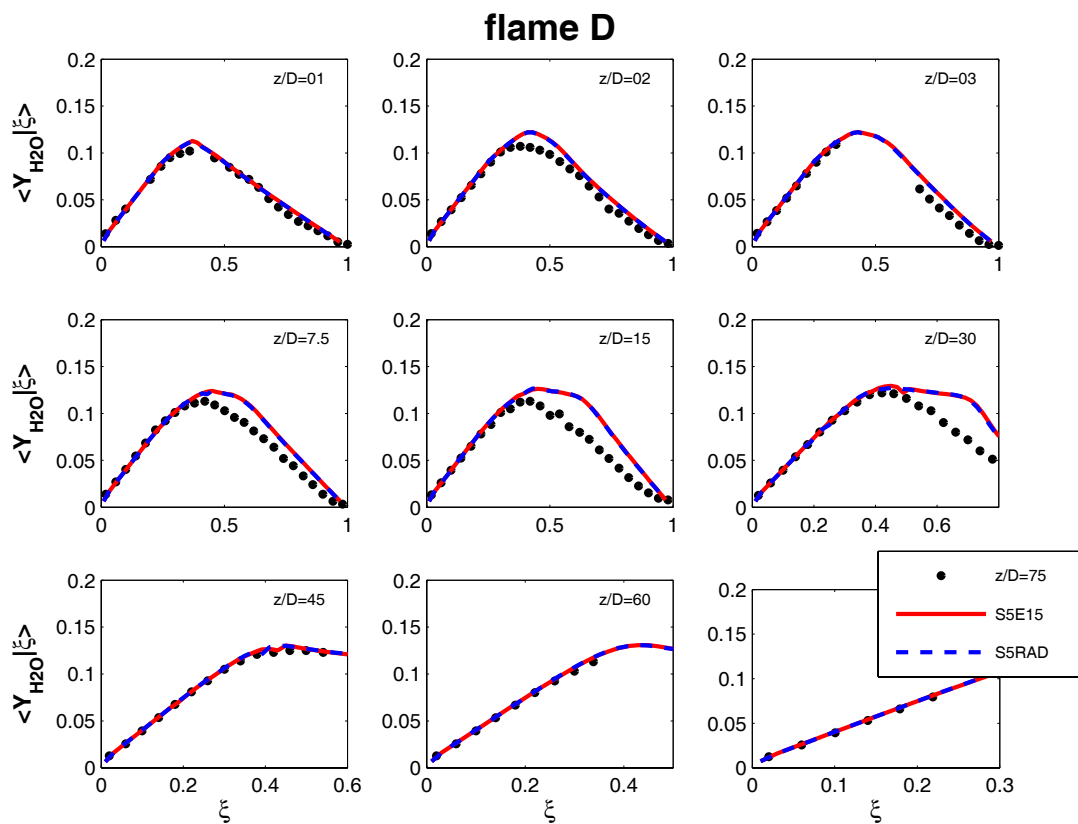


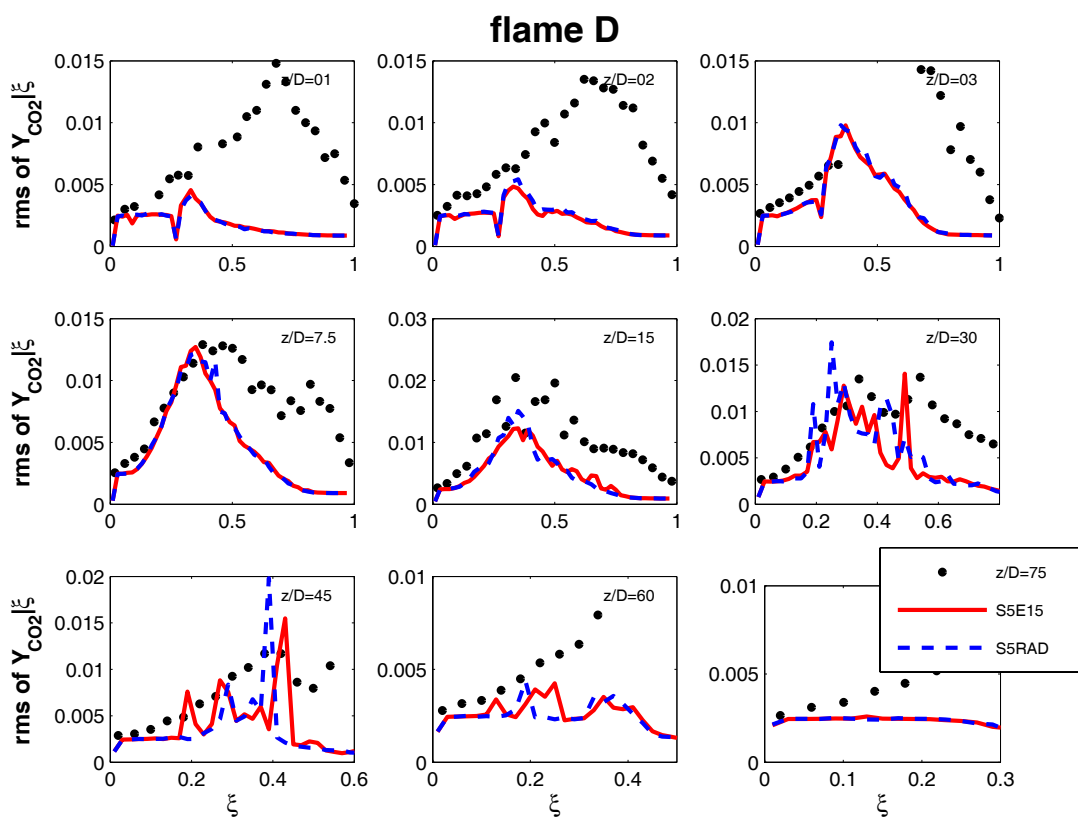
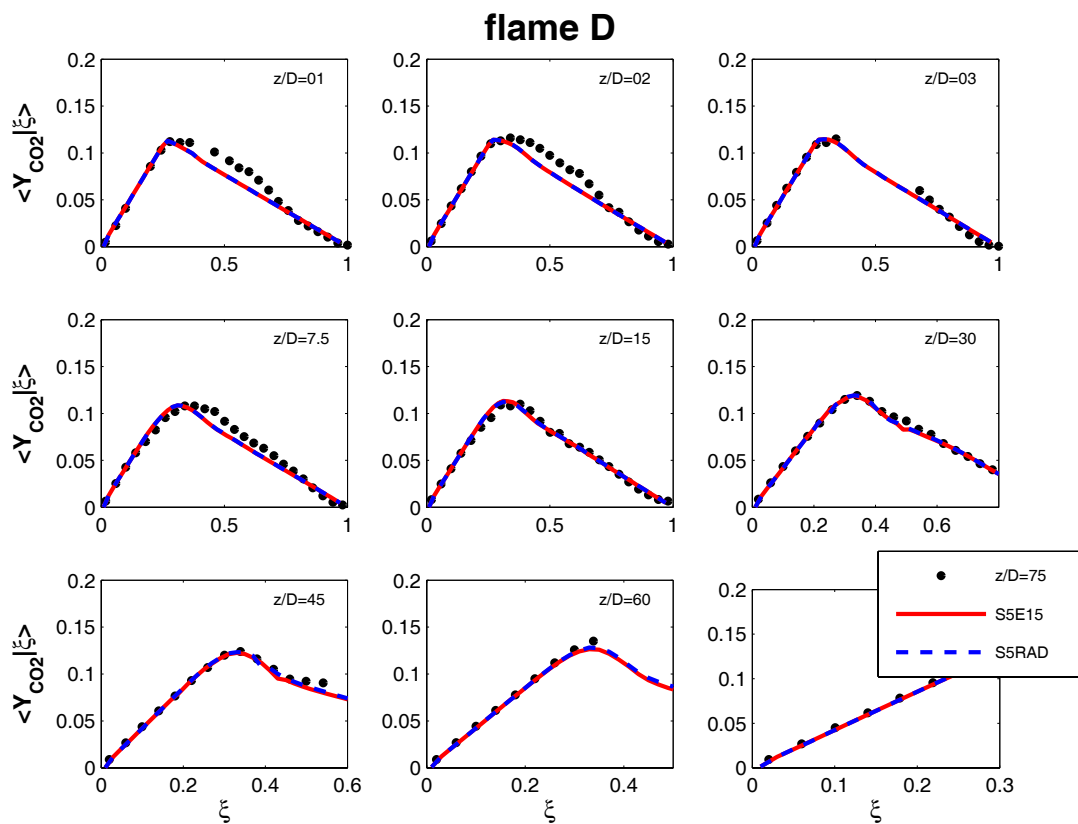


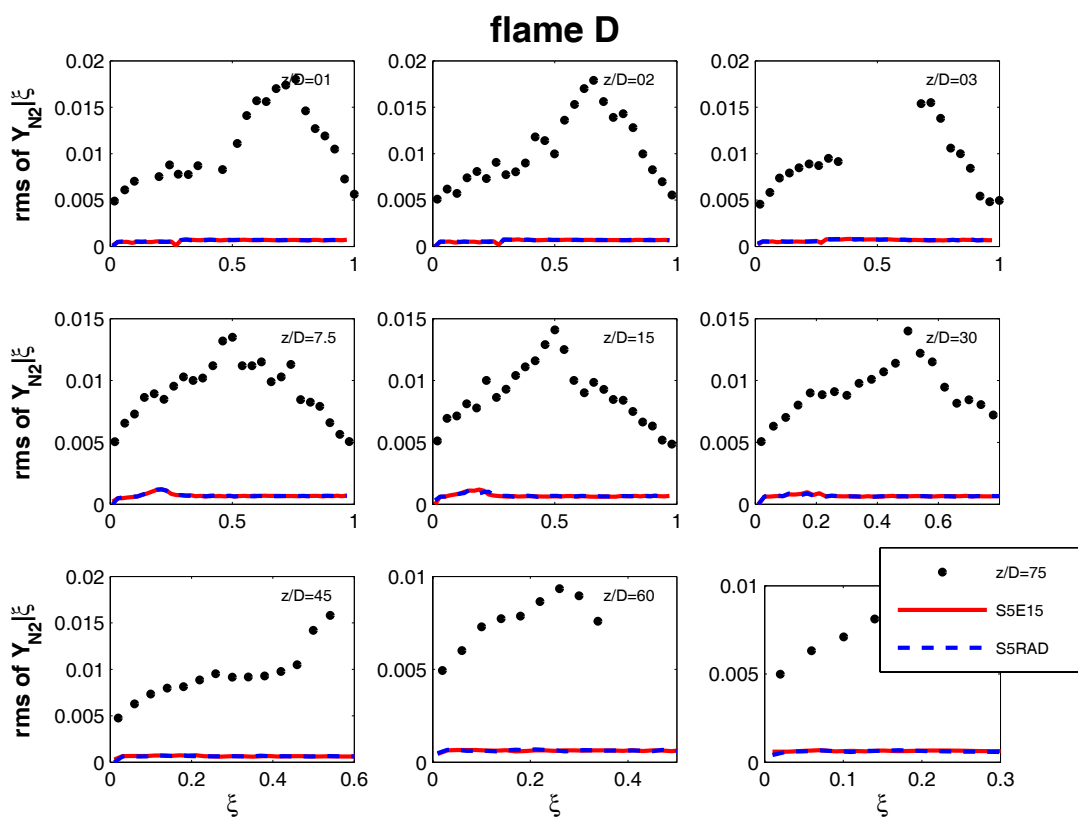
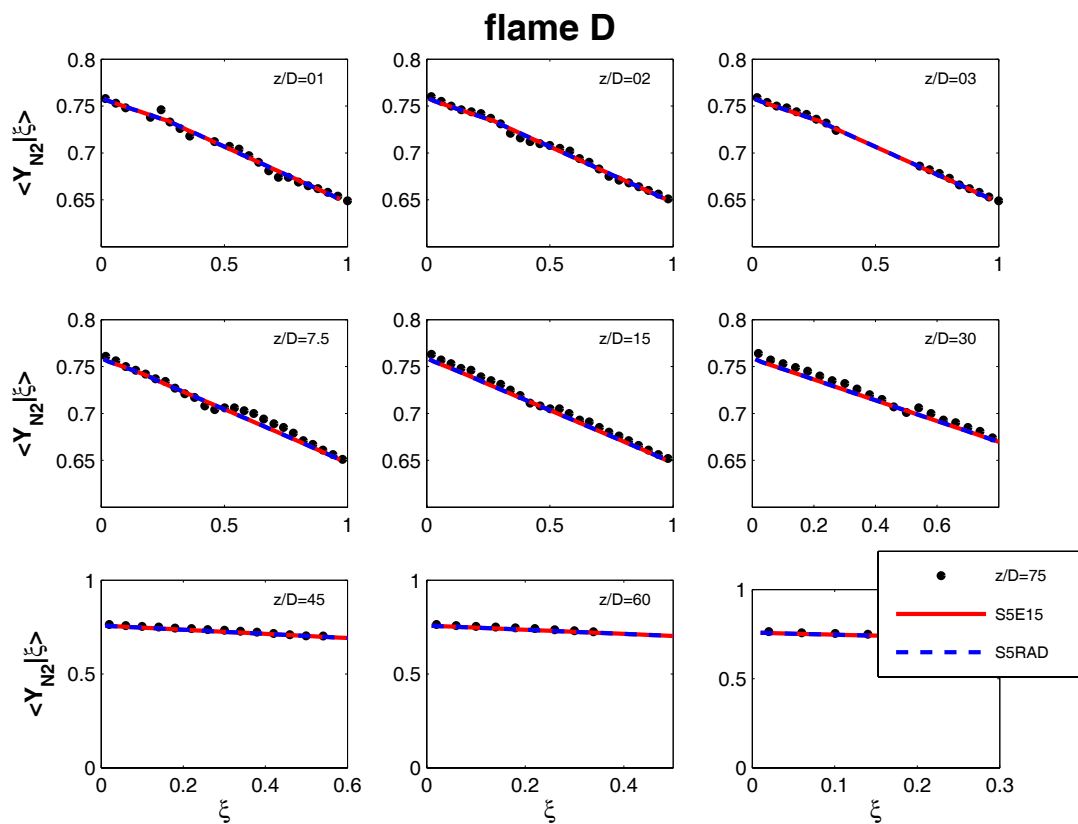


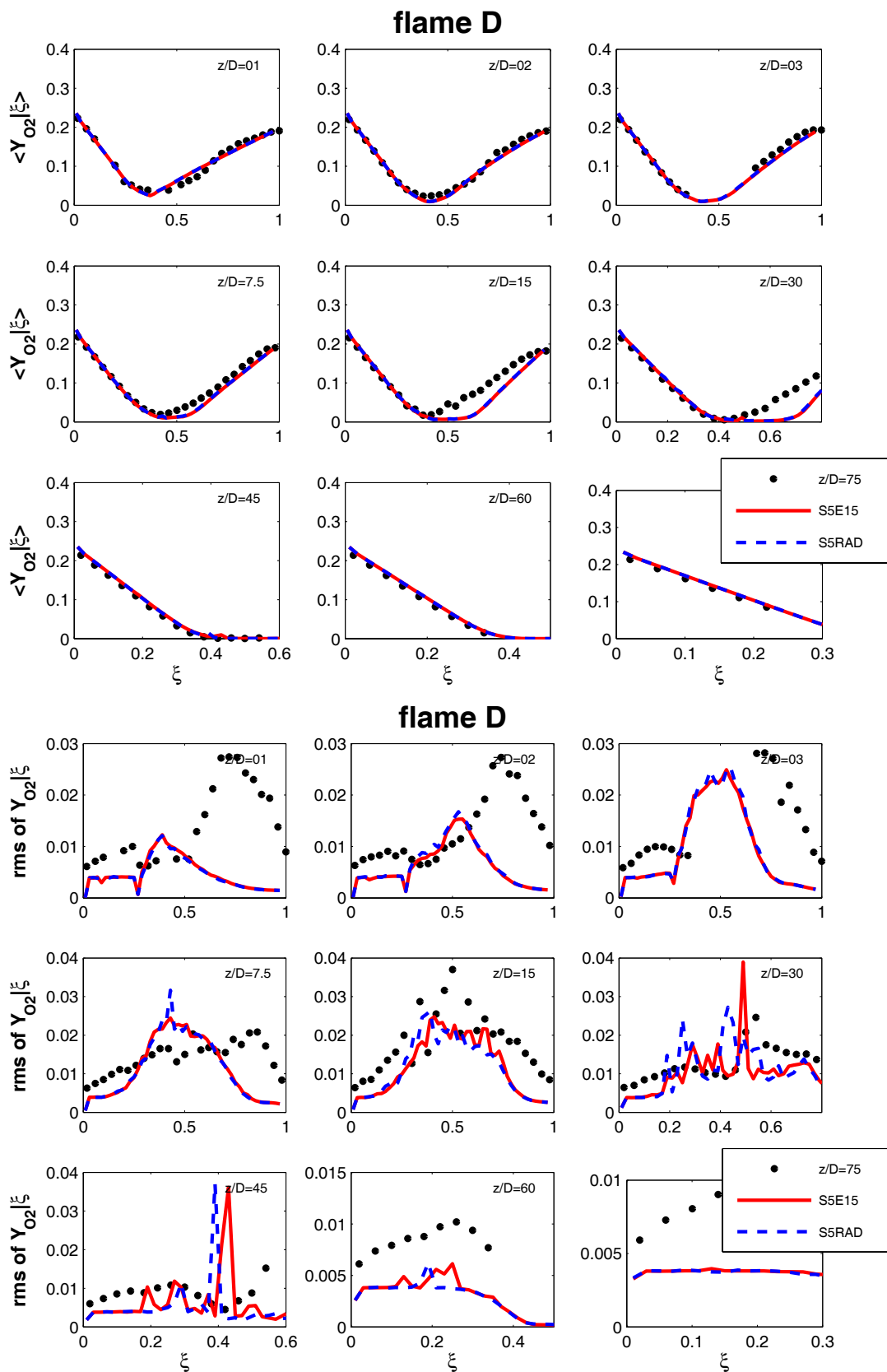
(6) S5E15 and S5RAD

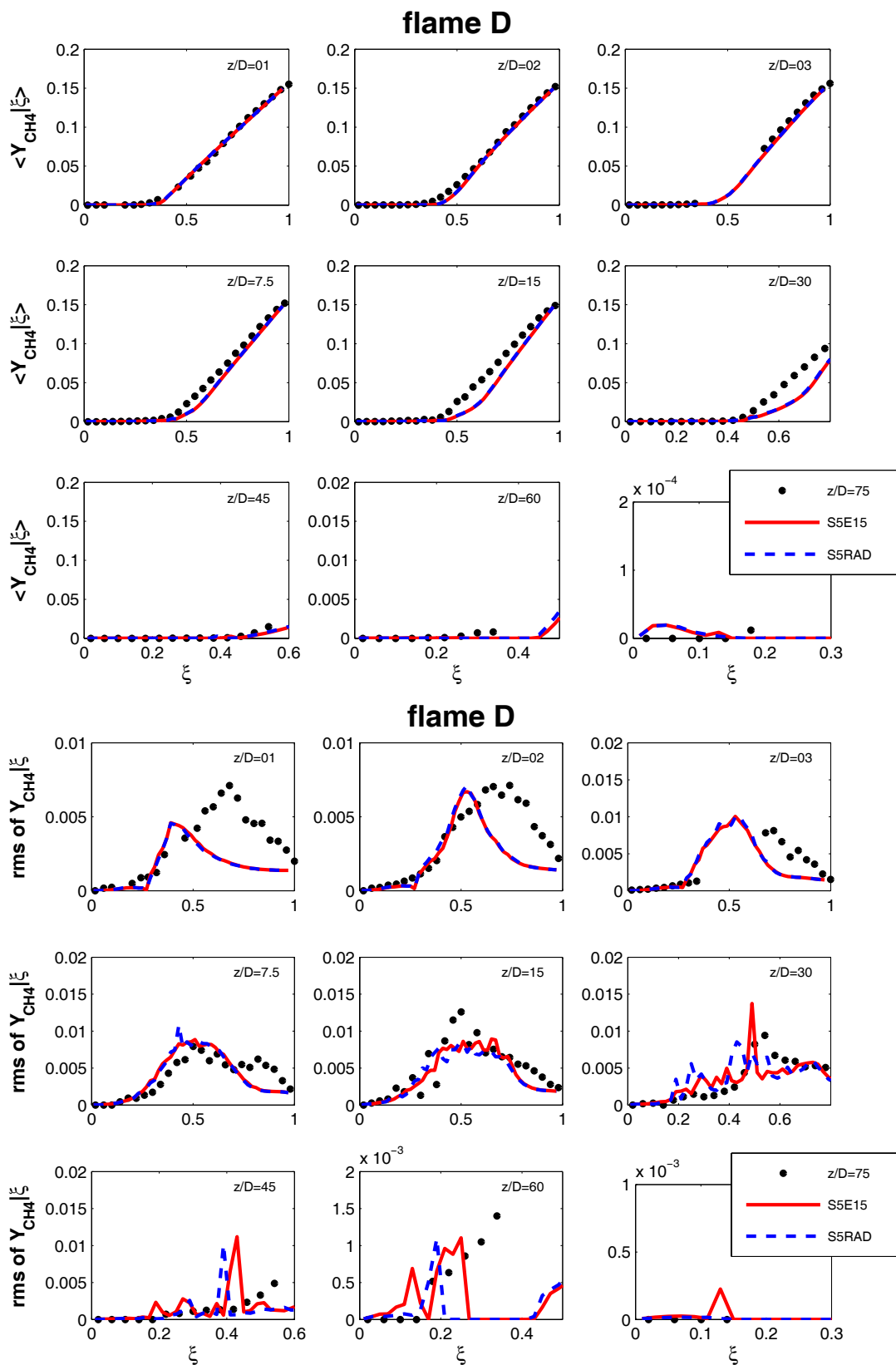


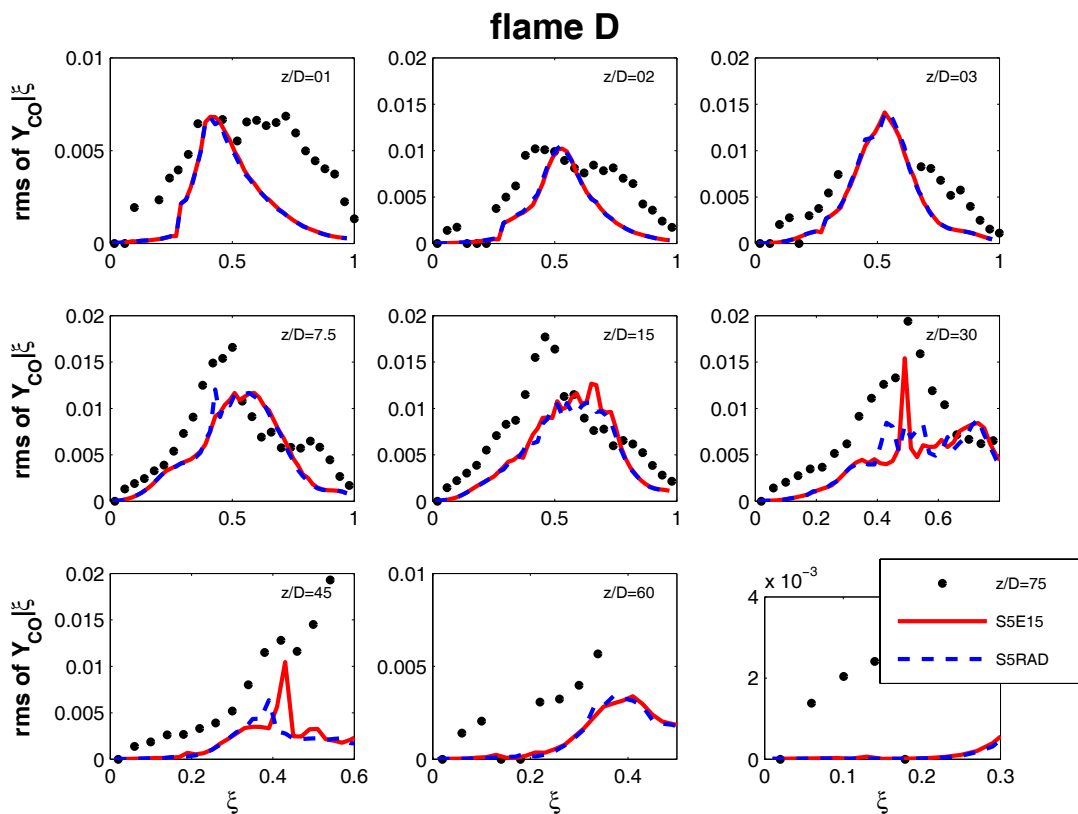
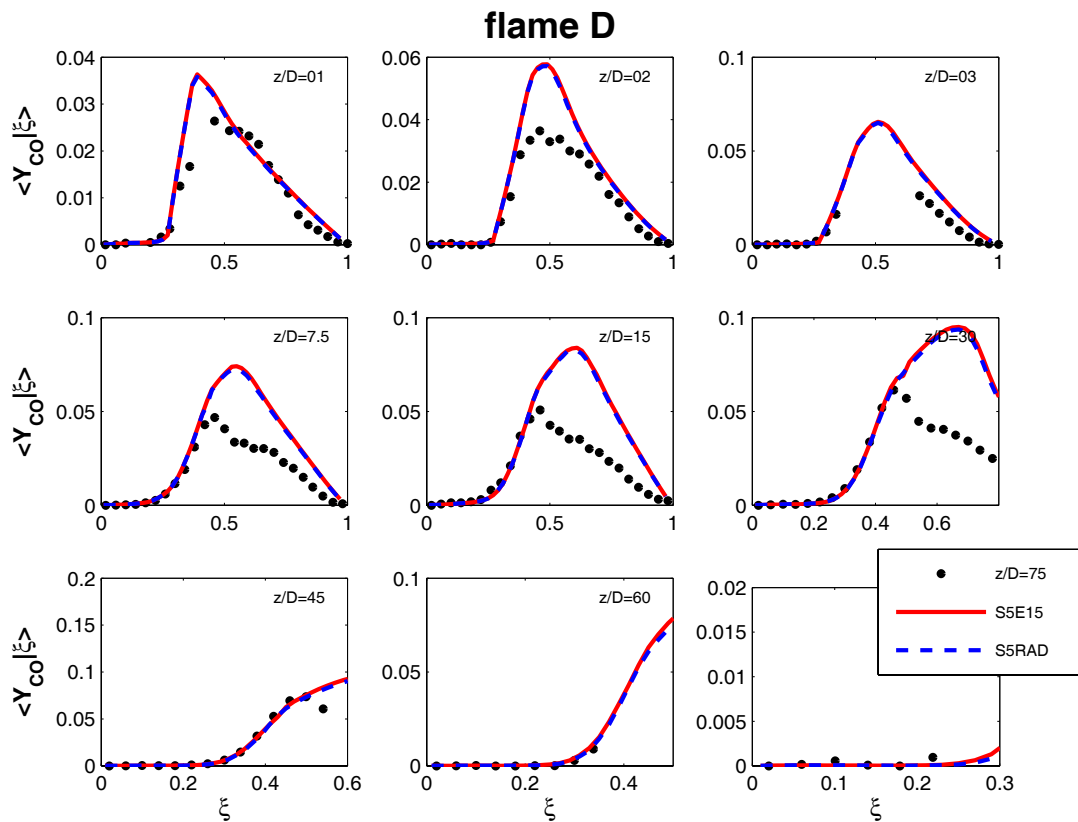


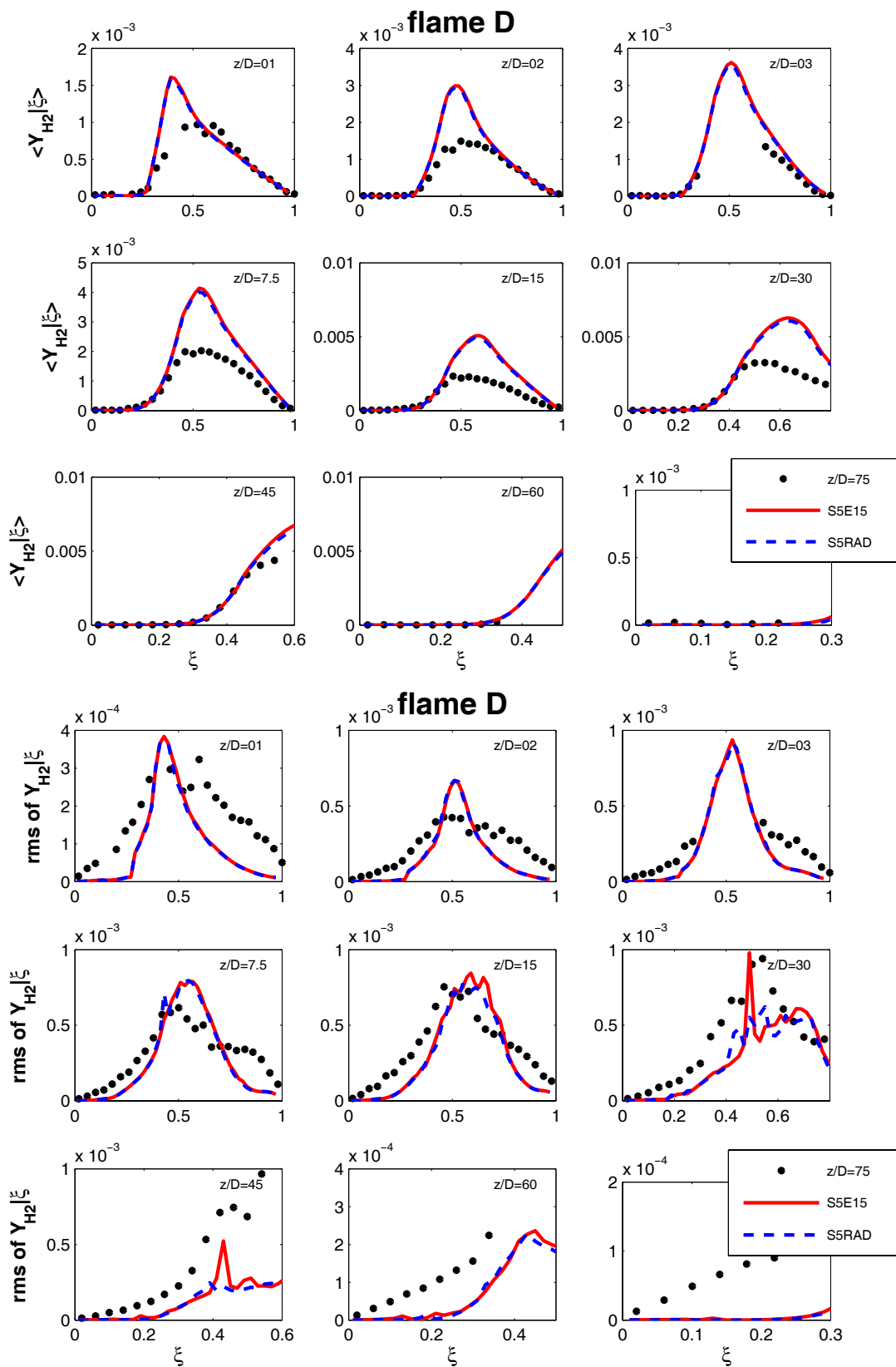


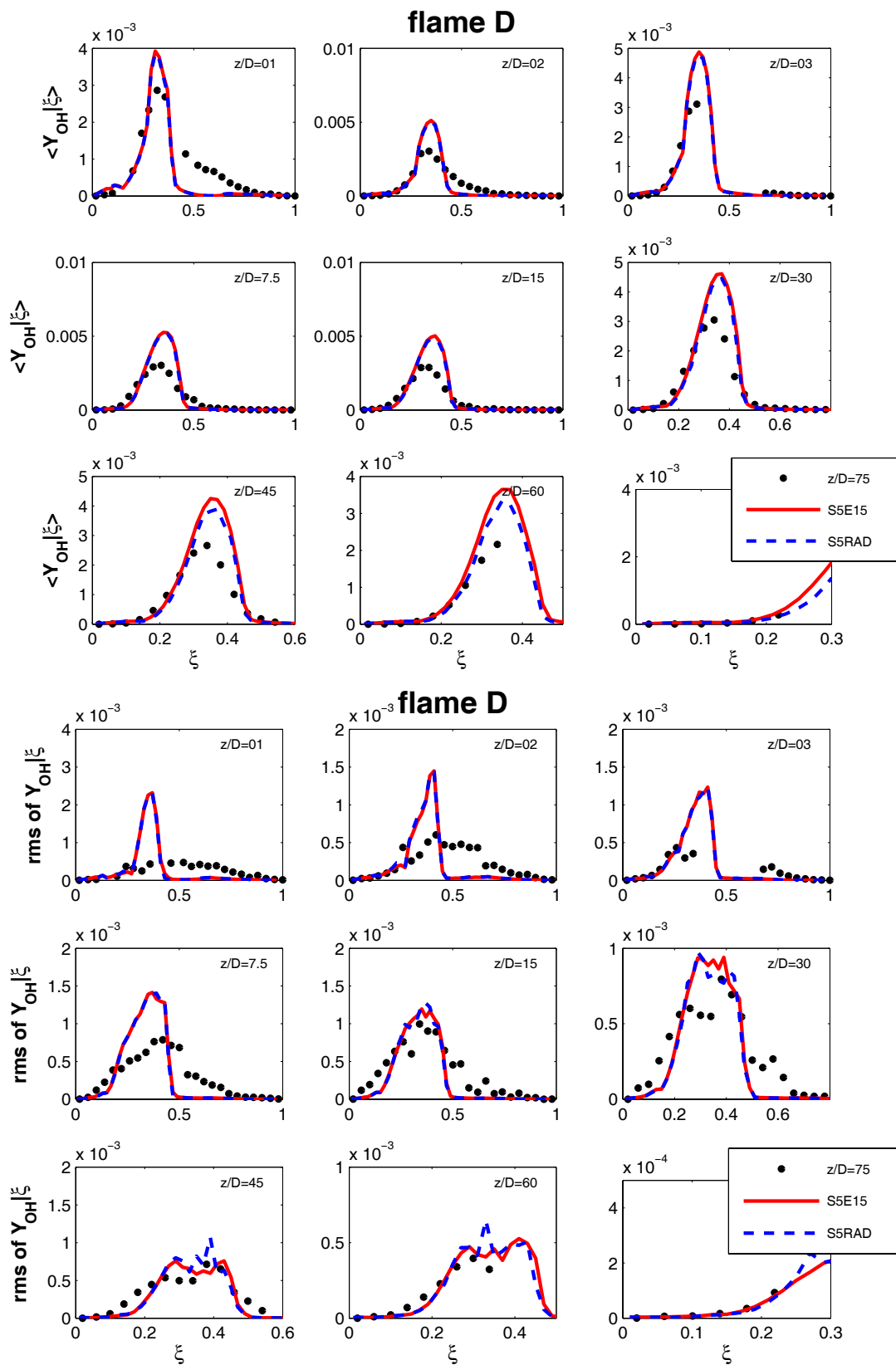


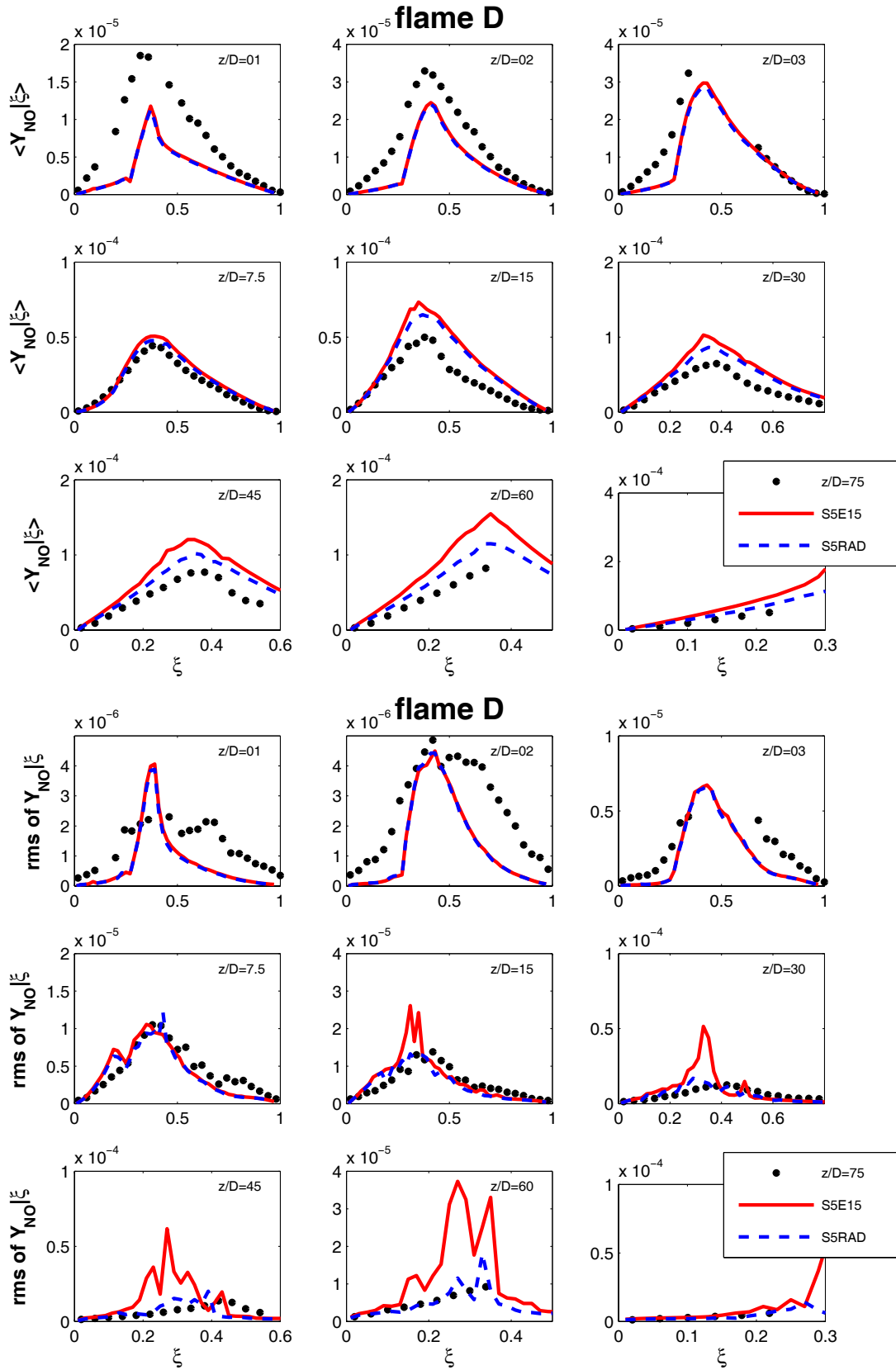




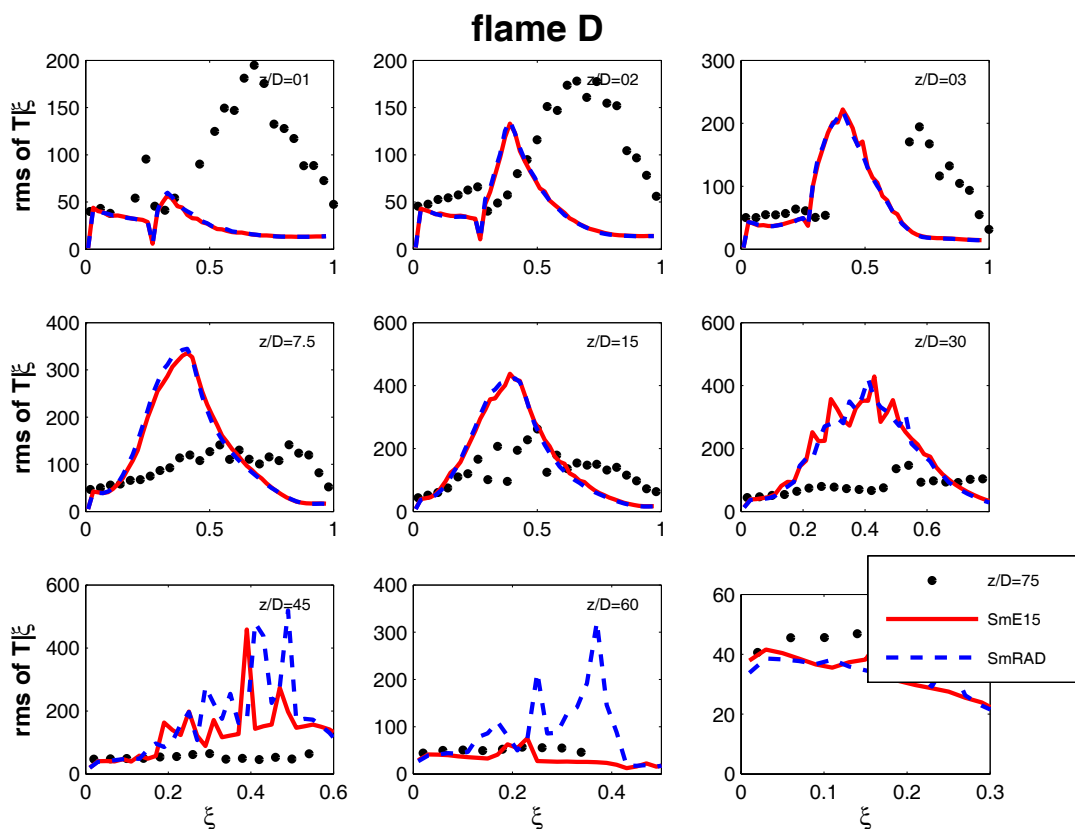
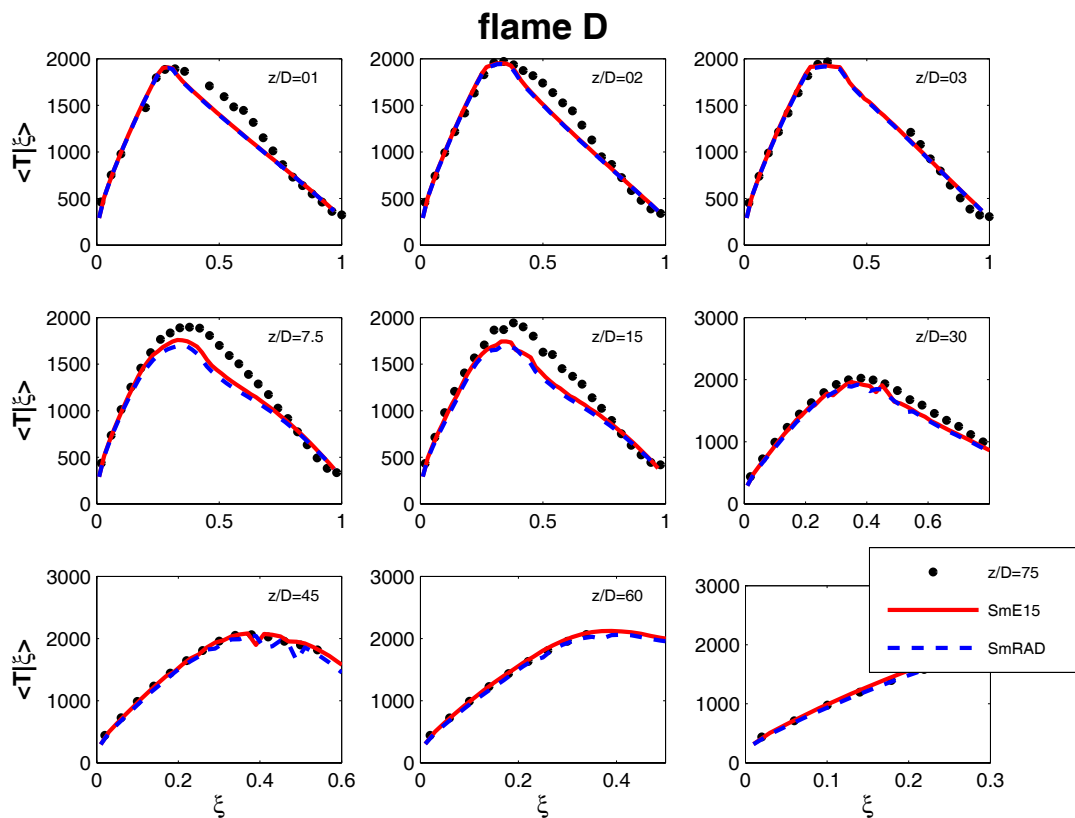


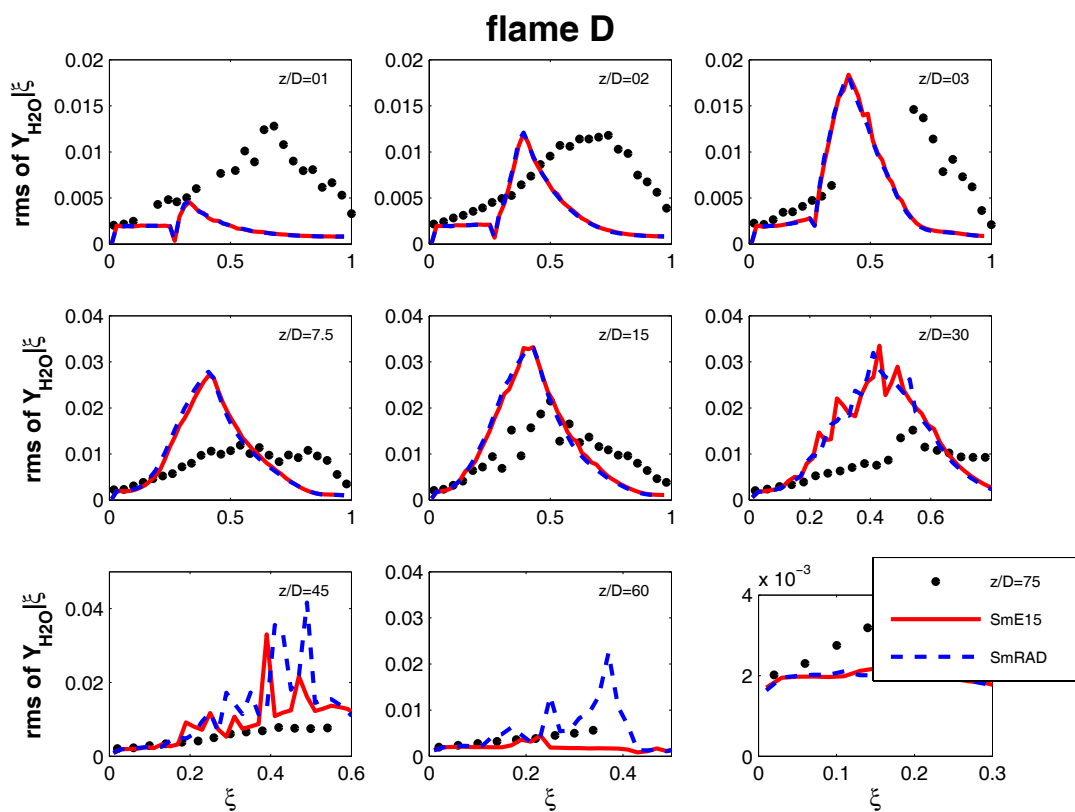
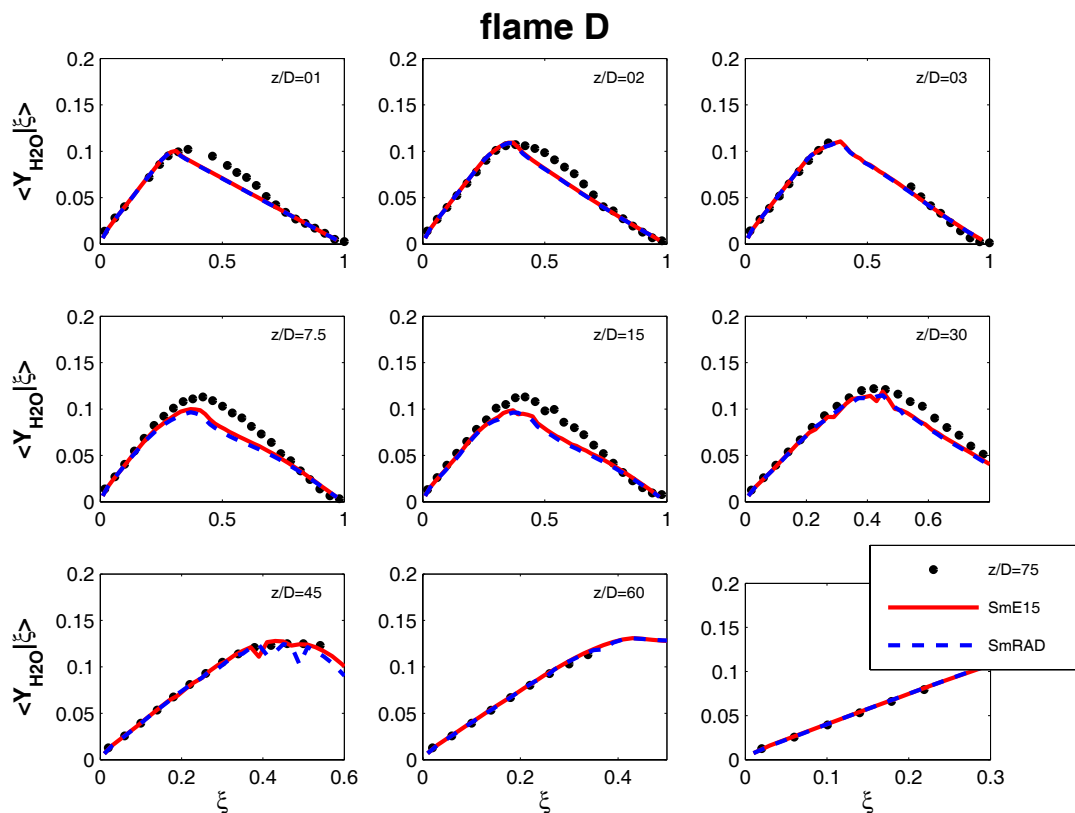


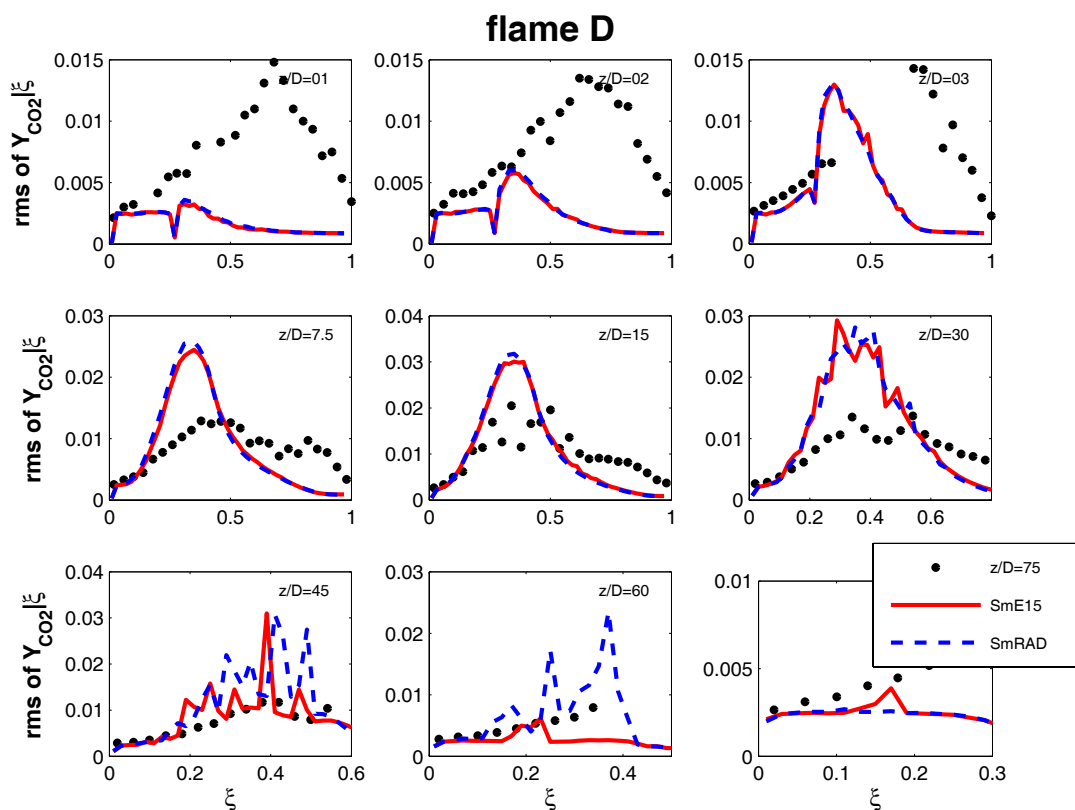
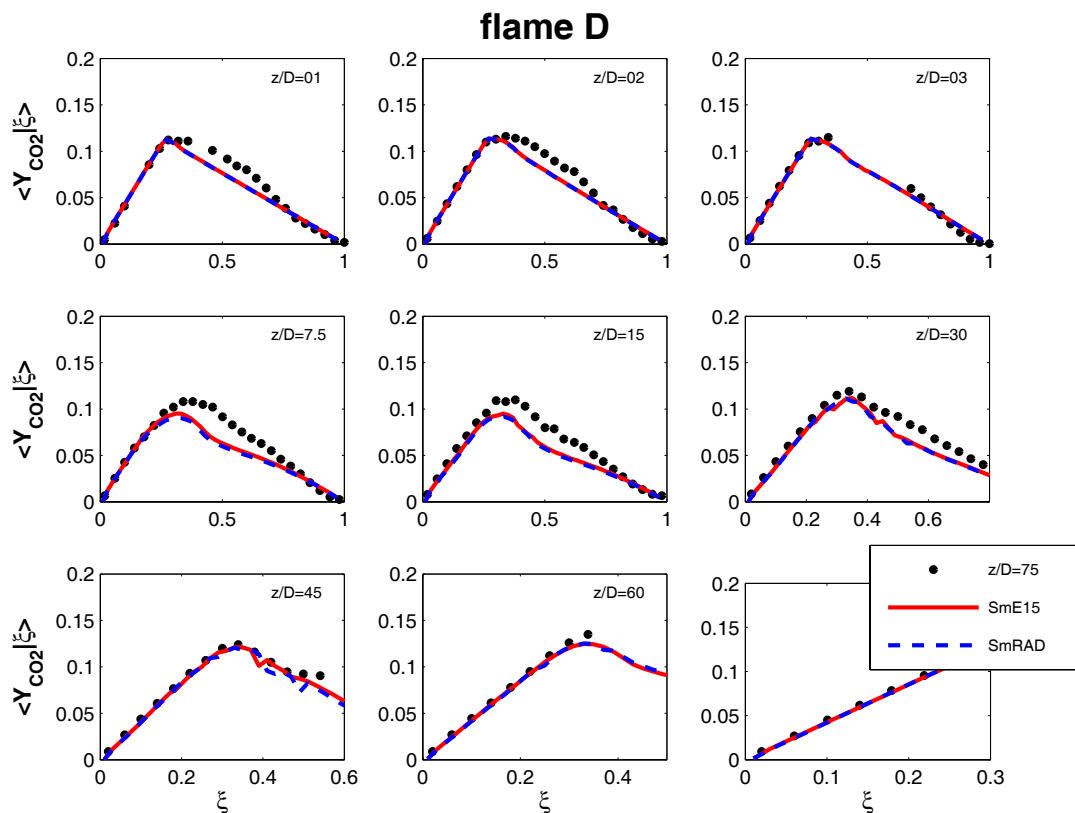


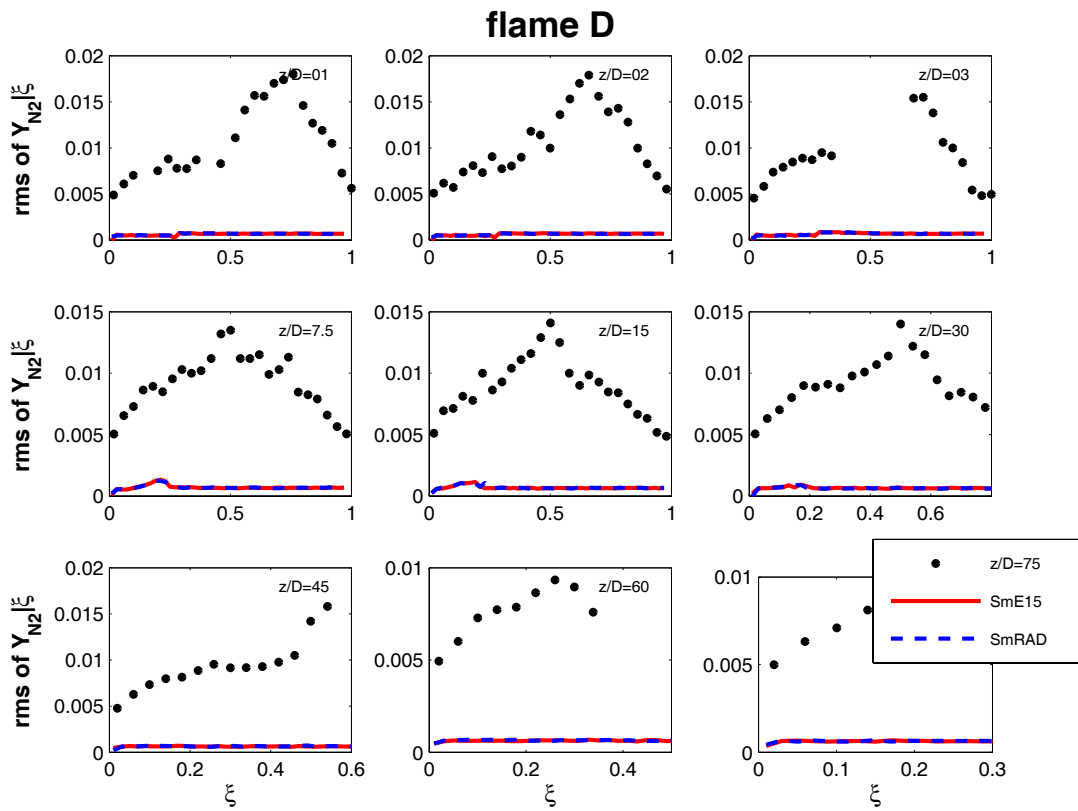
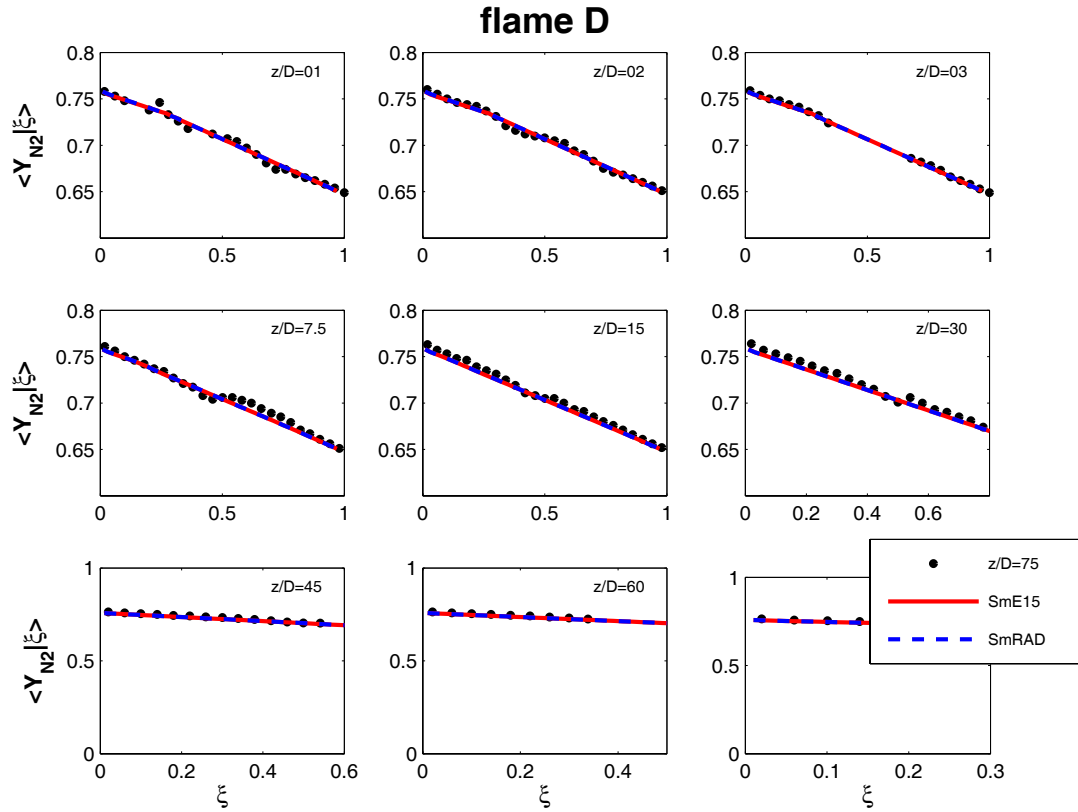


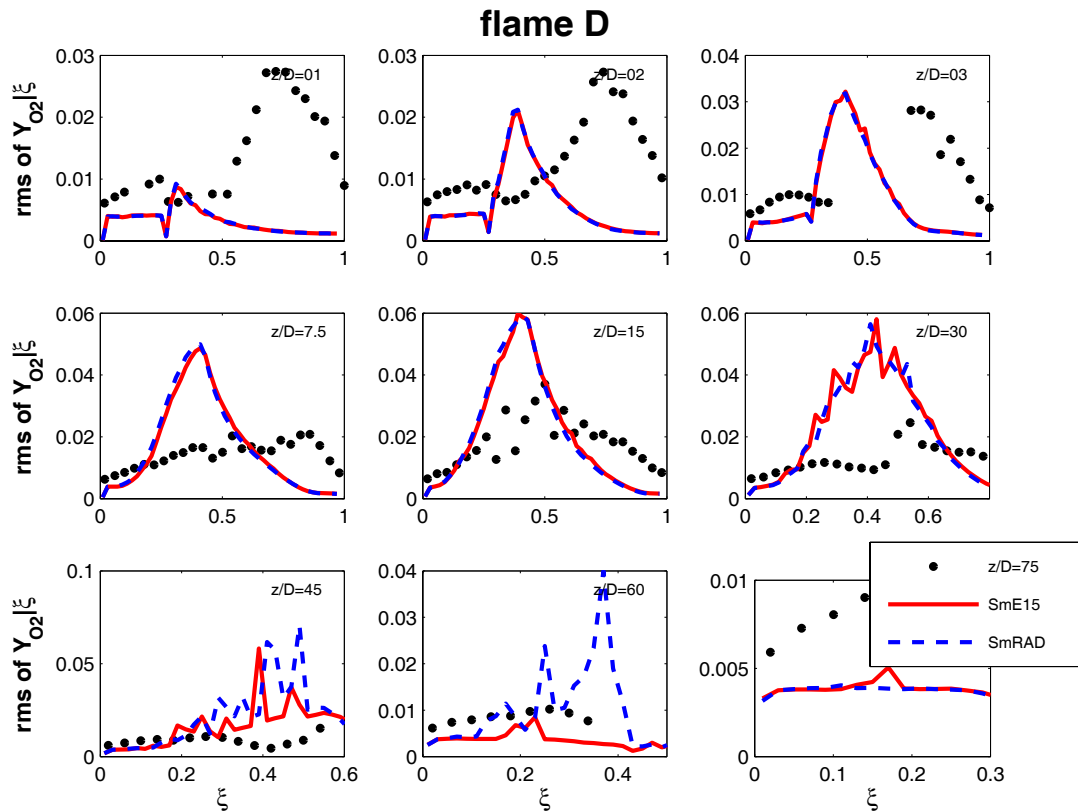
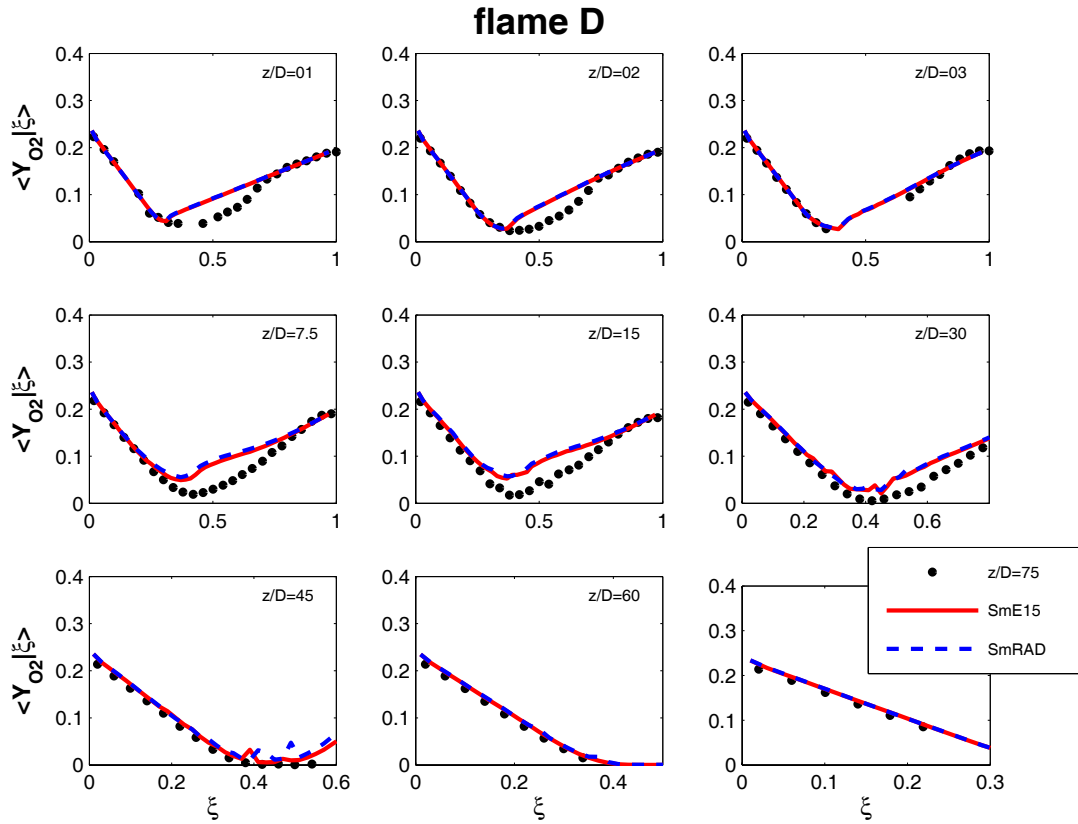
(7) SmE15 and SmRAD

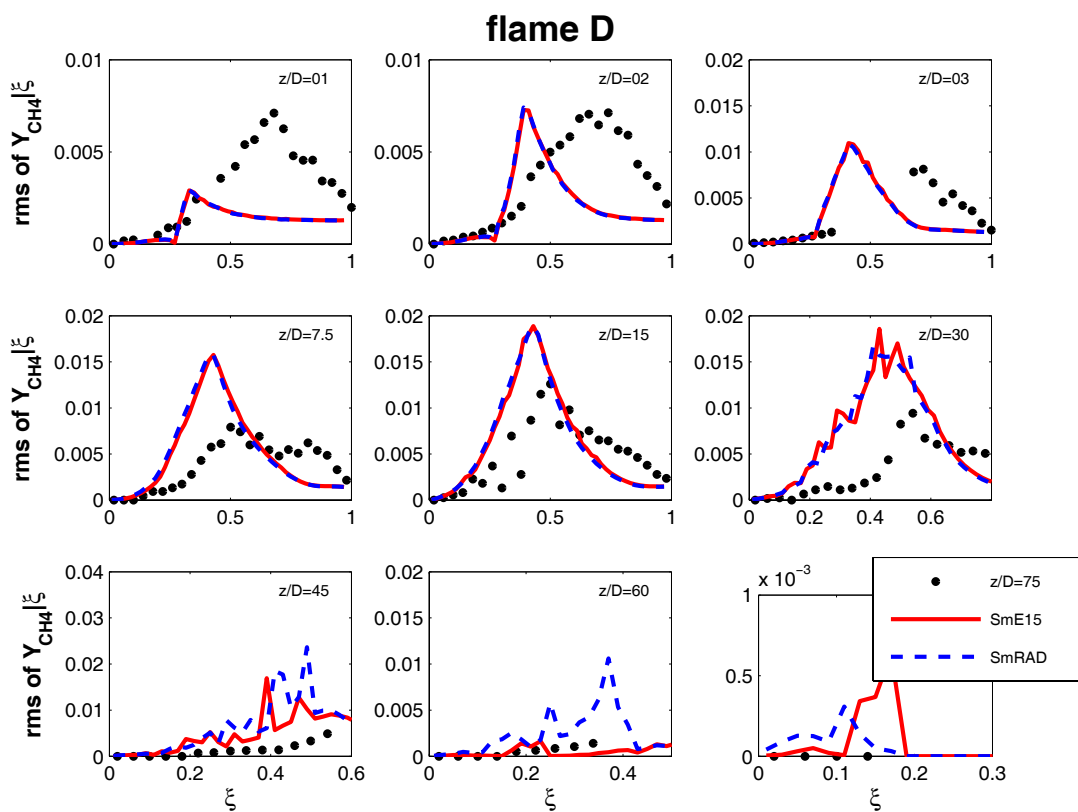
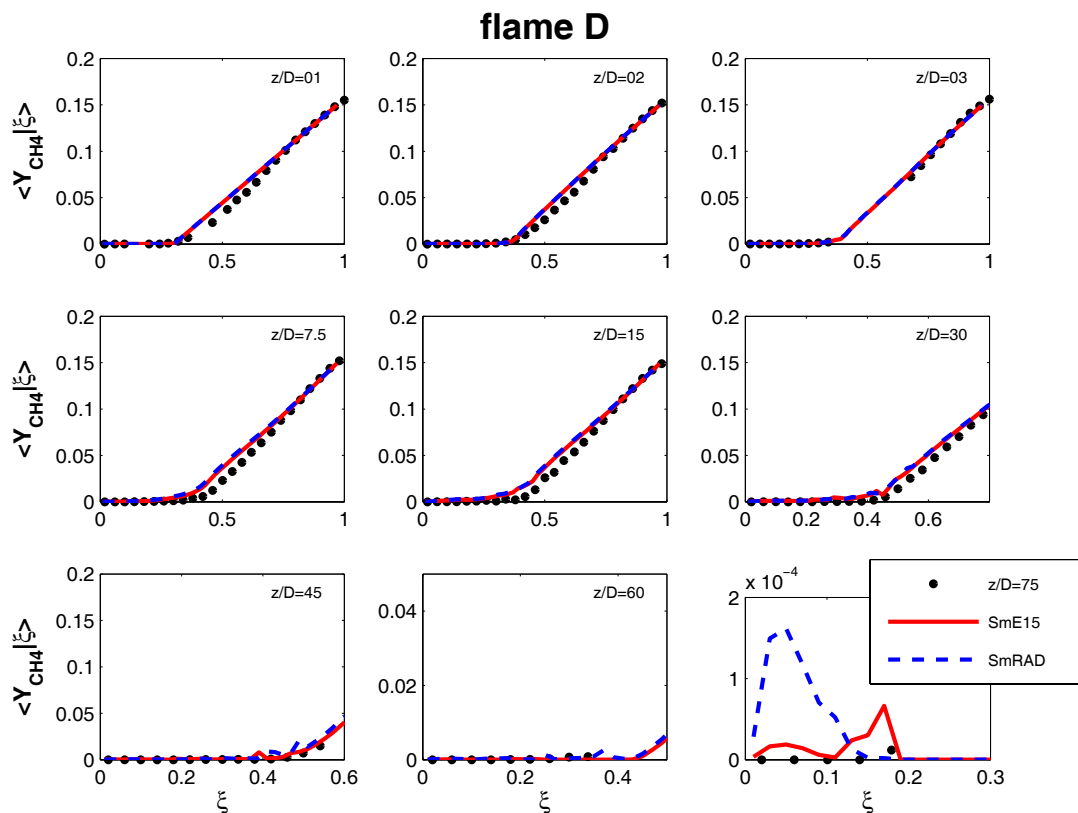


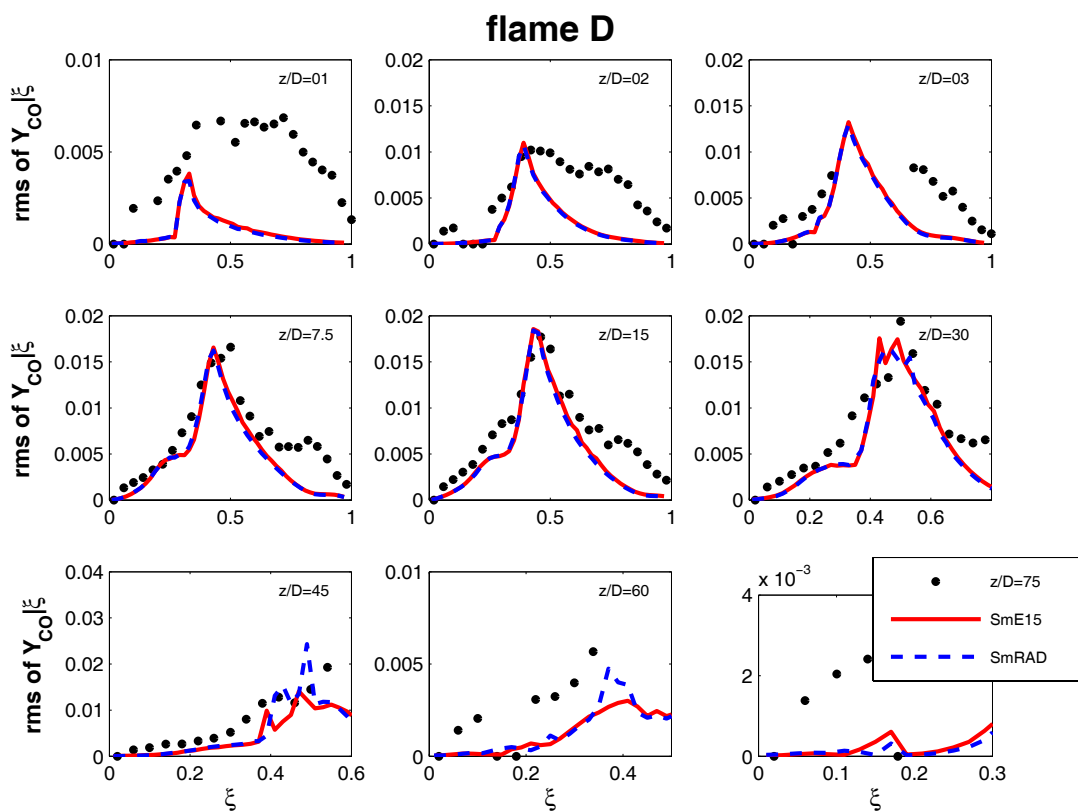
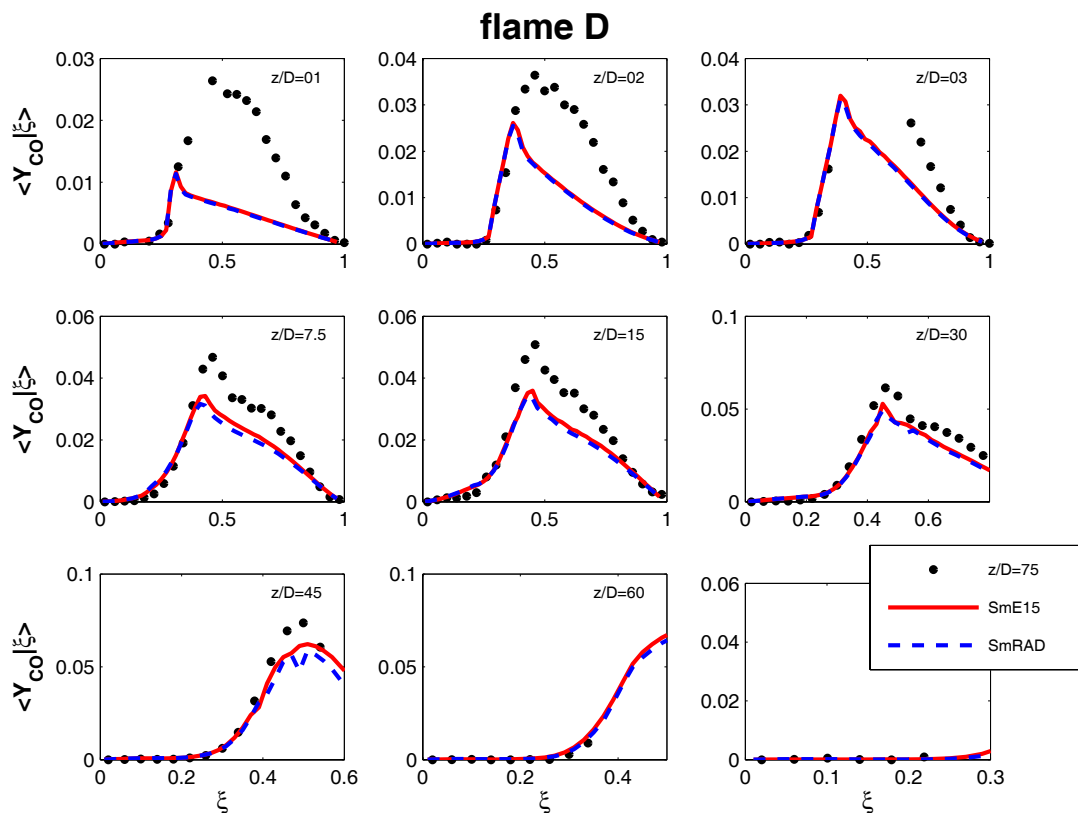


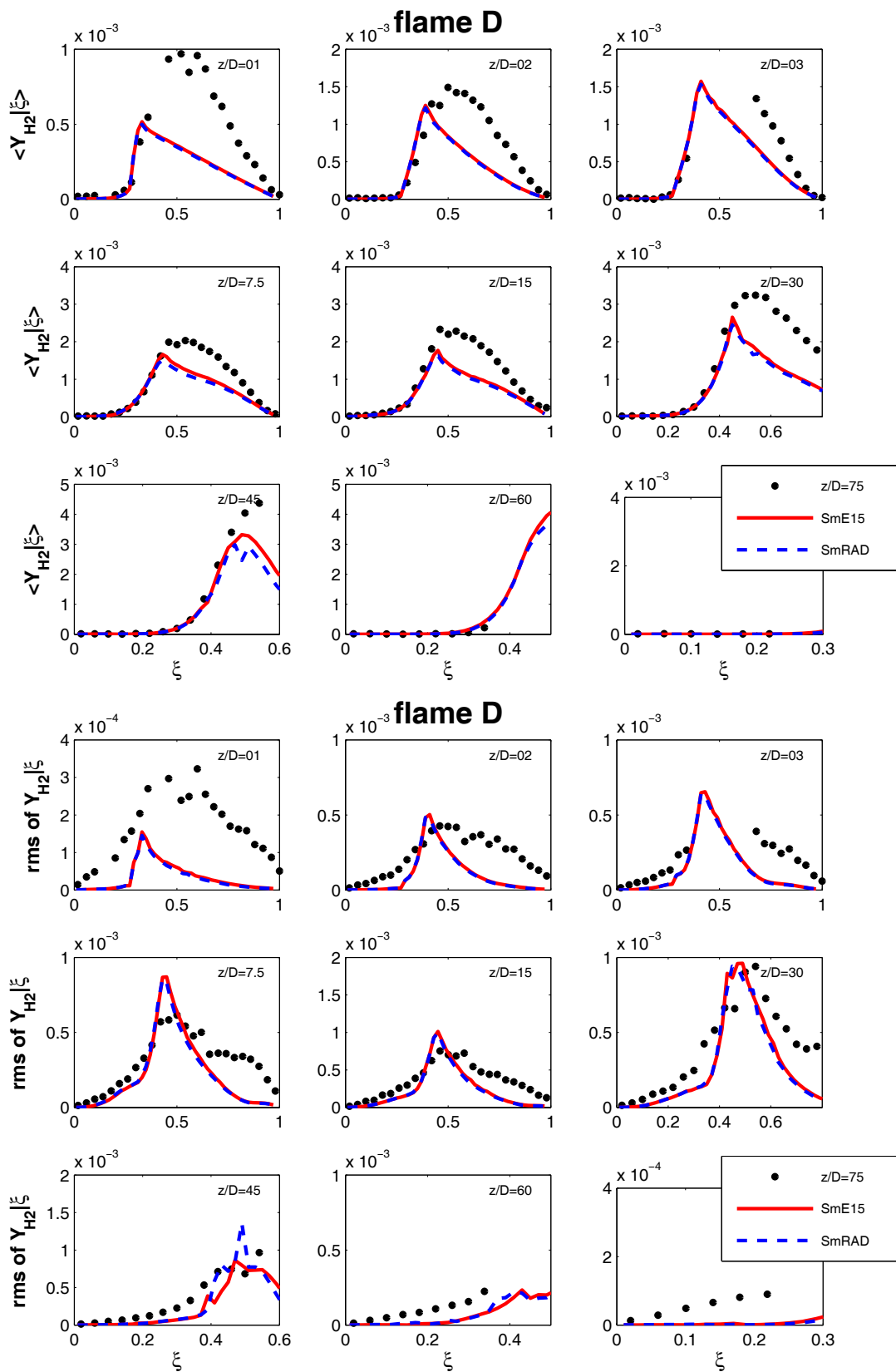


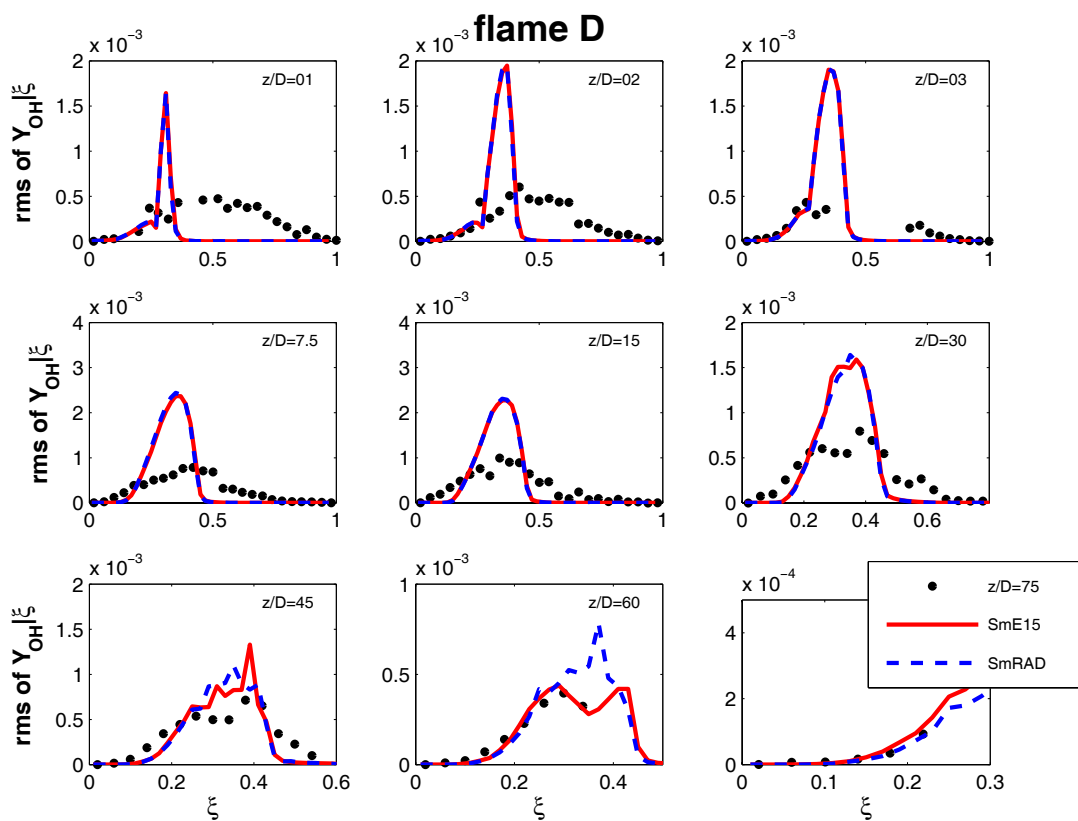
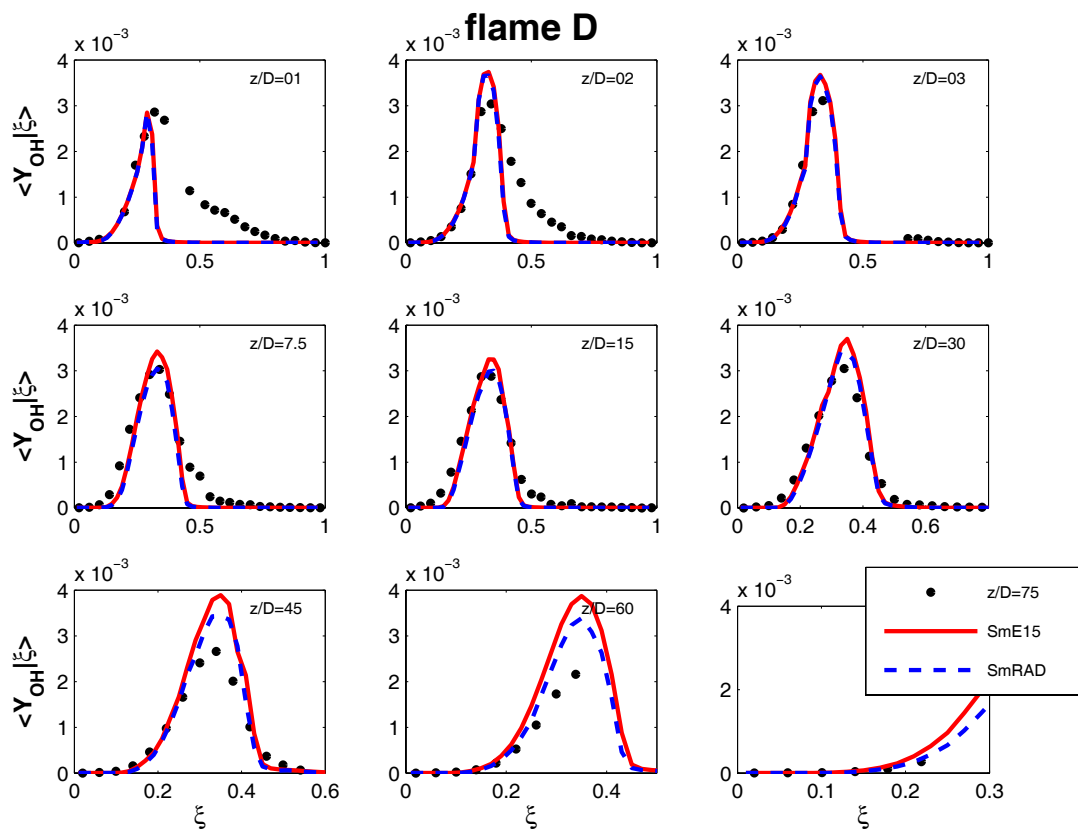






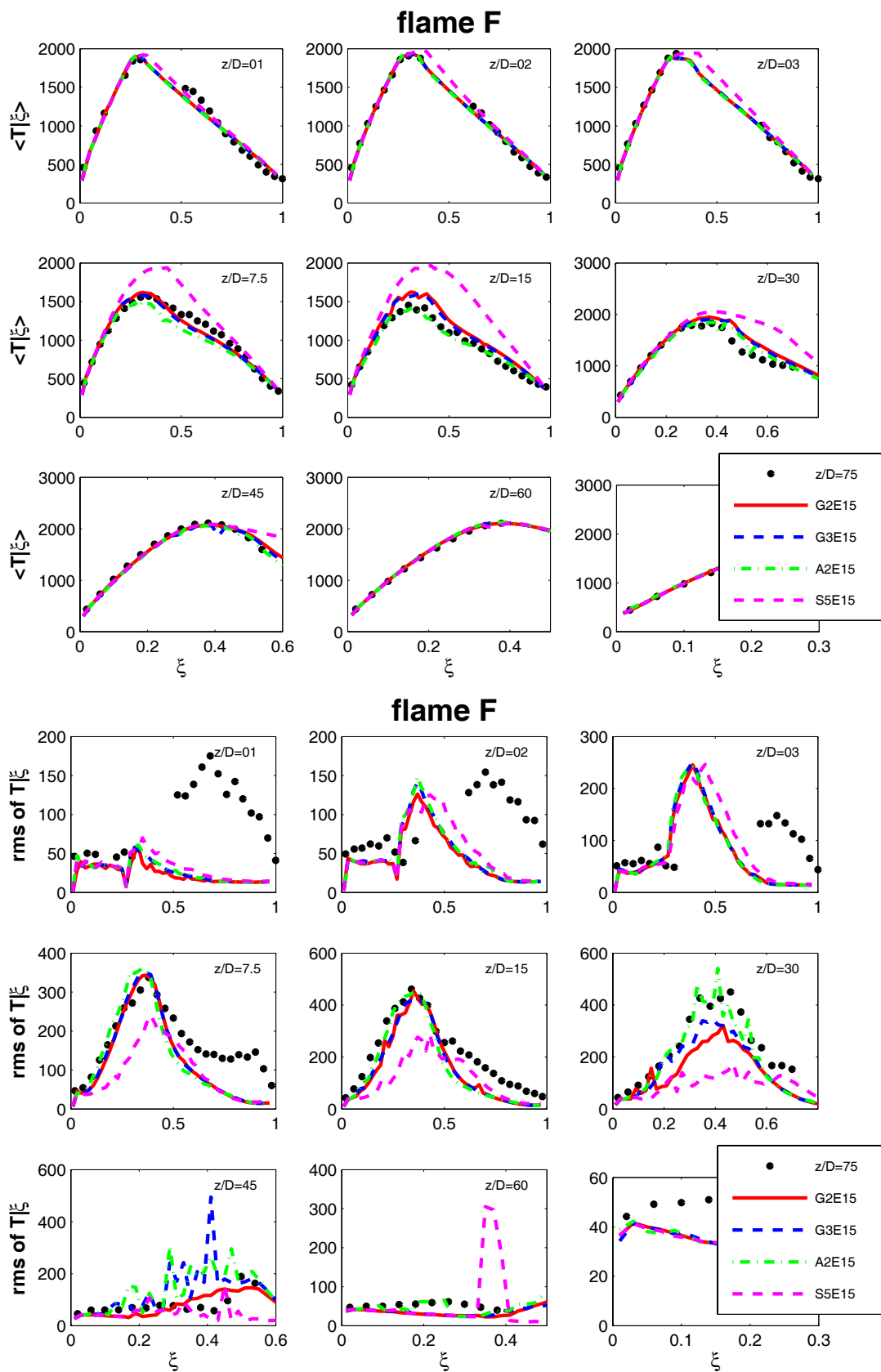


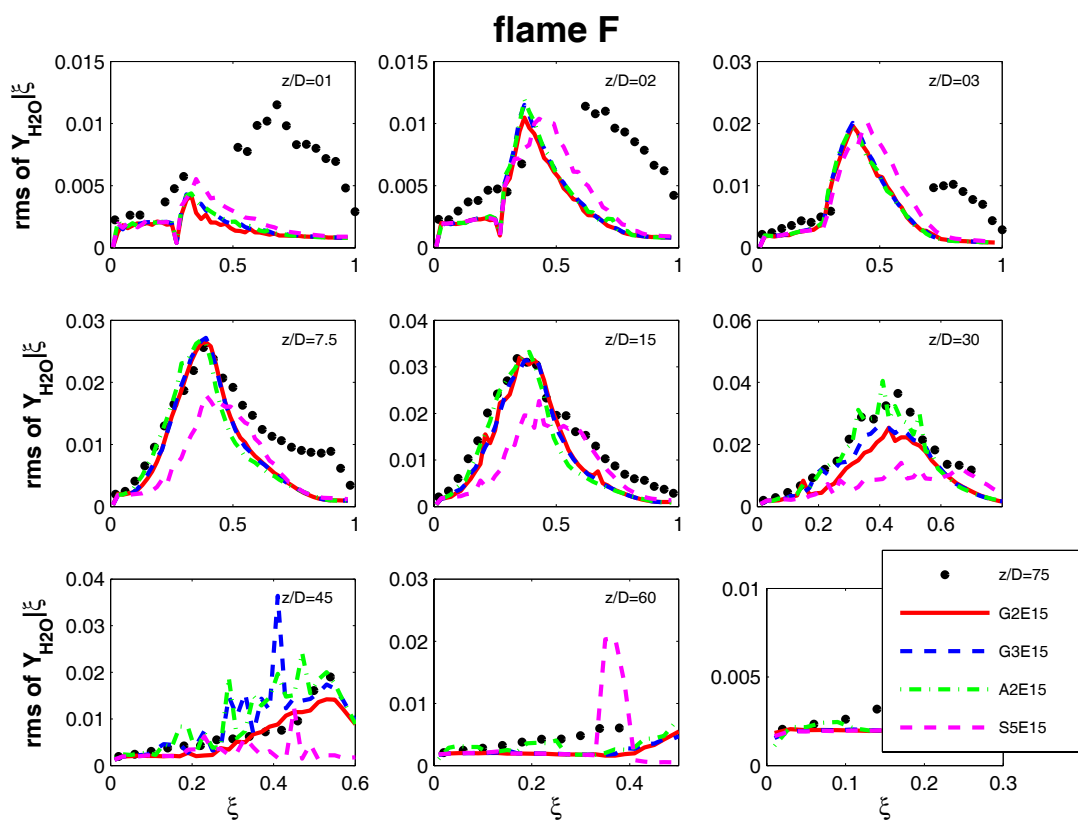
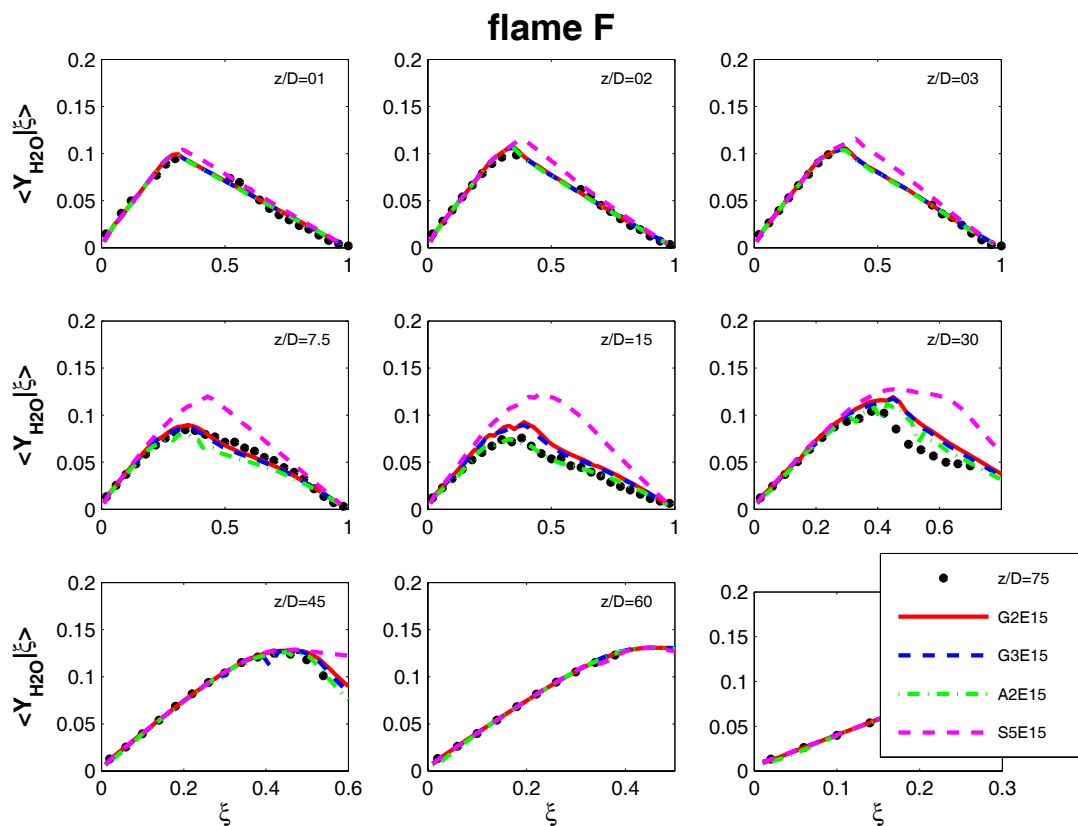


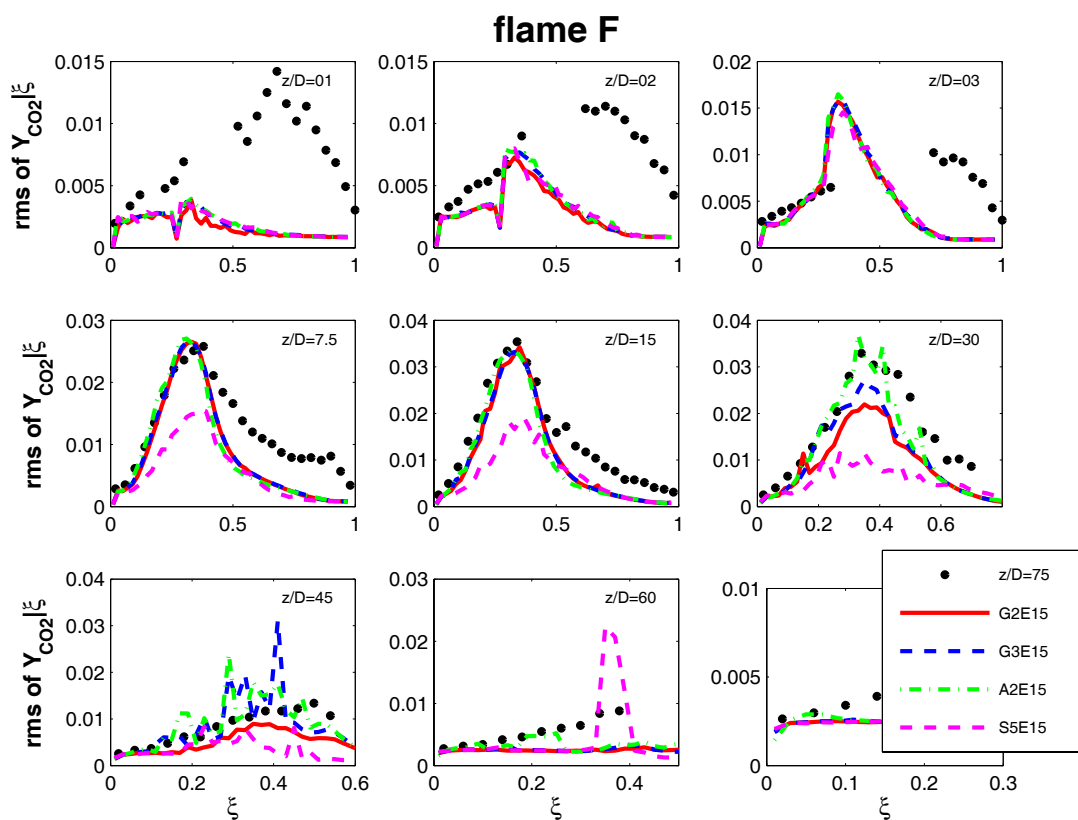
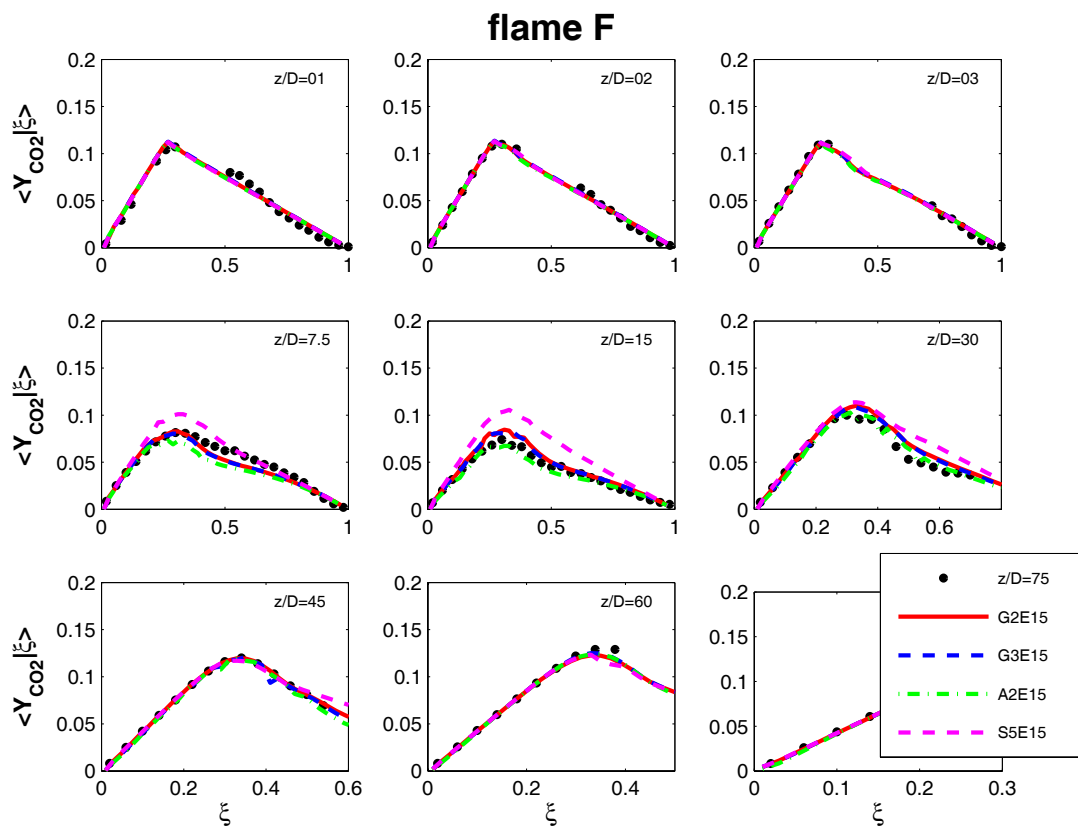


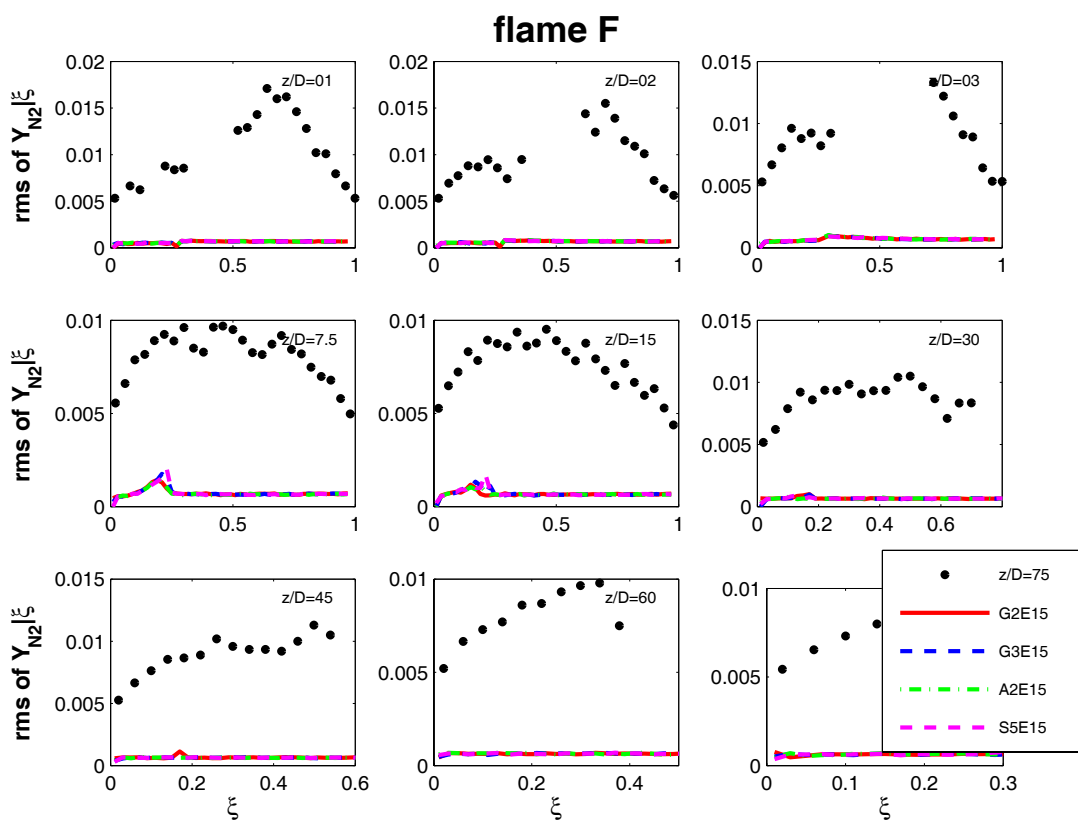
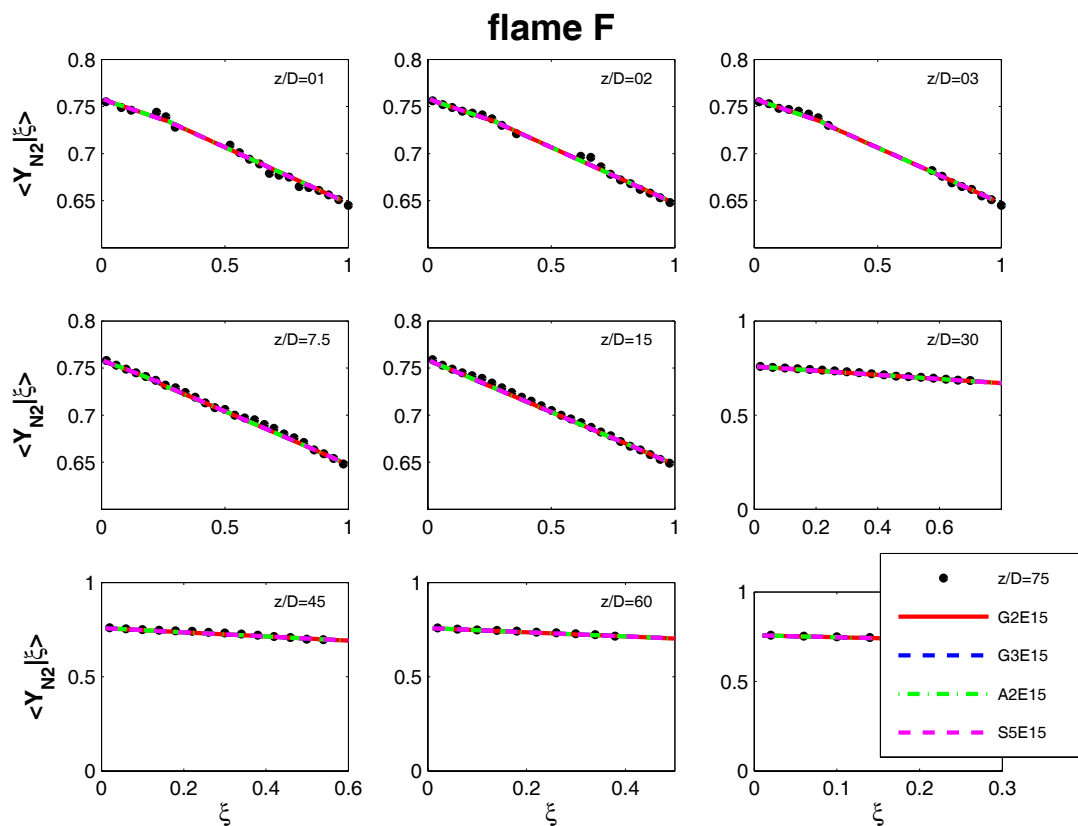
B-5 Calculations of NO

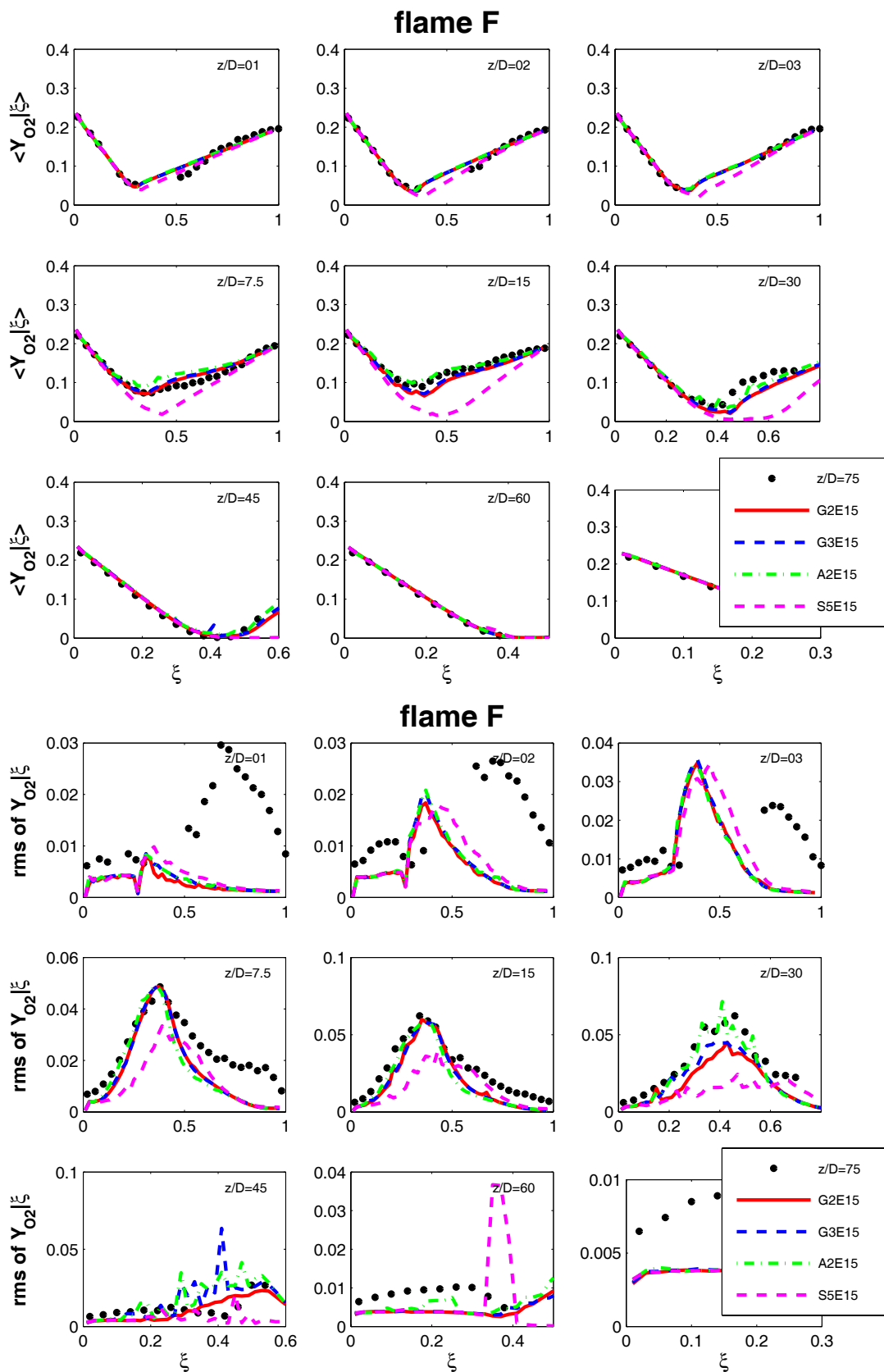
(1) Flame F without radiation (G2, G3, A2, S5)

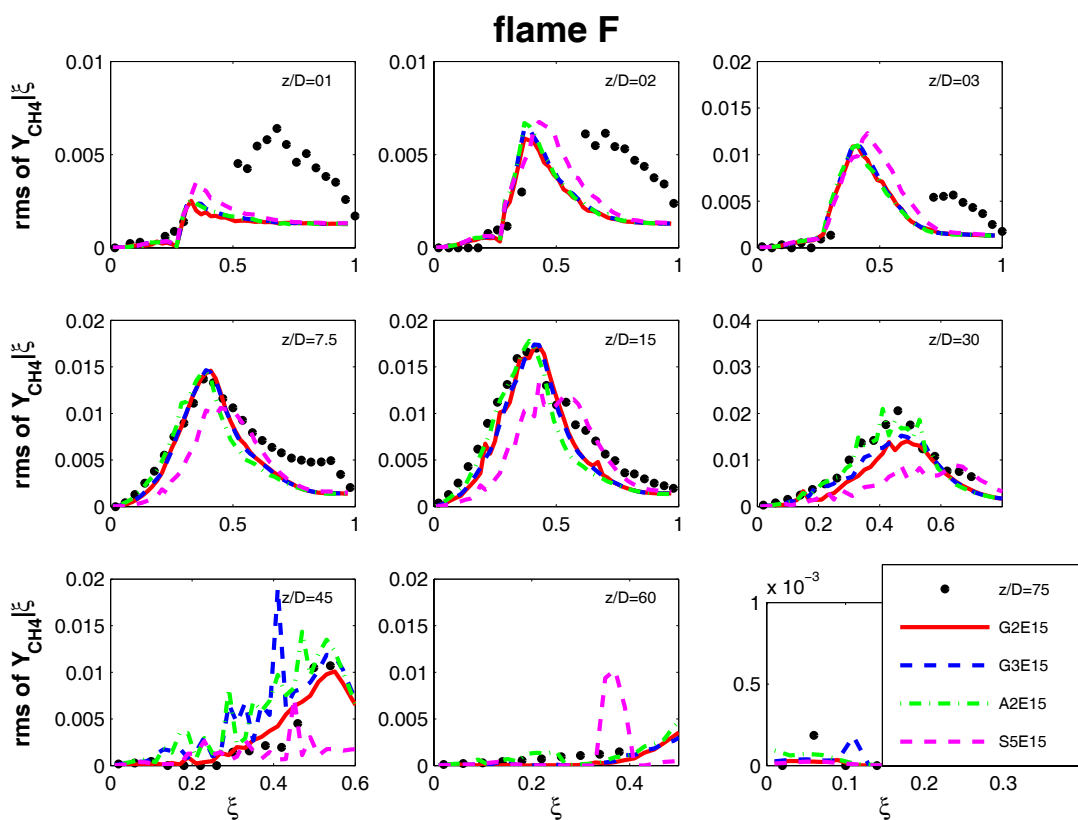
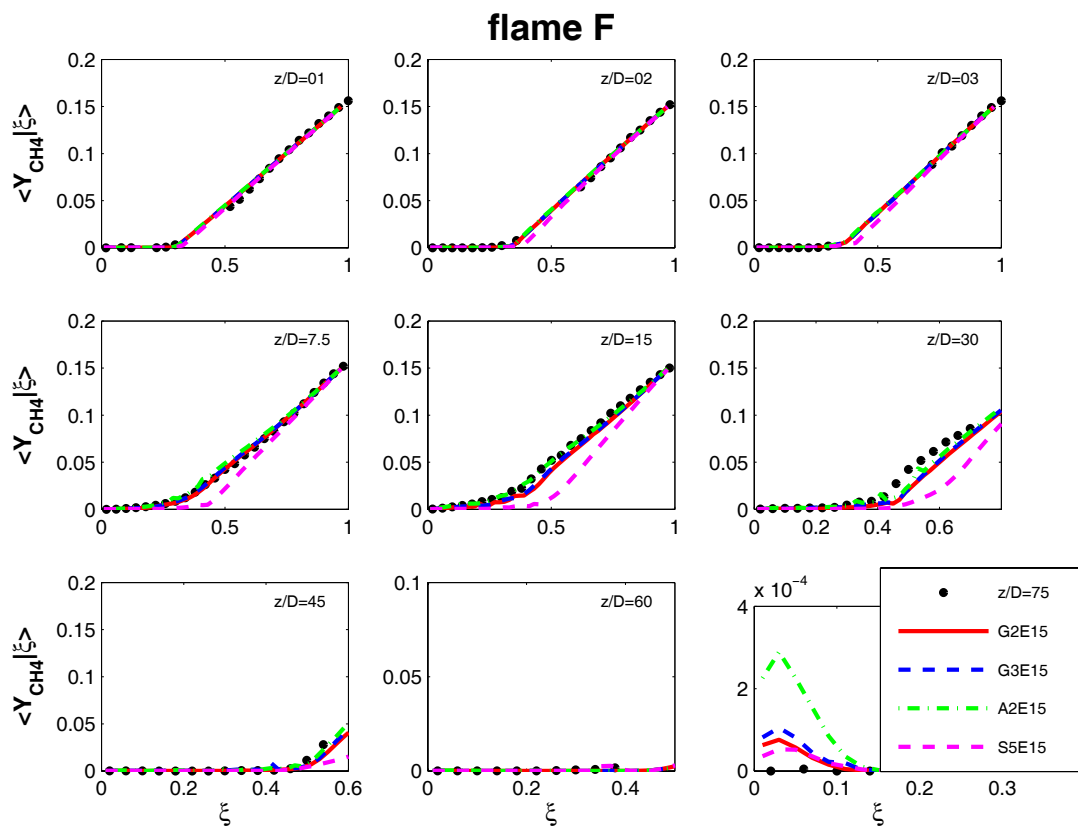


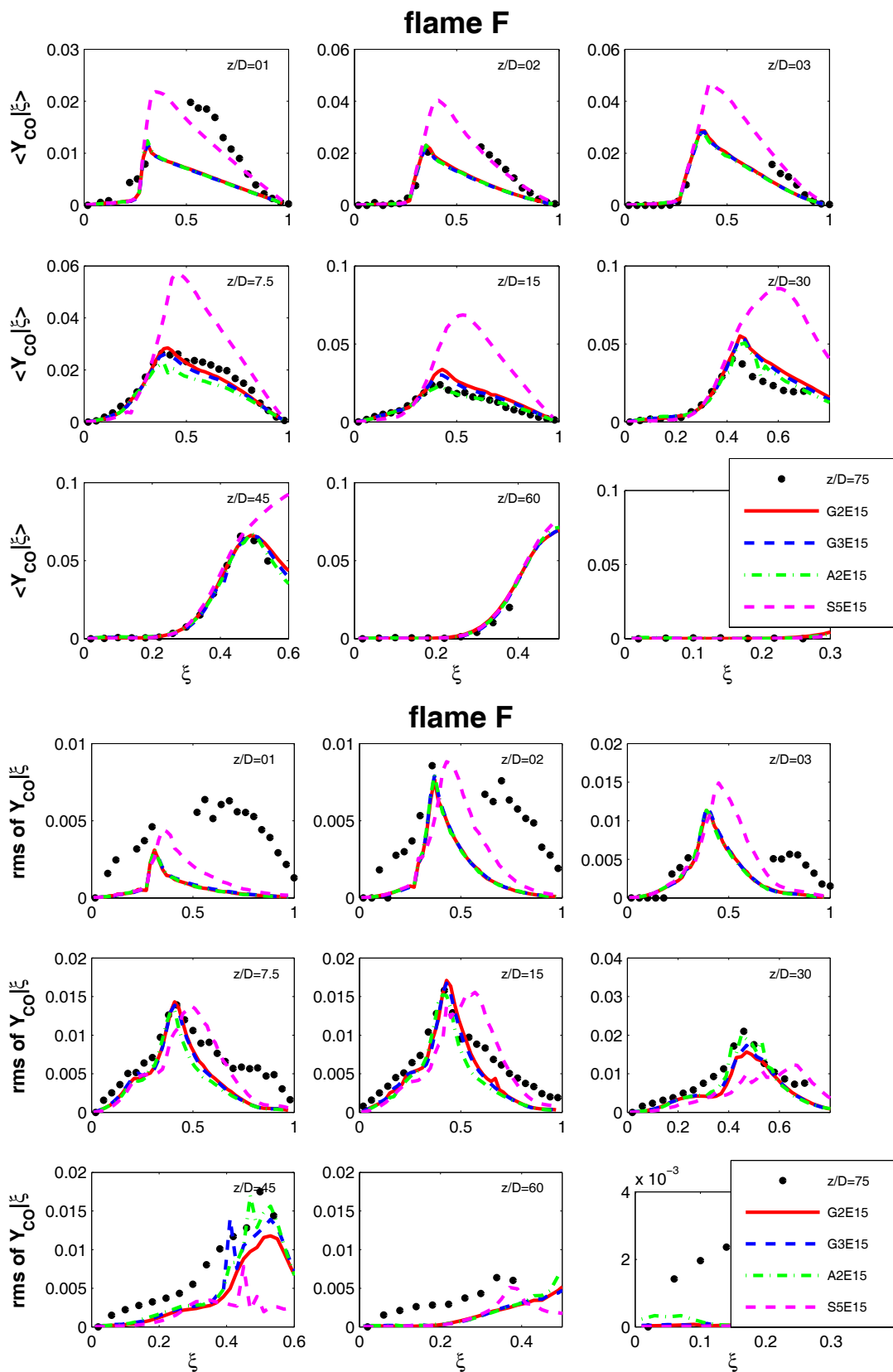


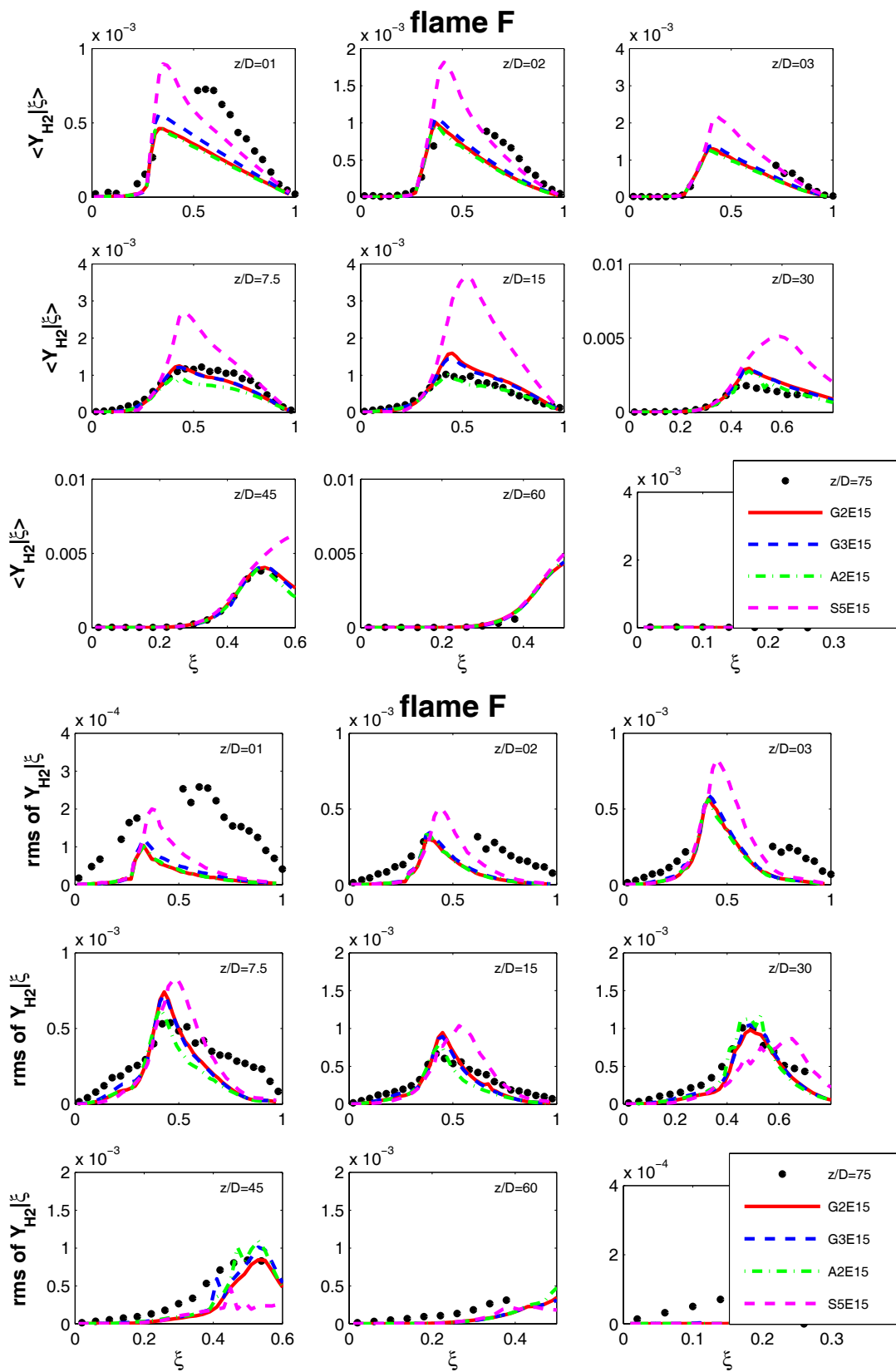


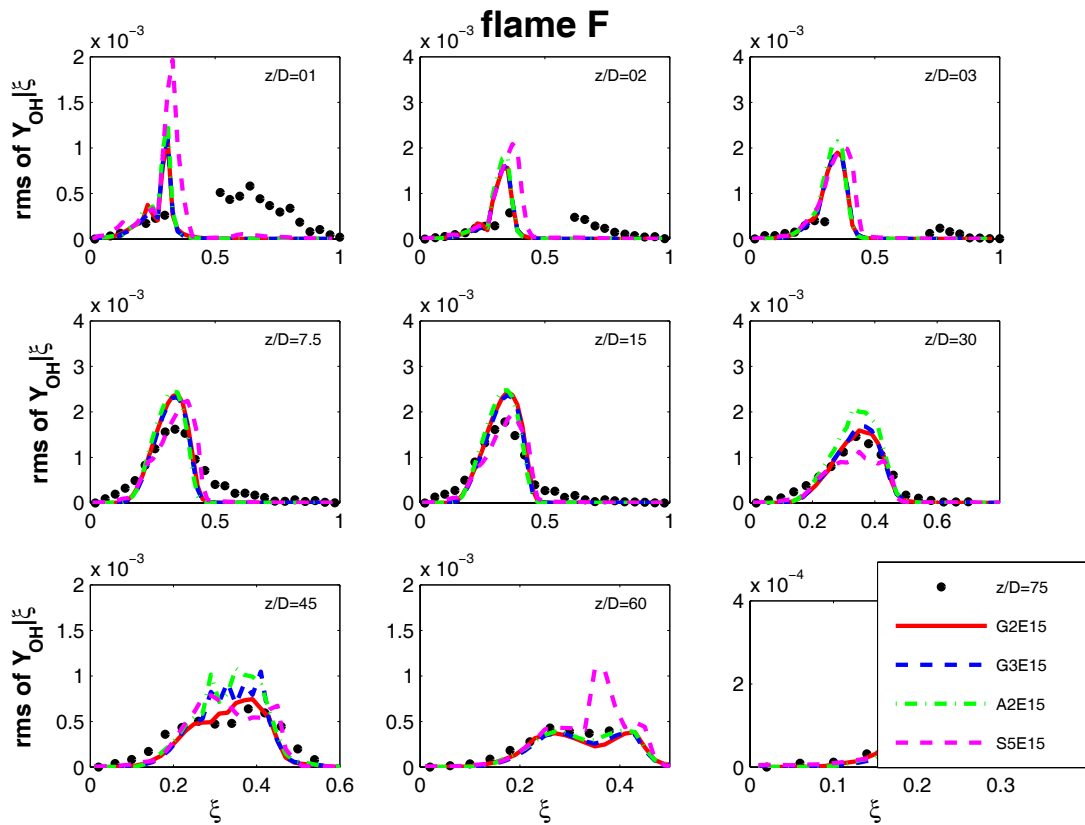
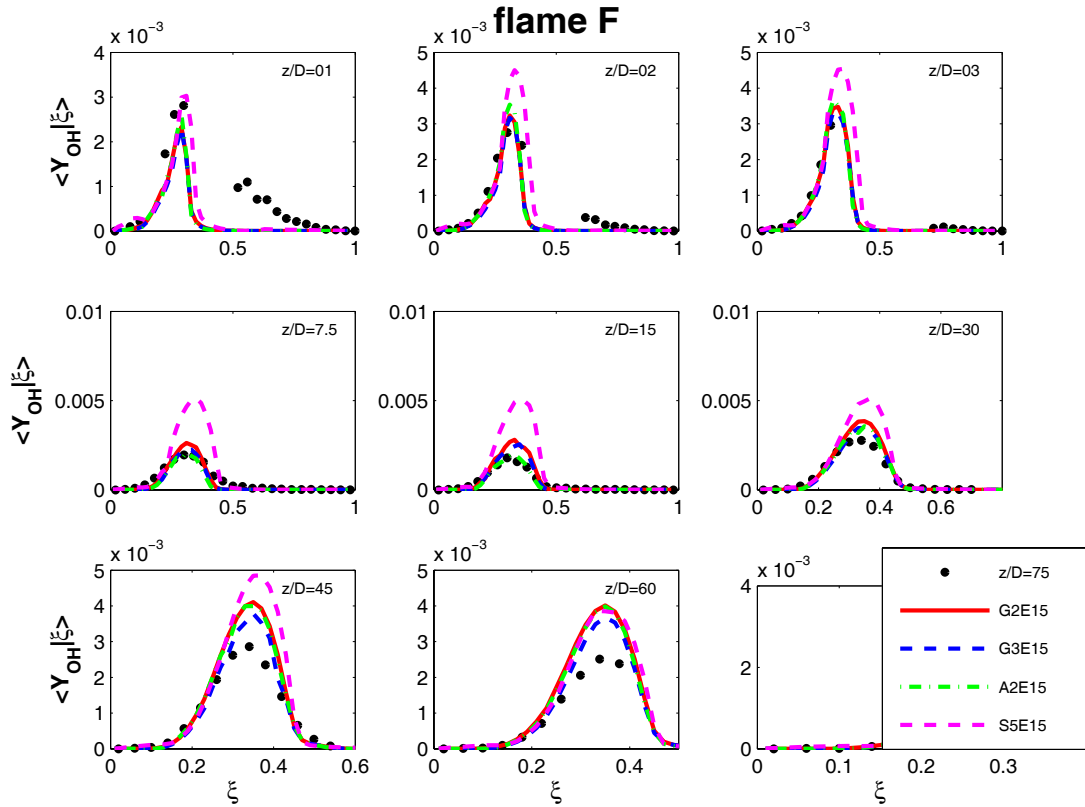


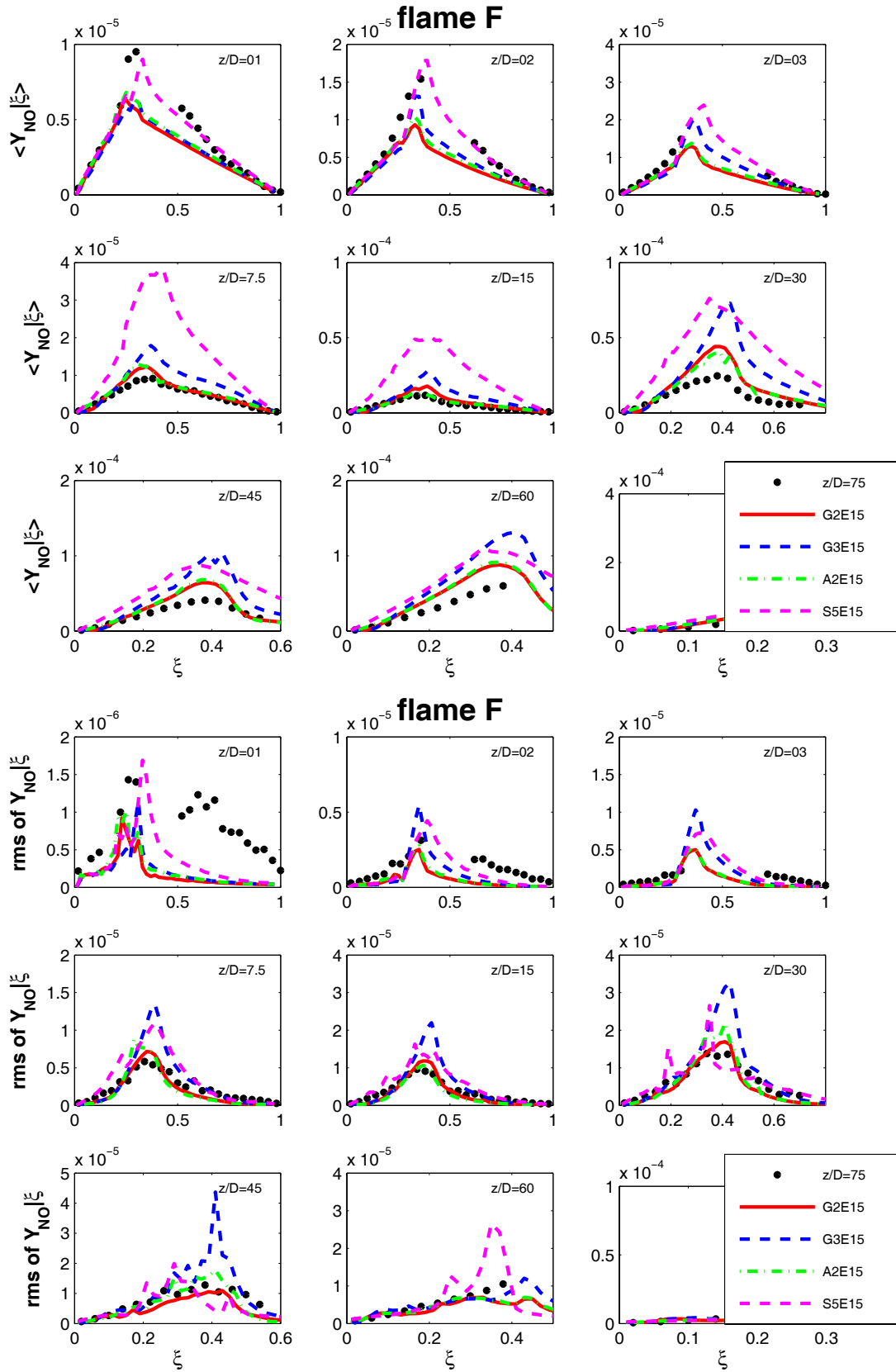




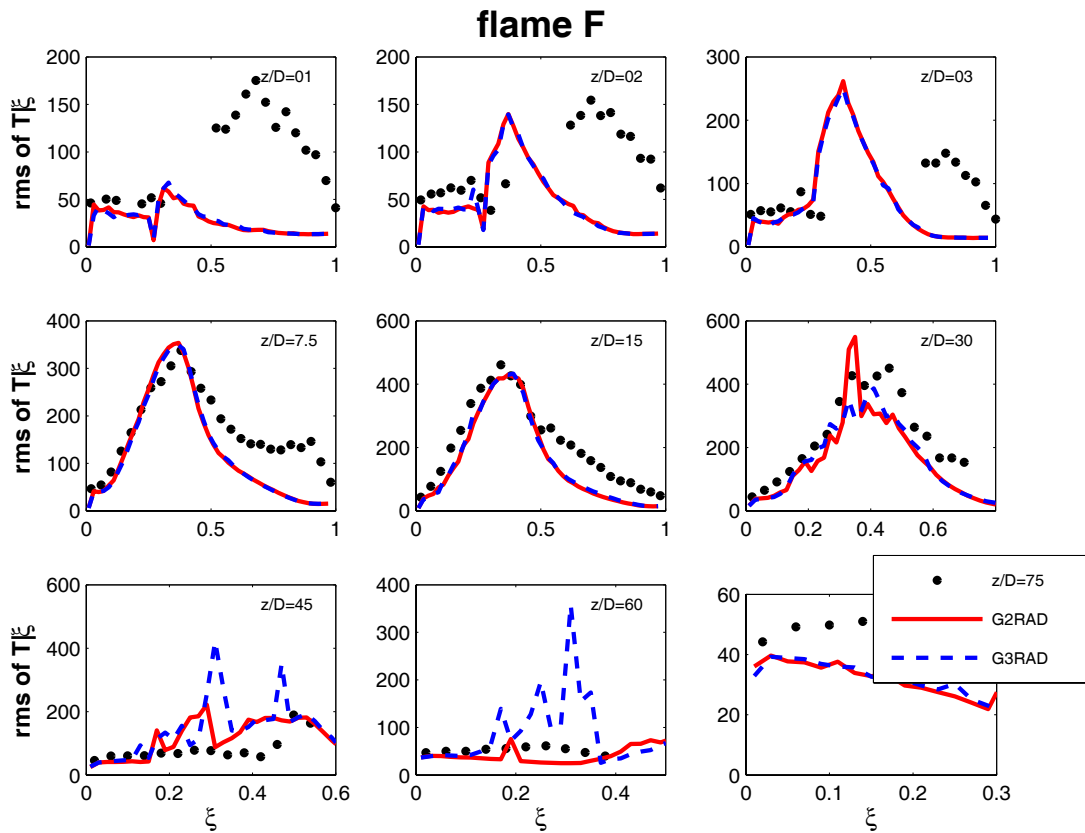
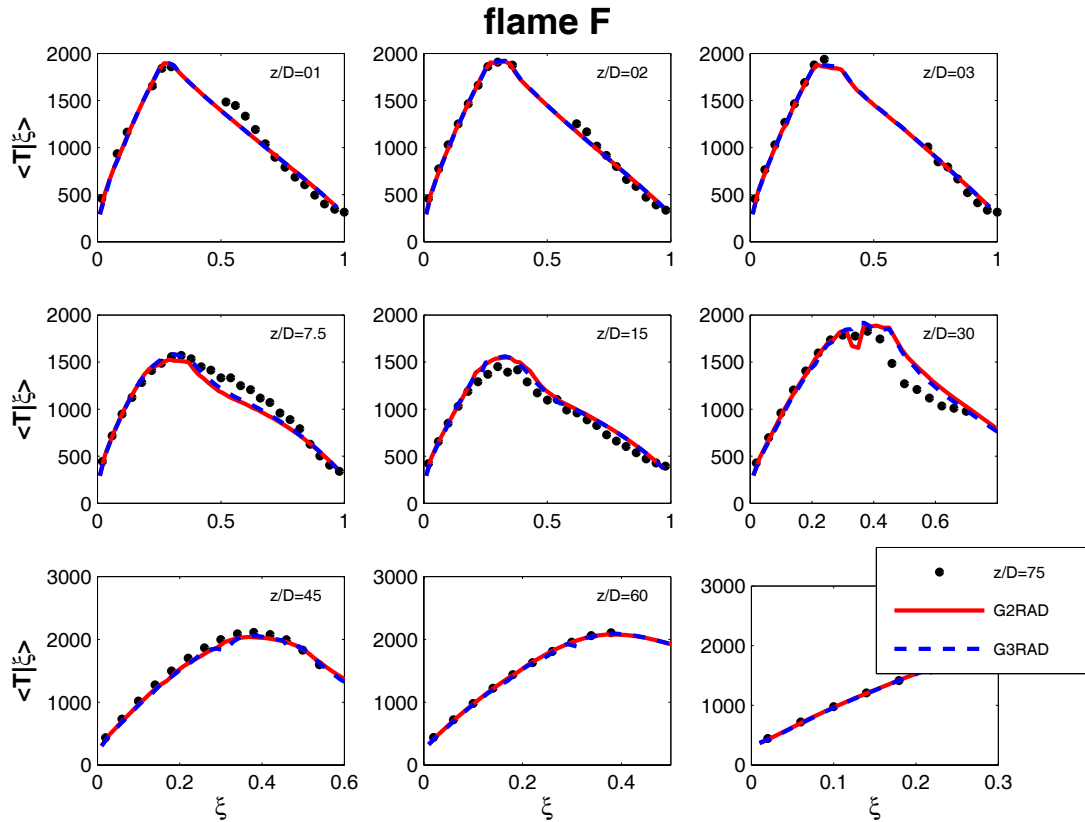


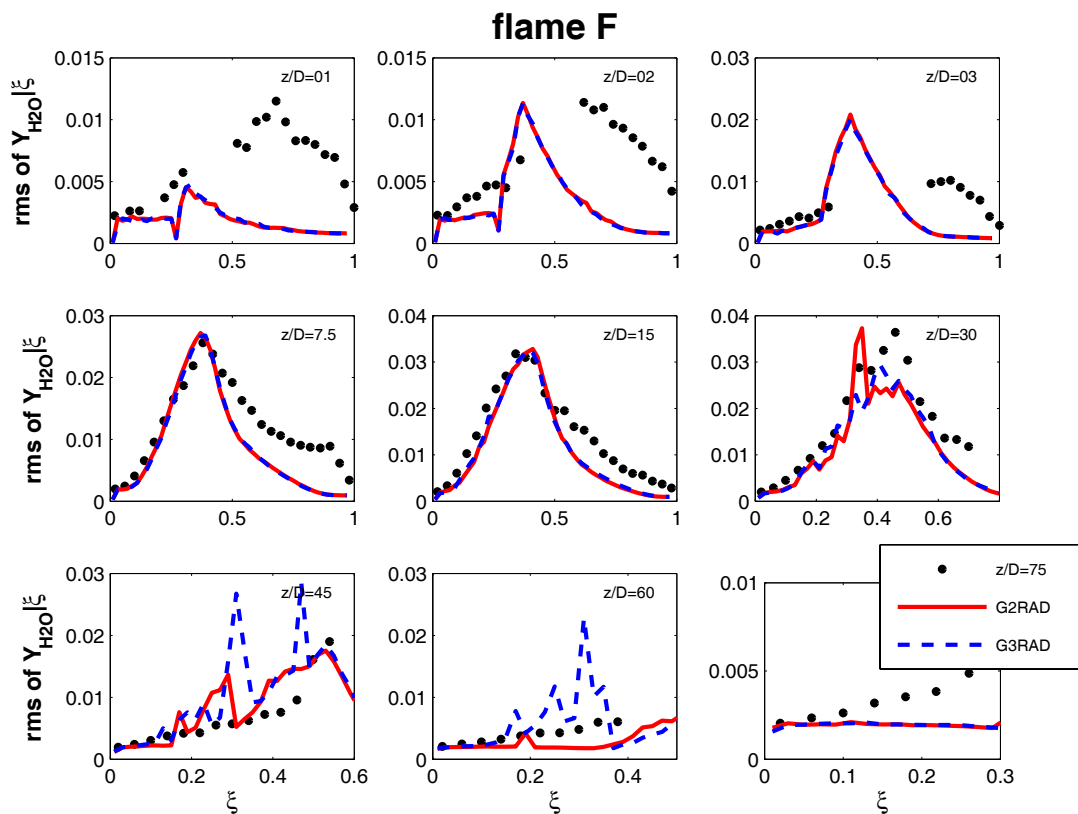
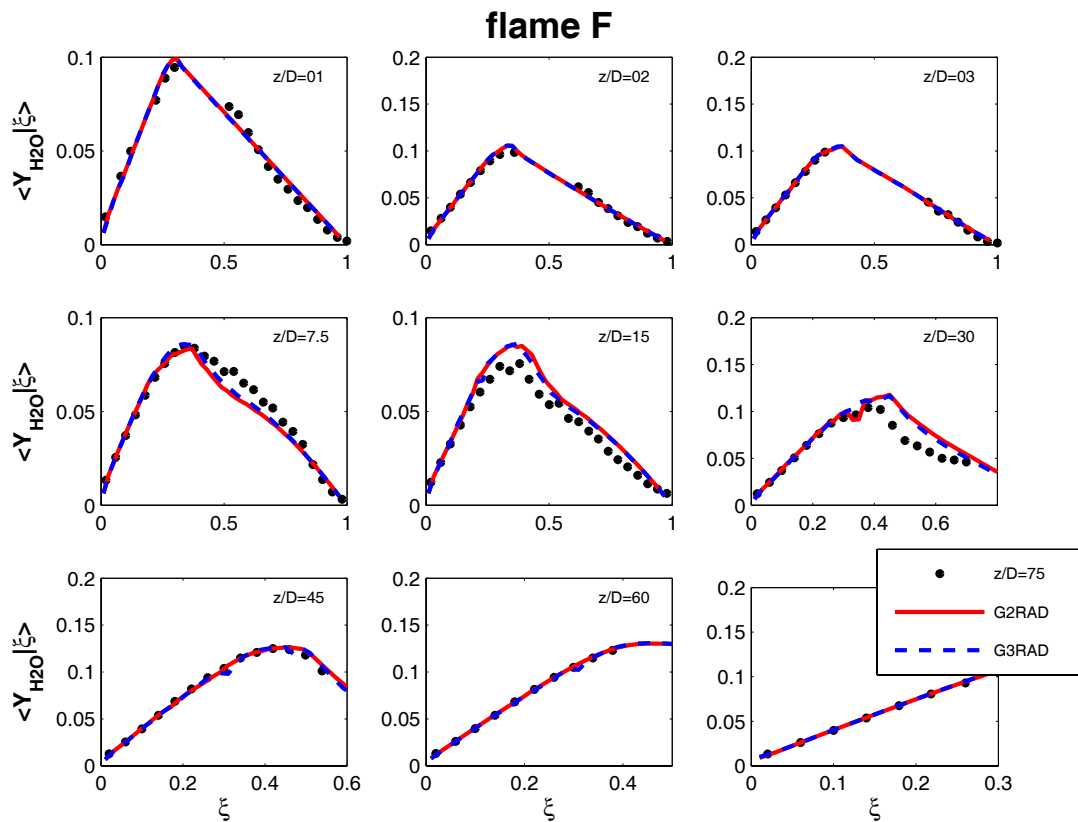


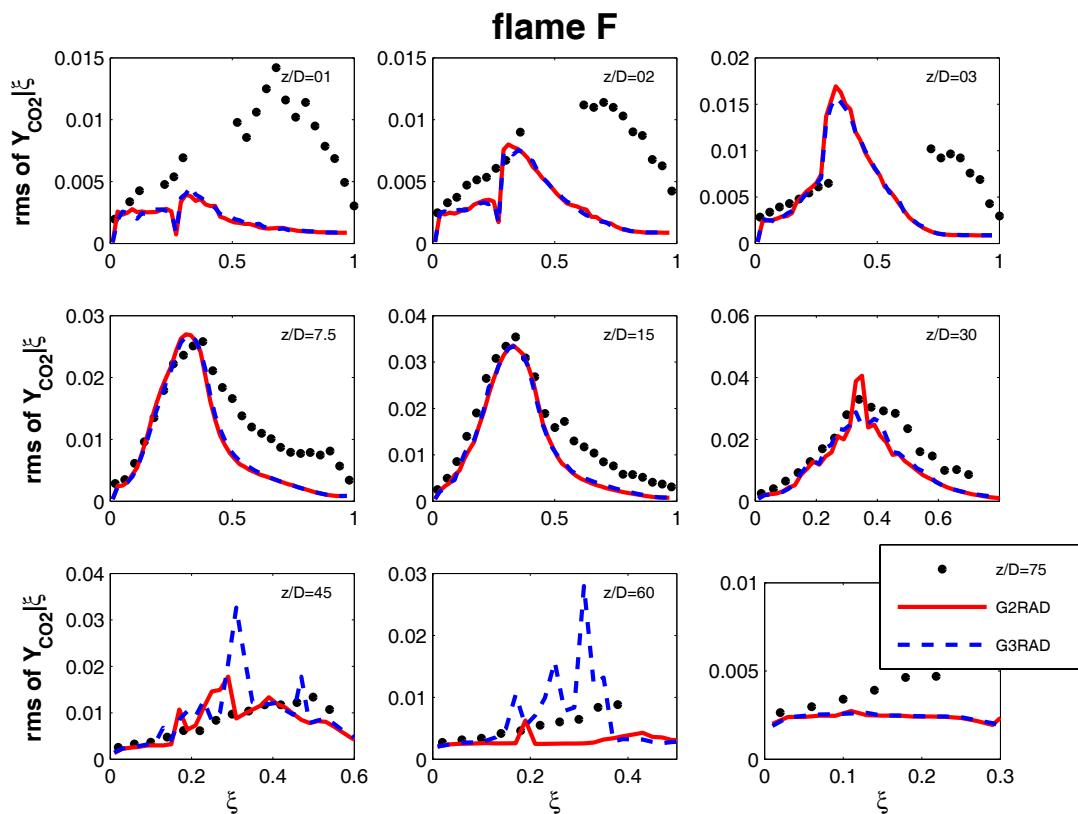
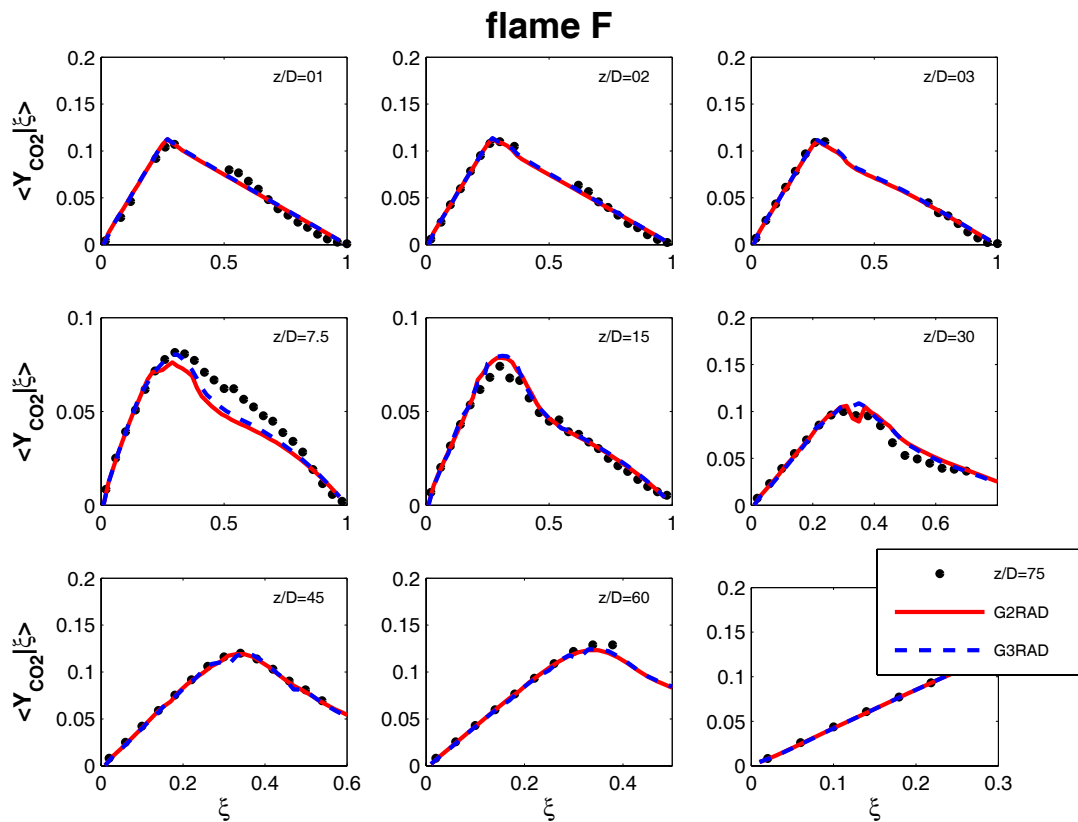


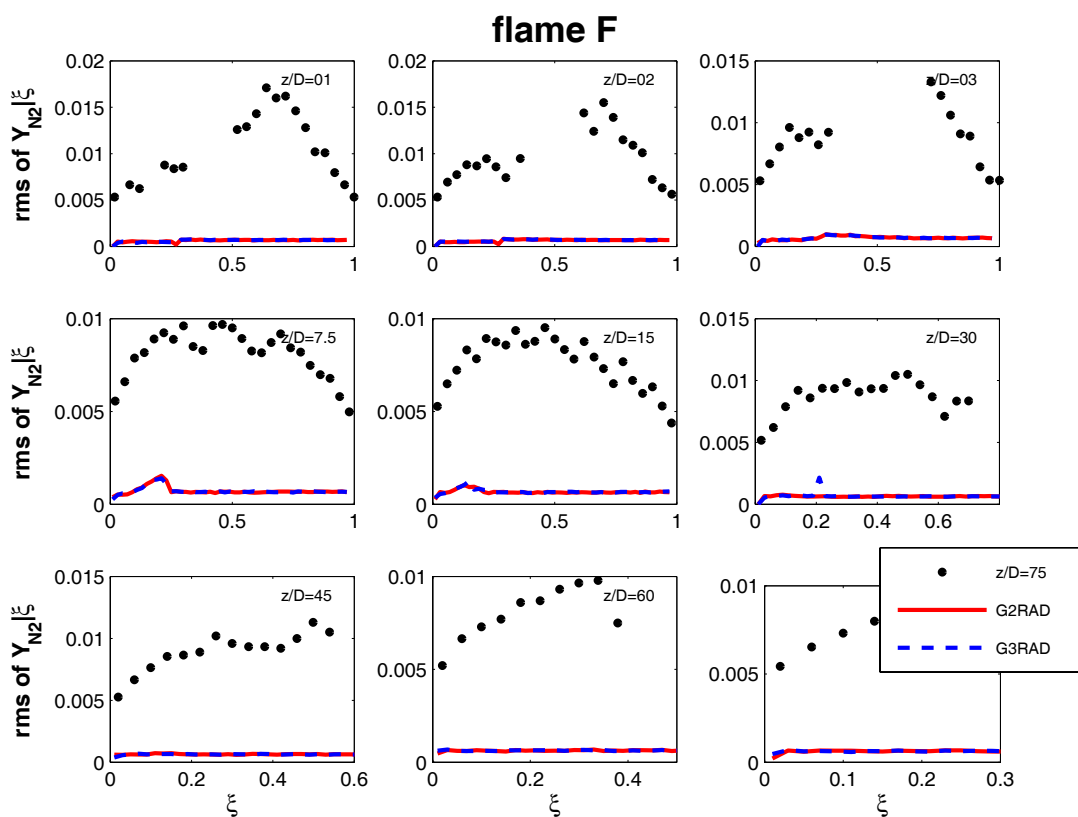
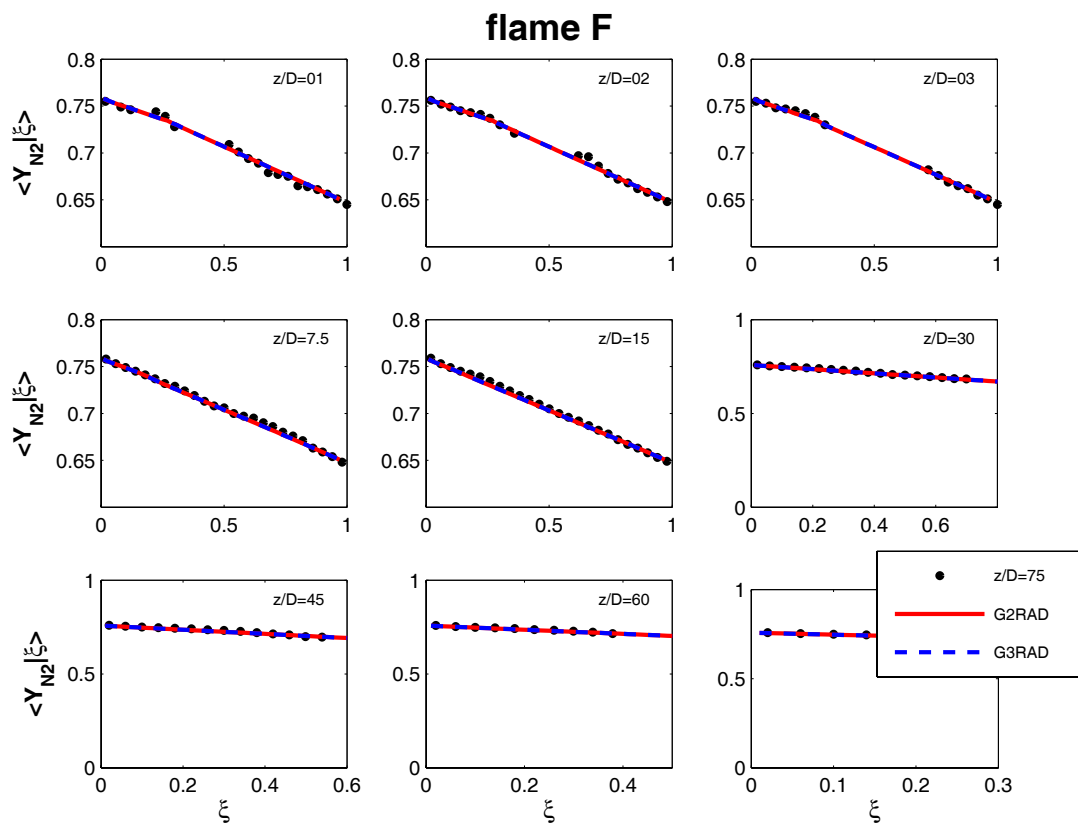


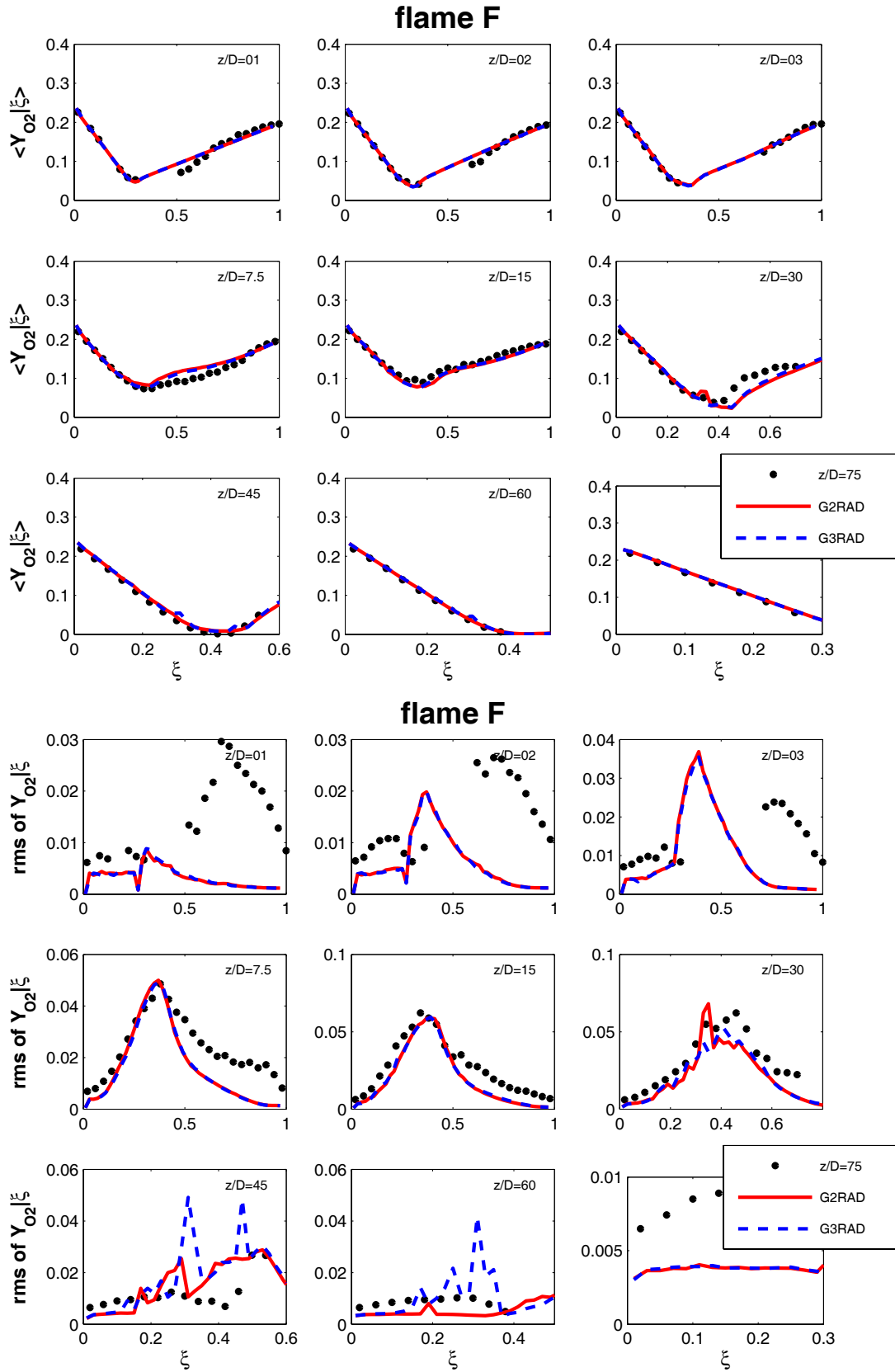
(2) Flame F with radiation (G2, G3)

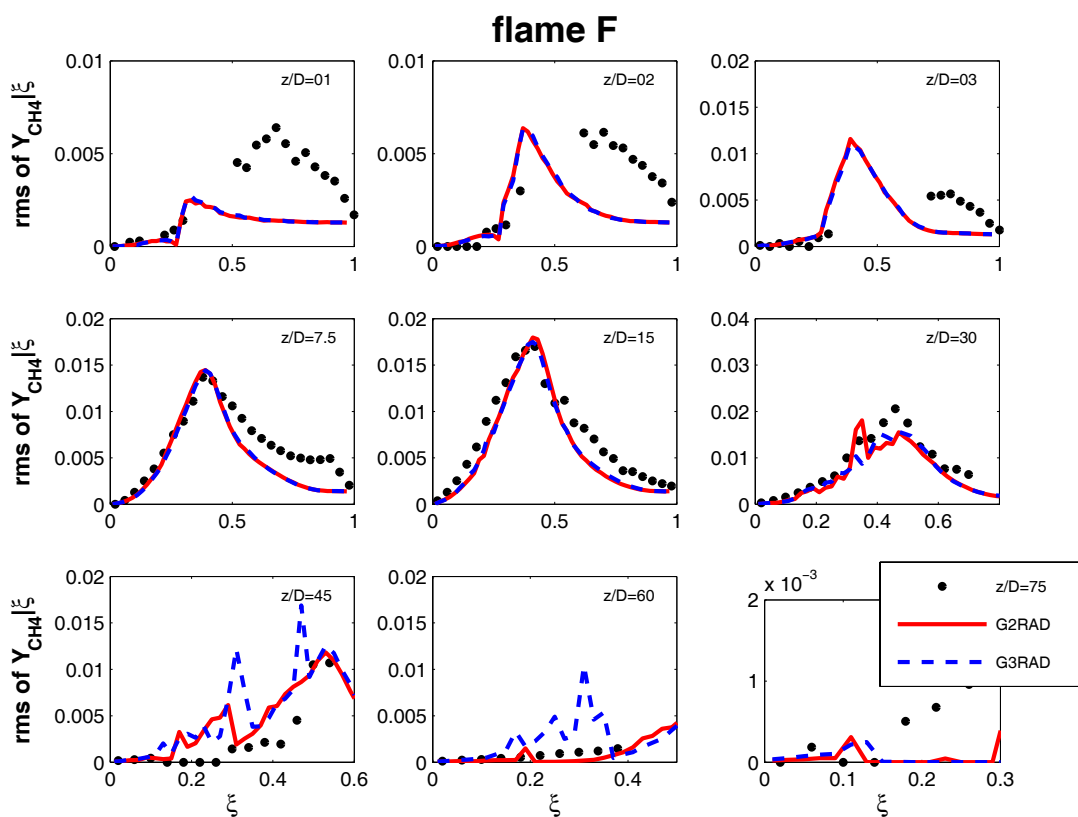
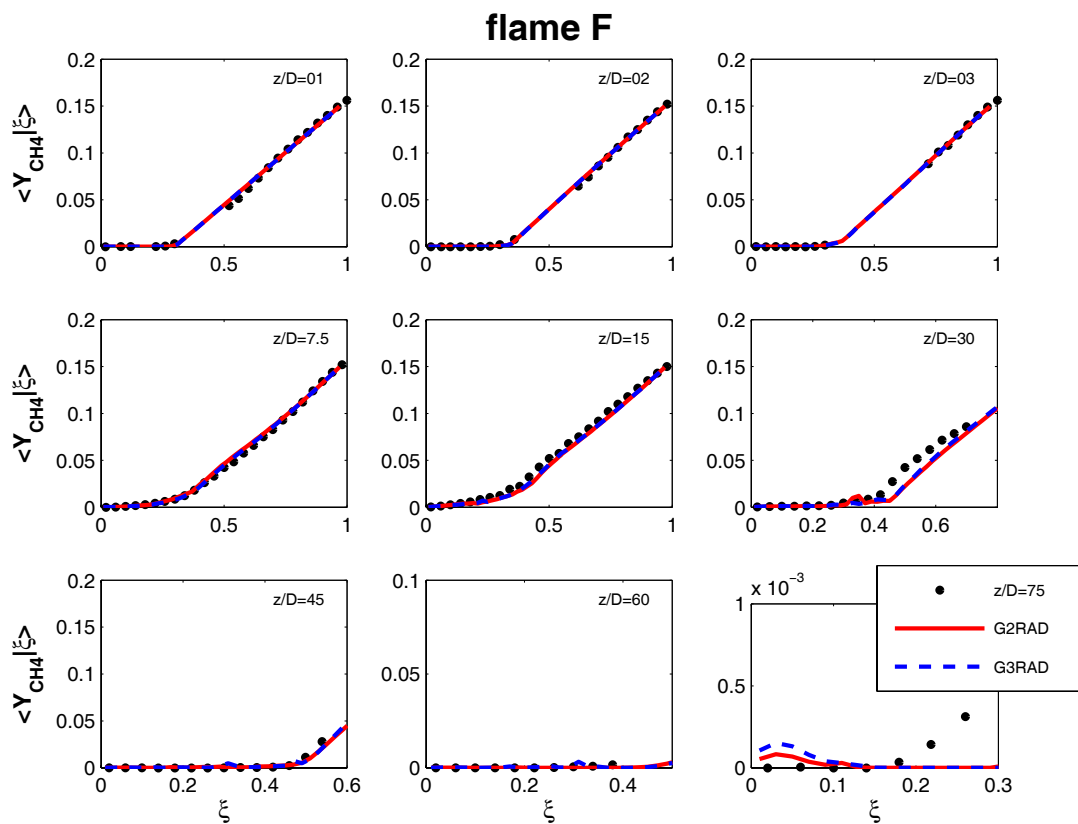


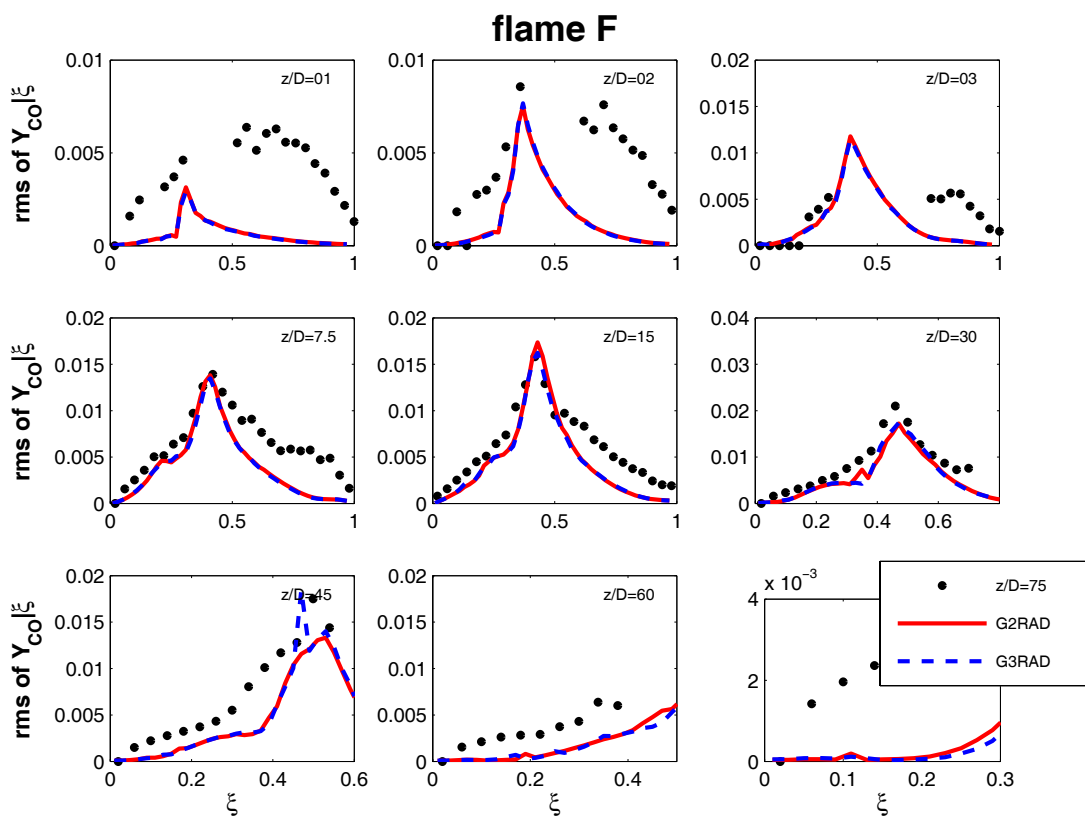
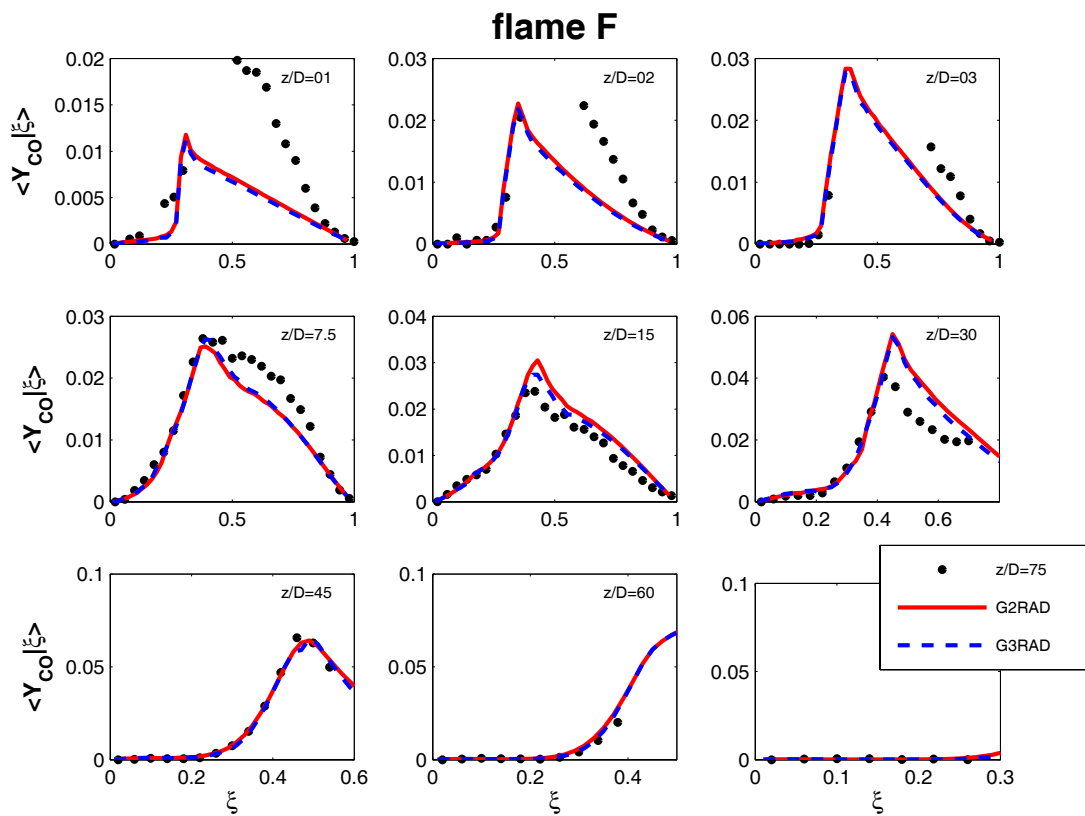


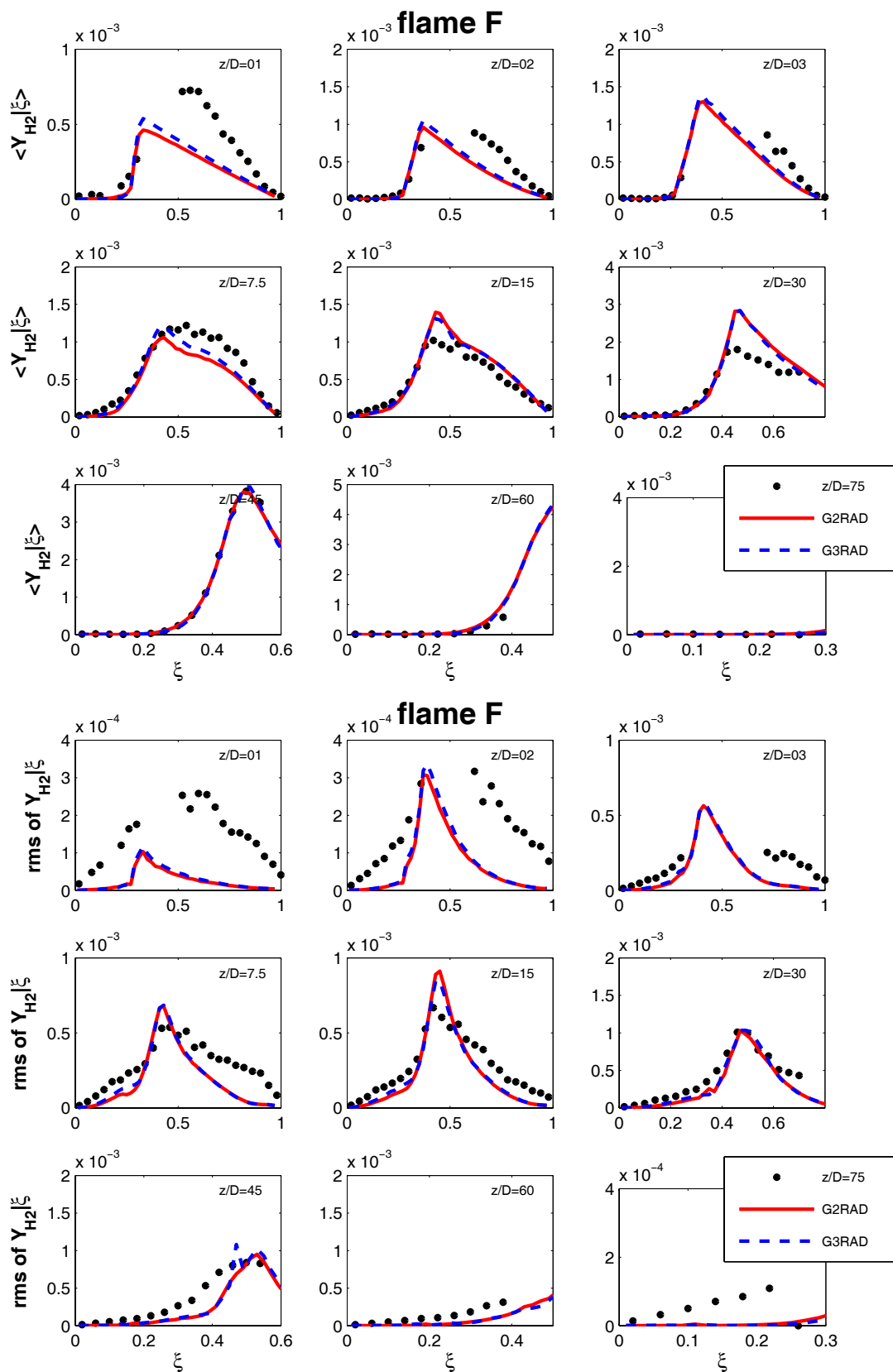


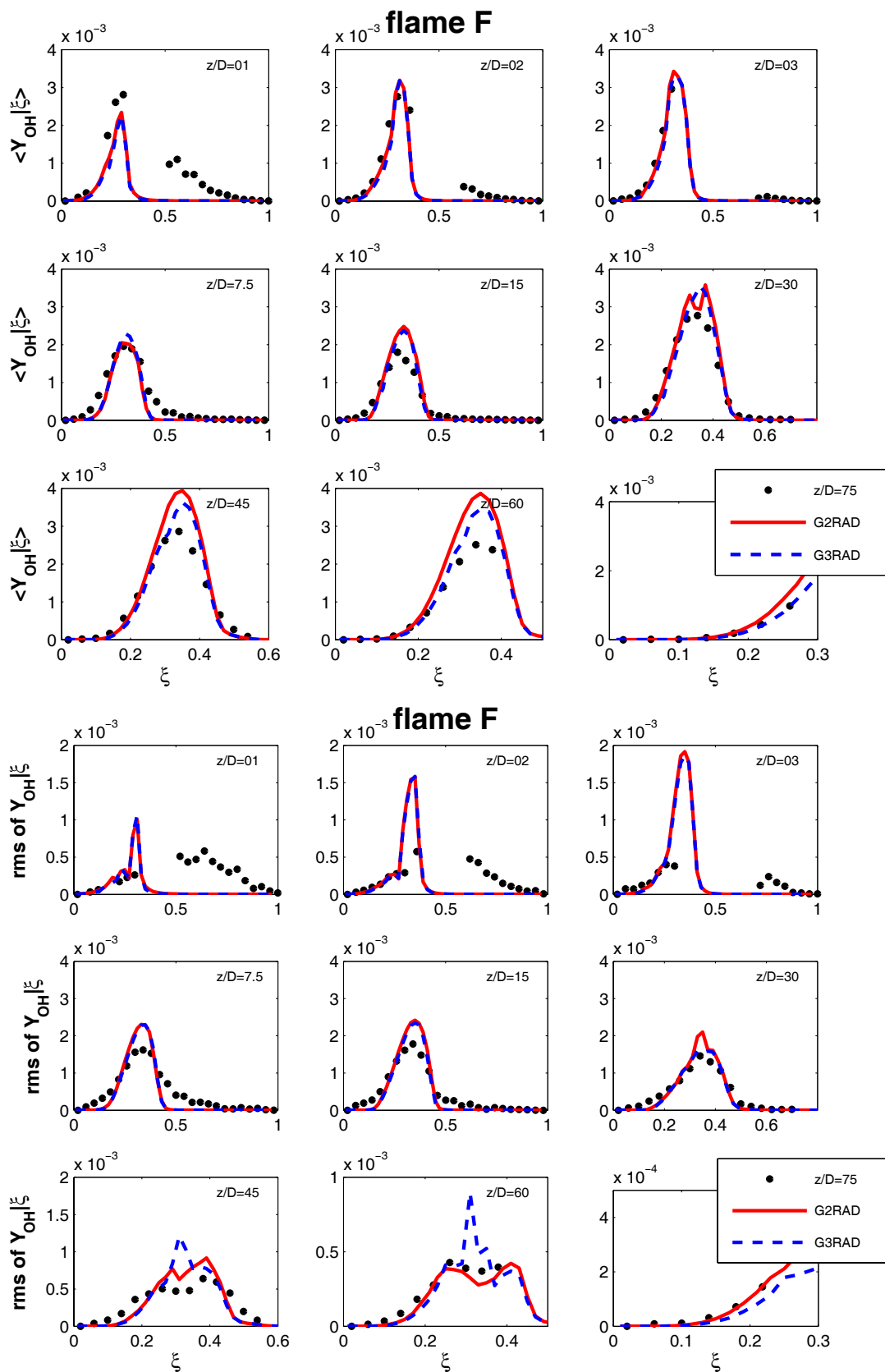


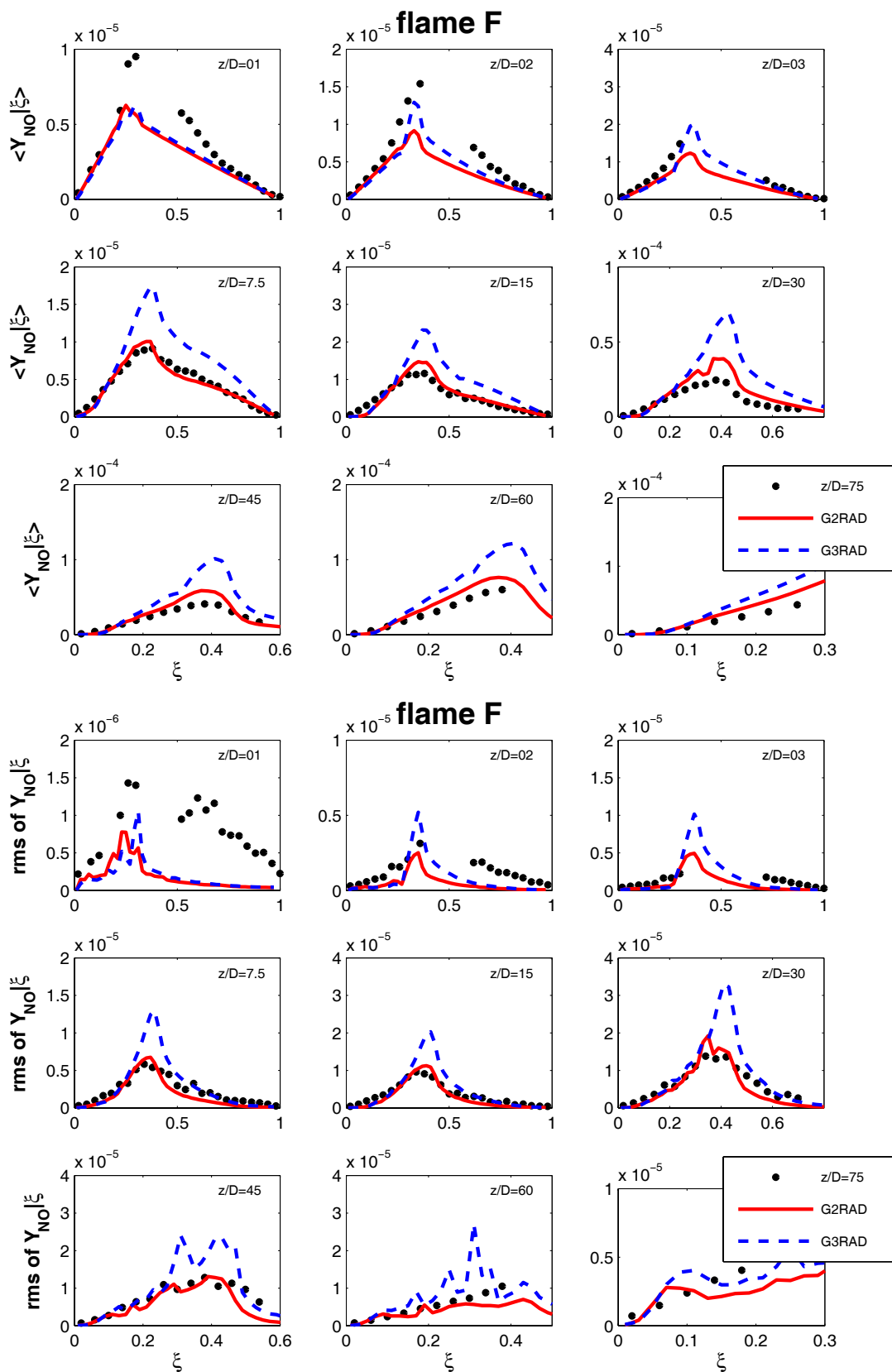




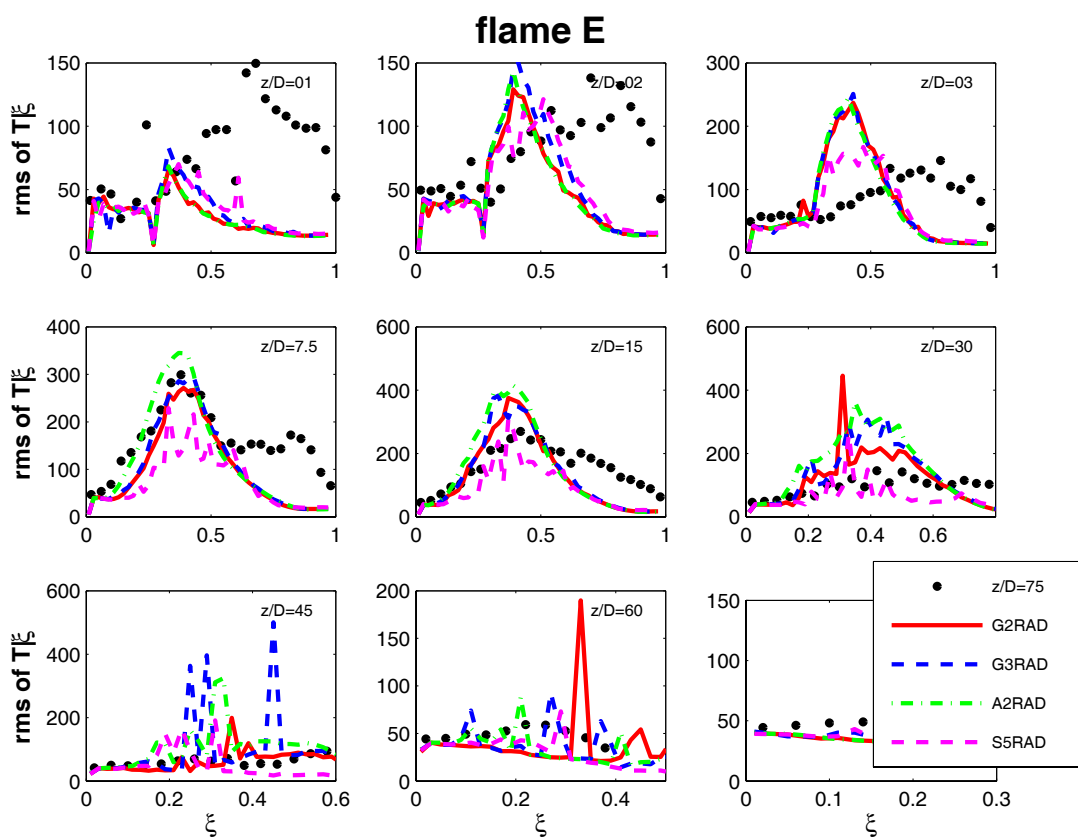
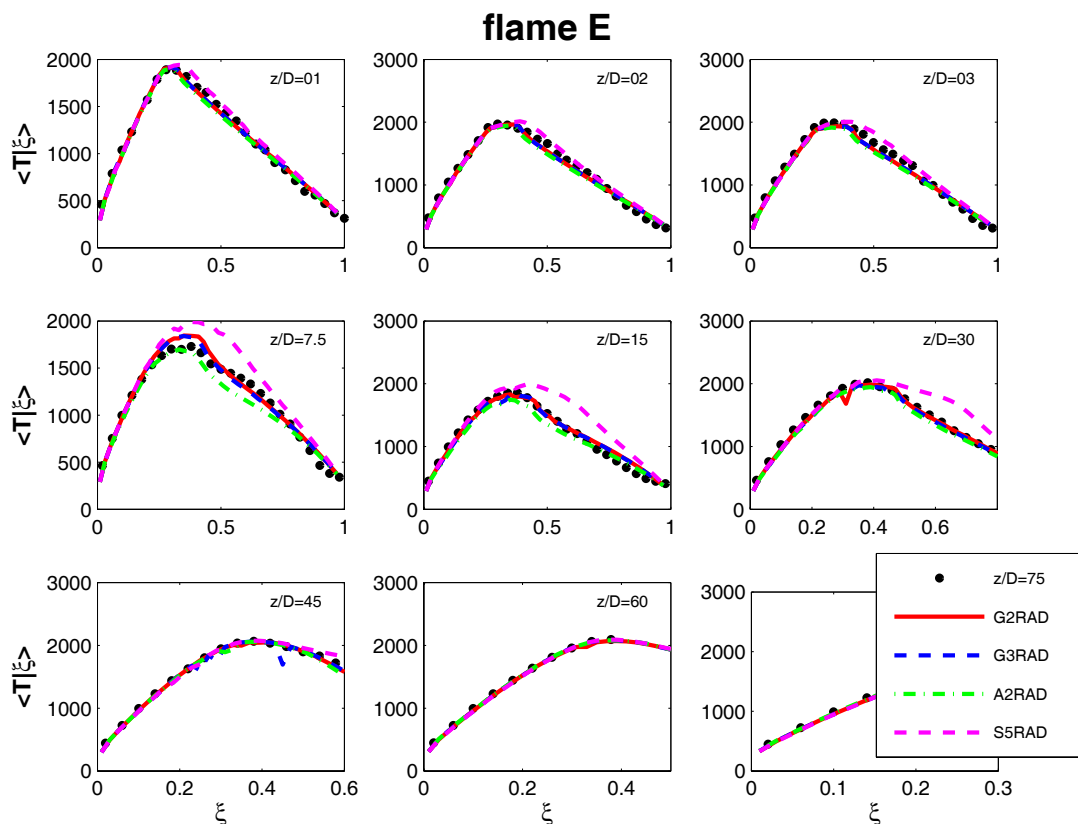


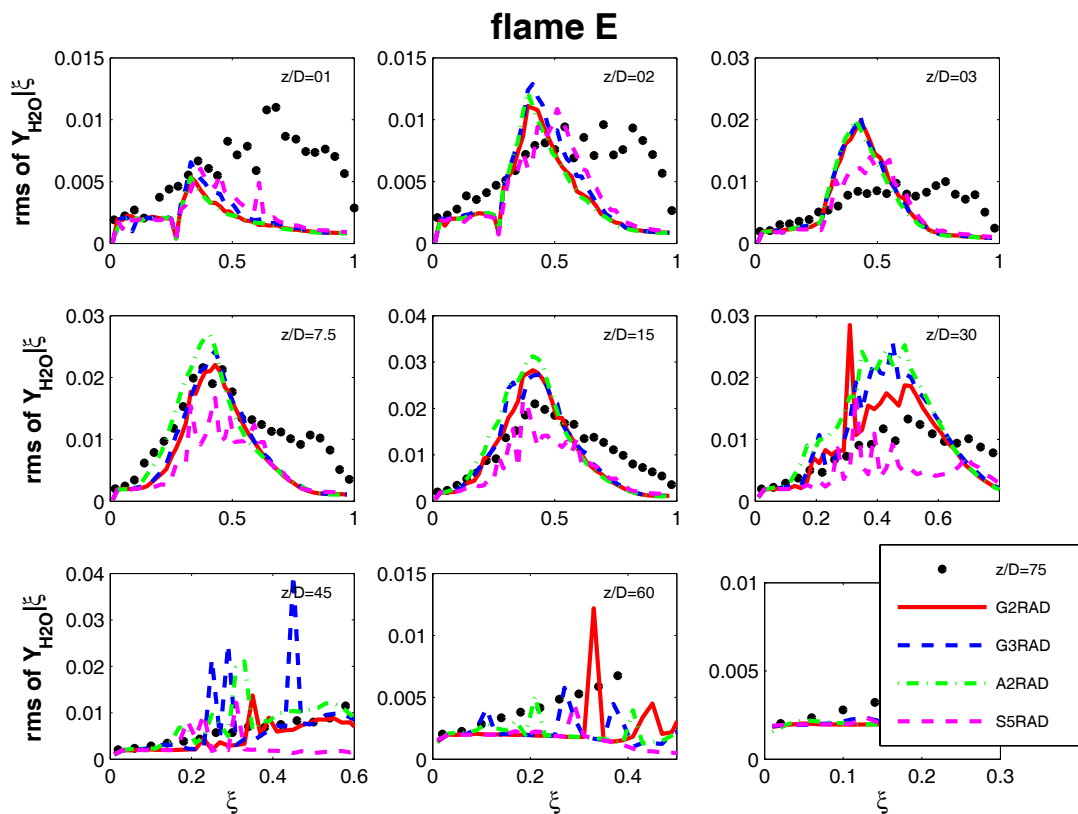
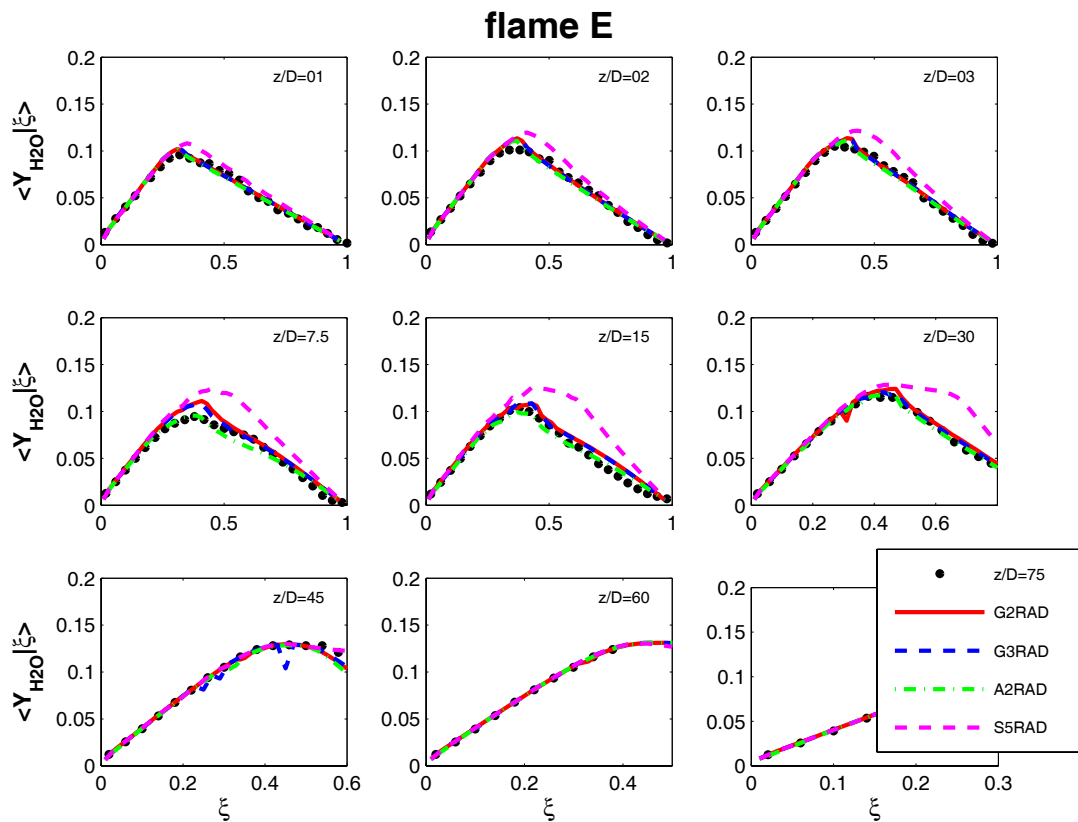


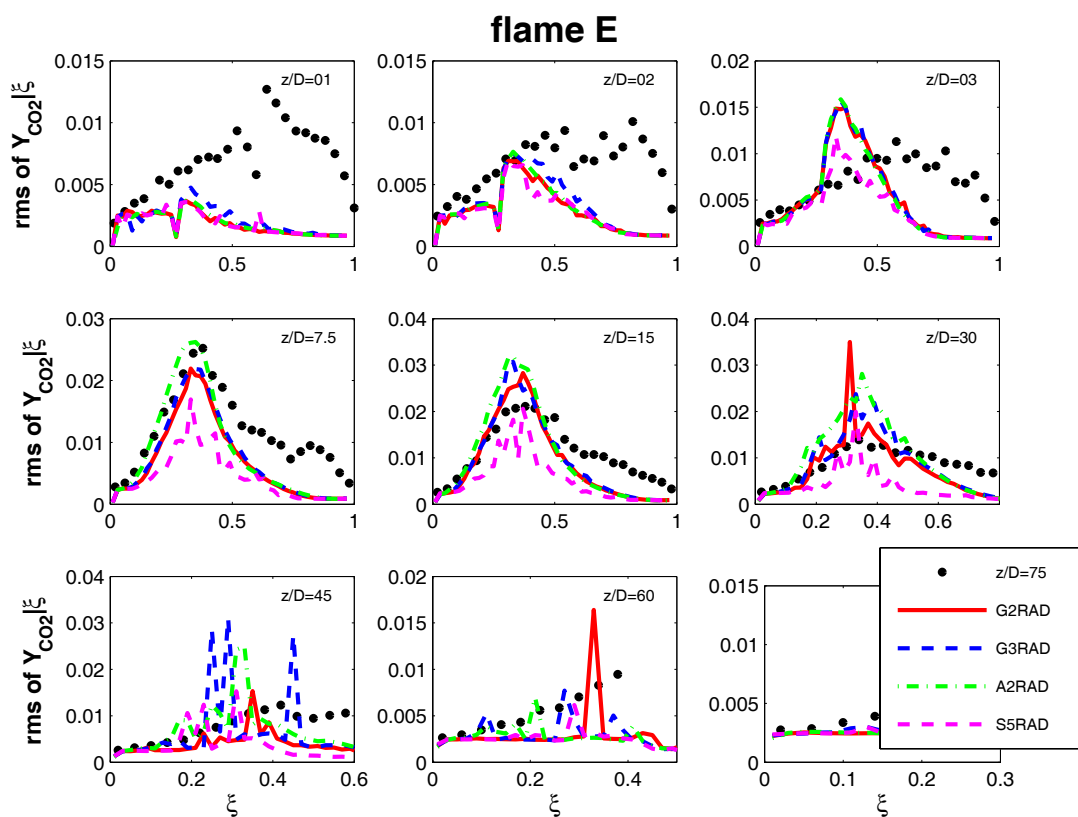
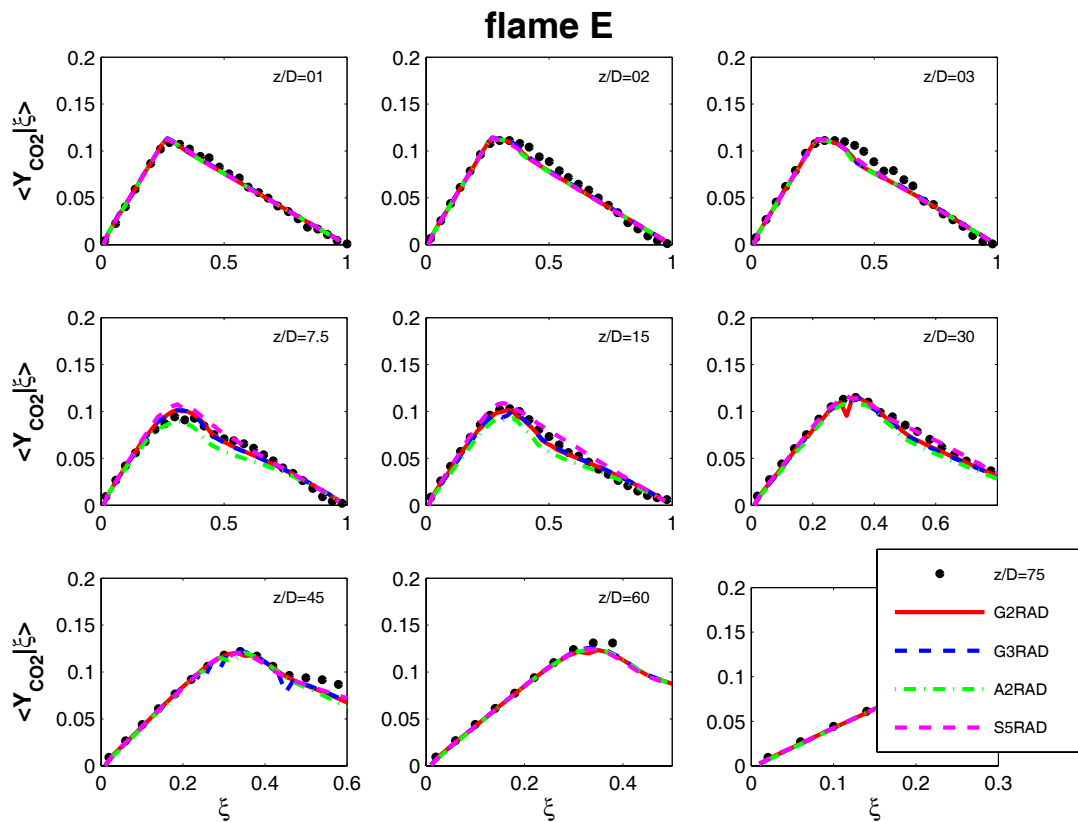


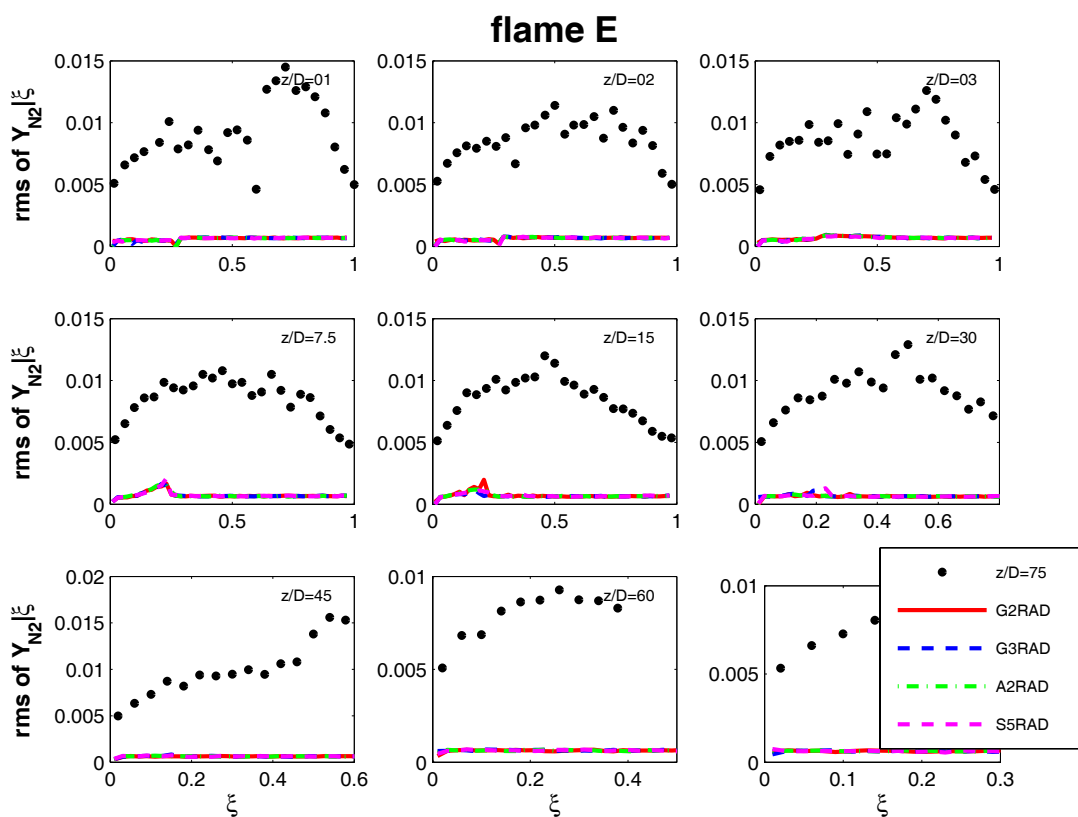
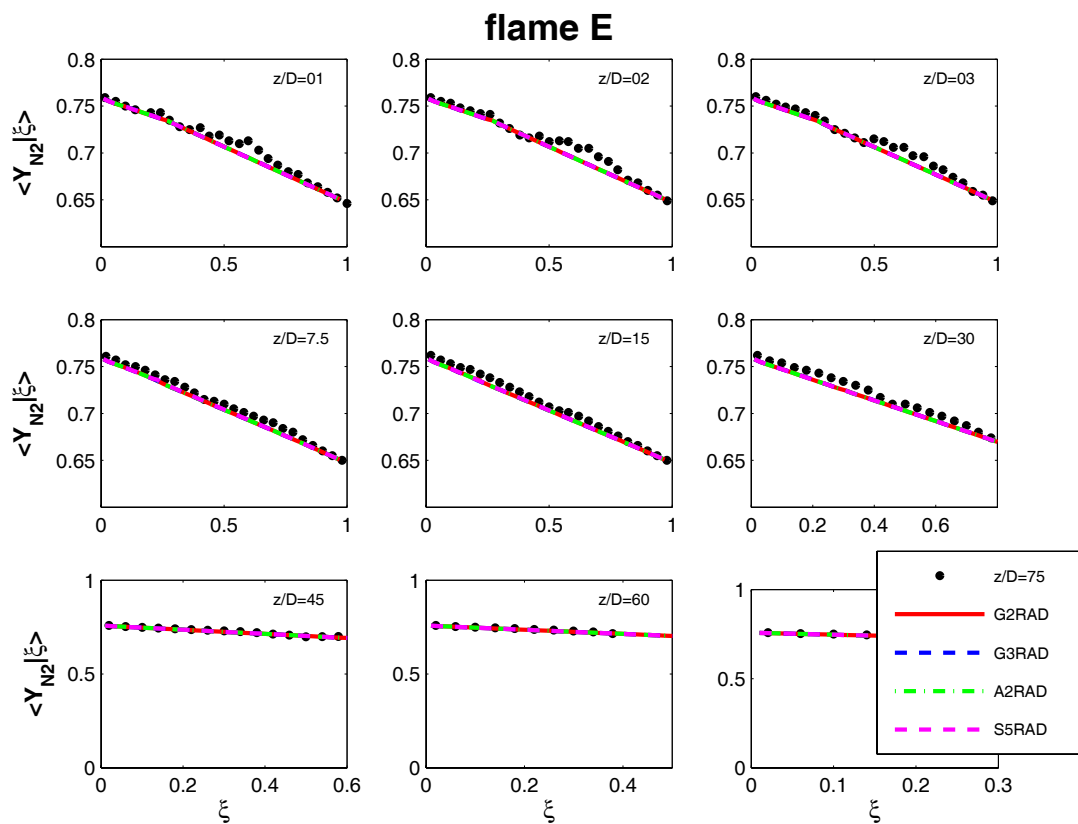


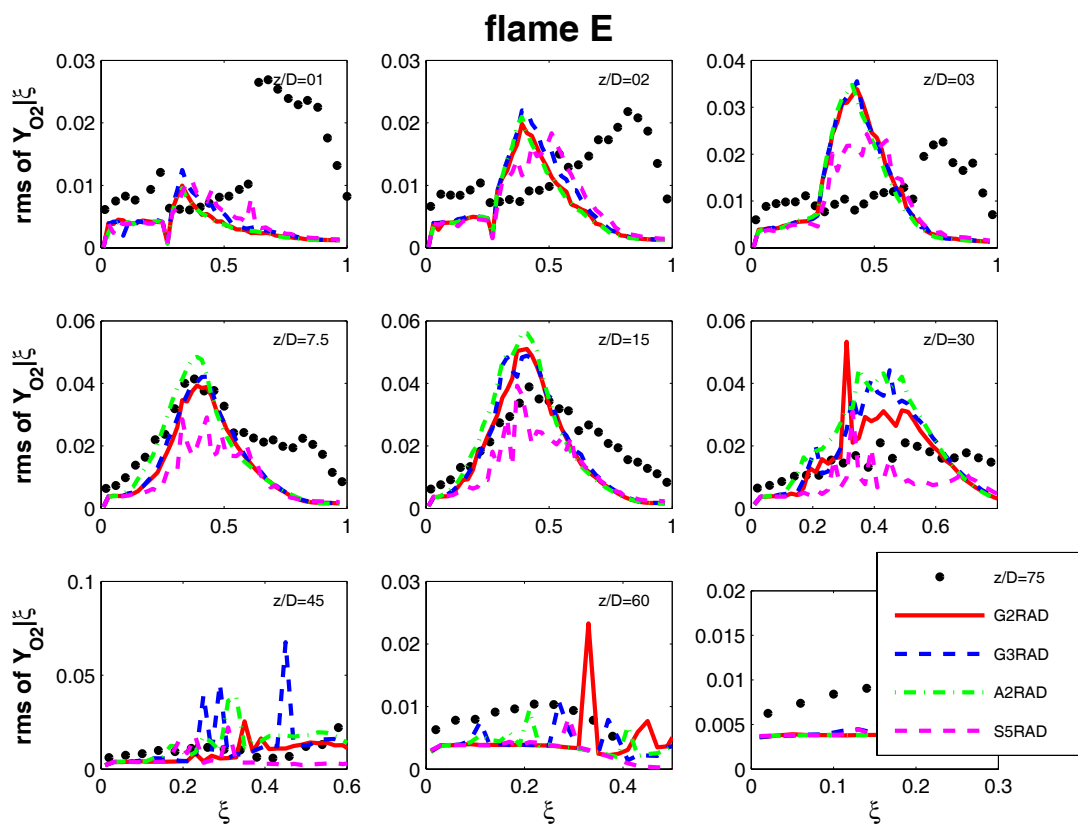
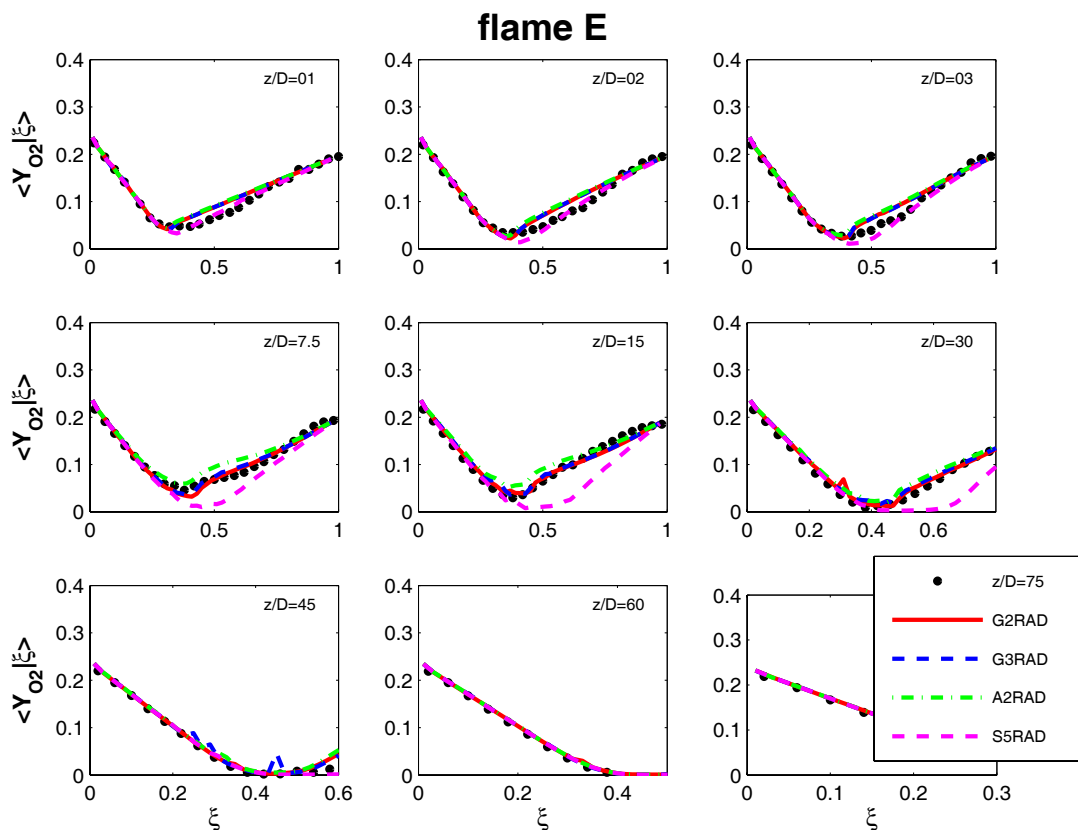
(3) Flame E with radiation (G2, G3, A2, S5)

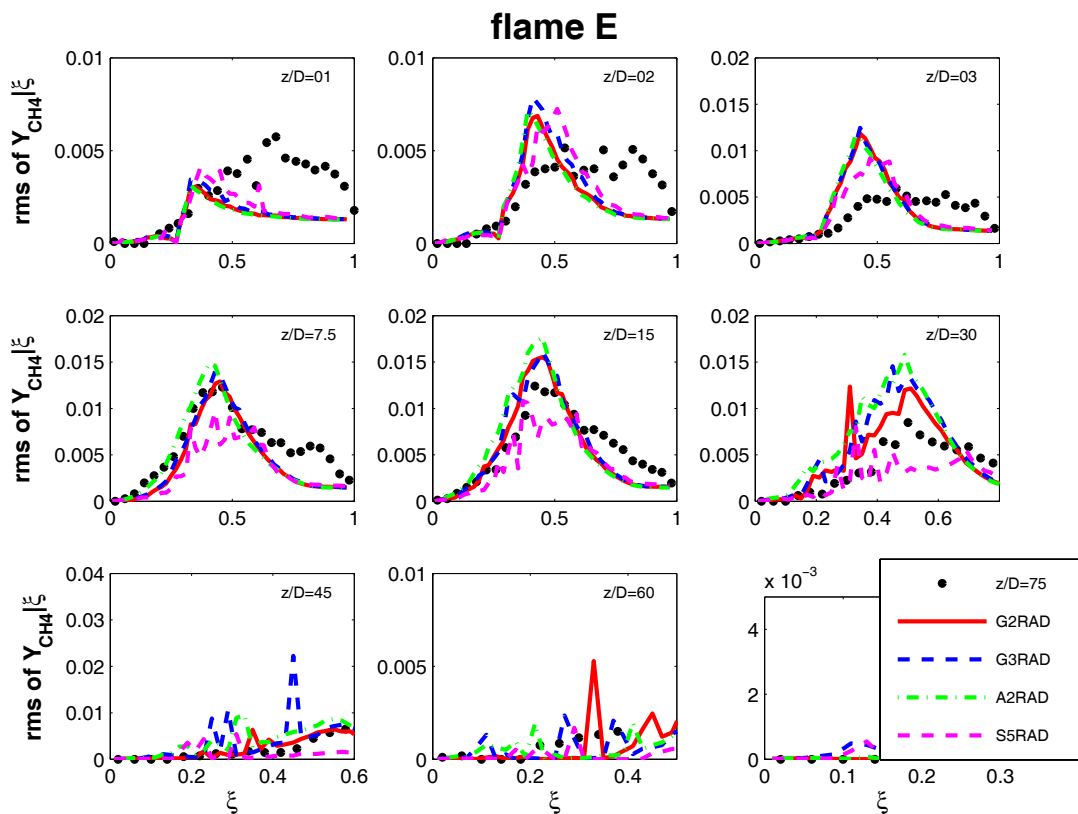
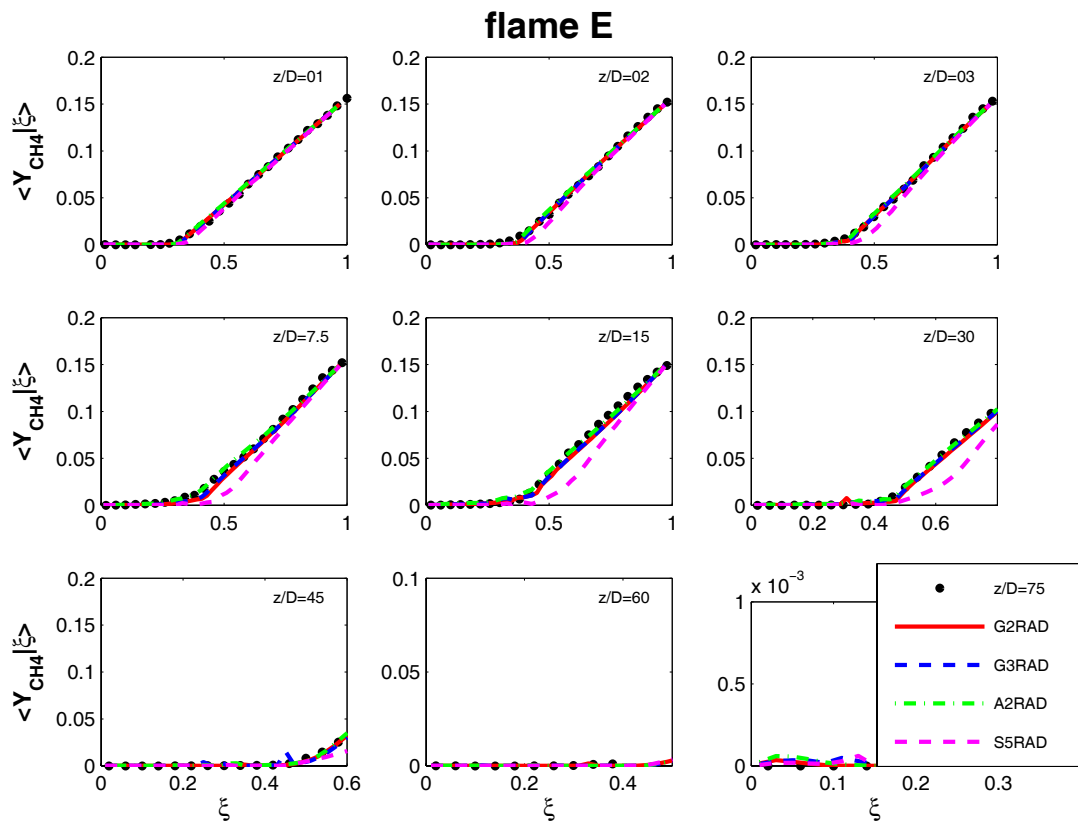


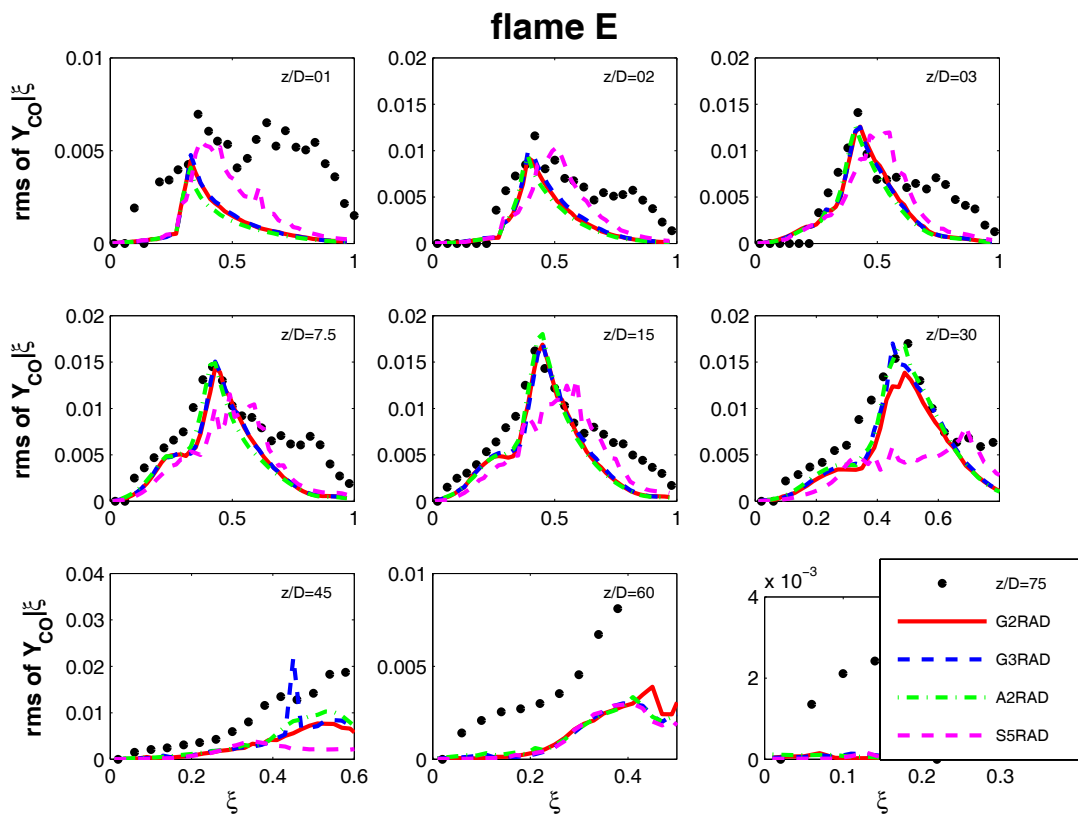
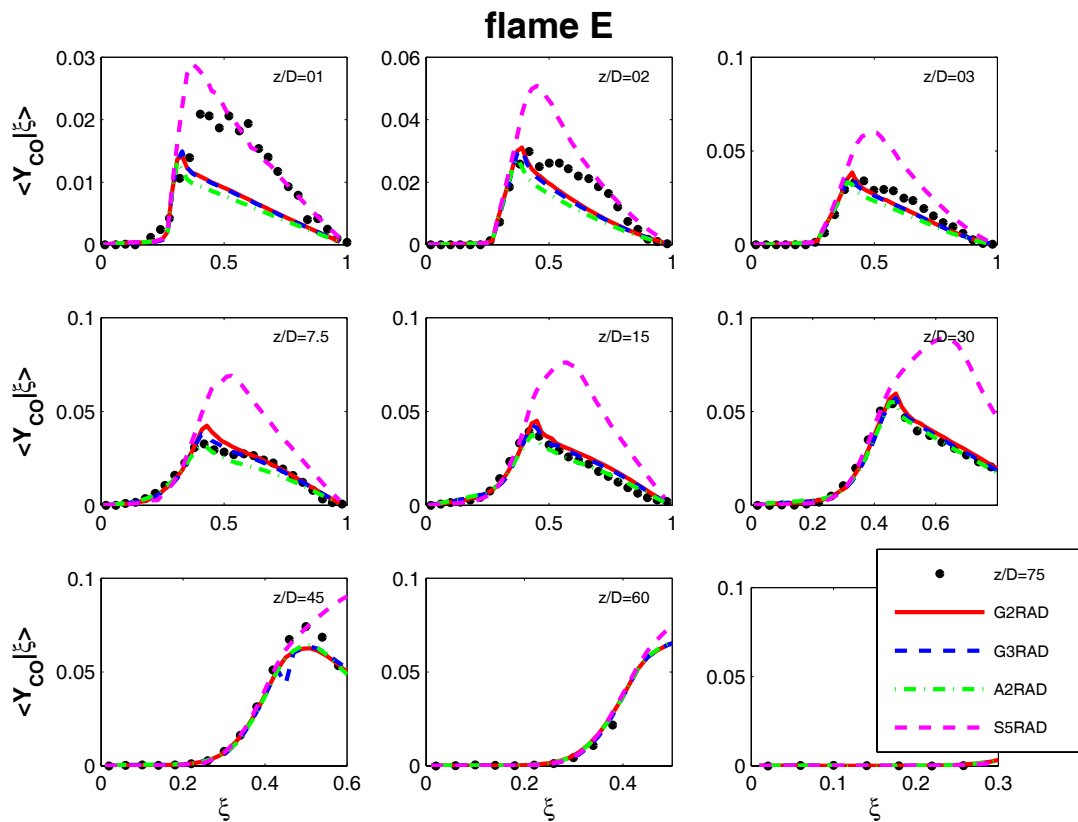


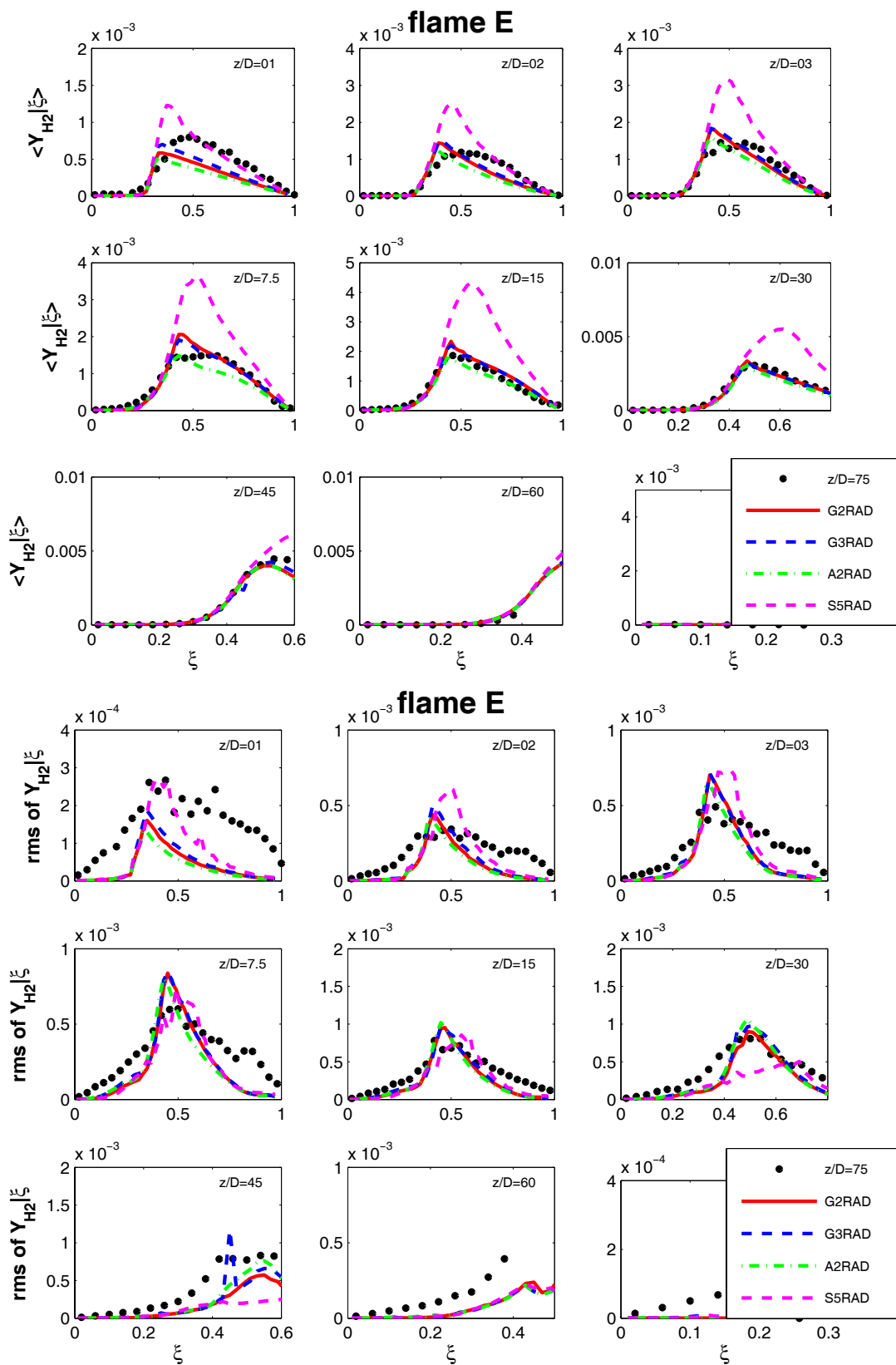


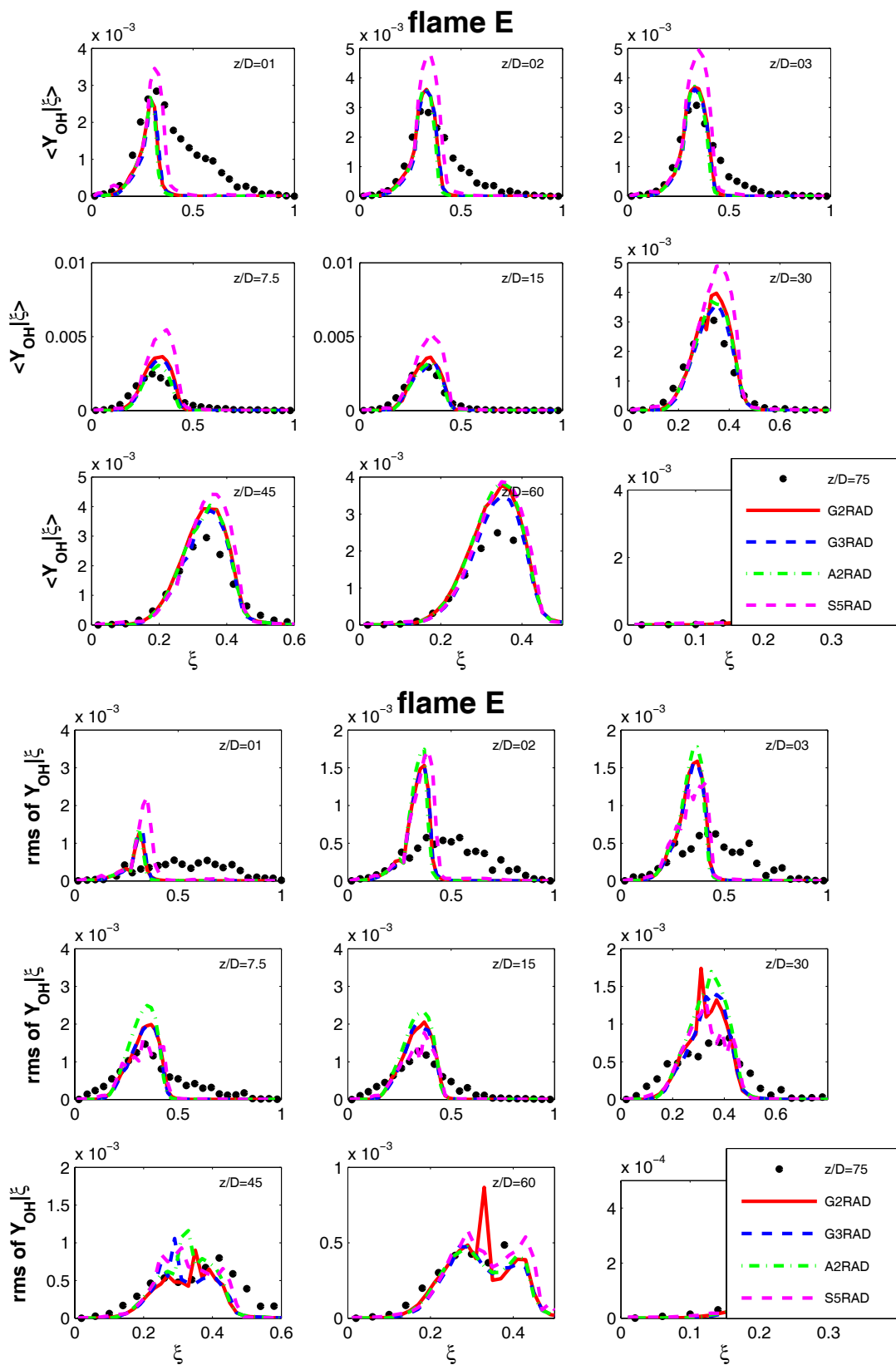


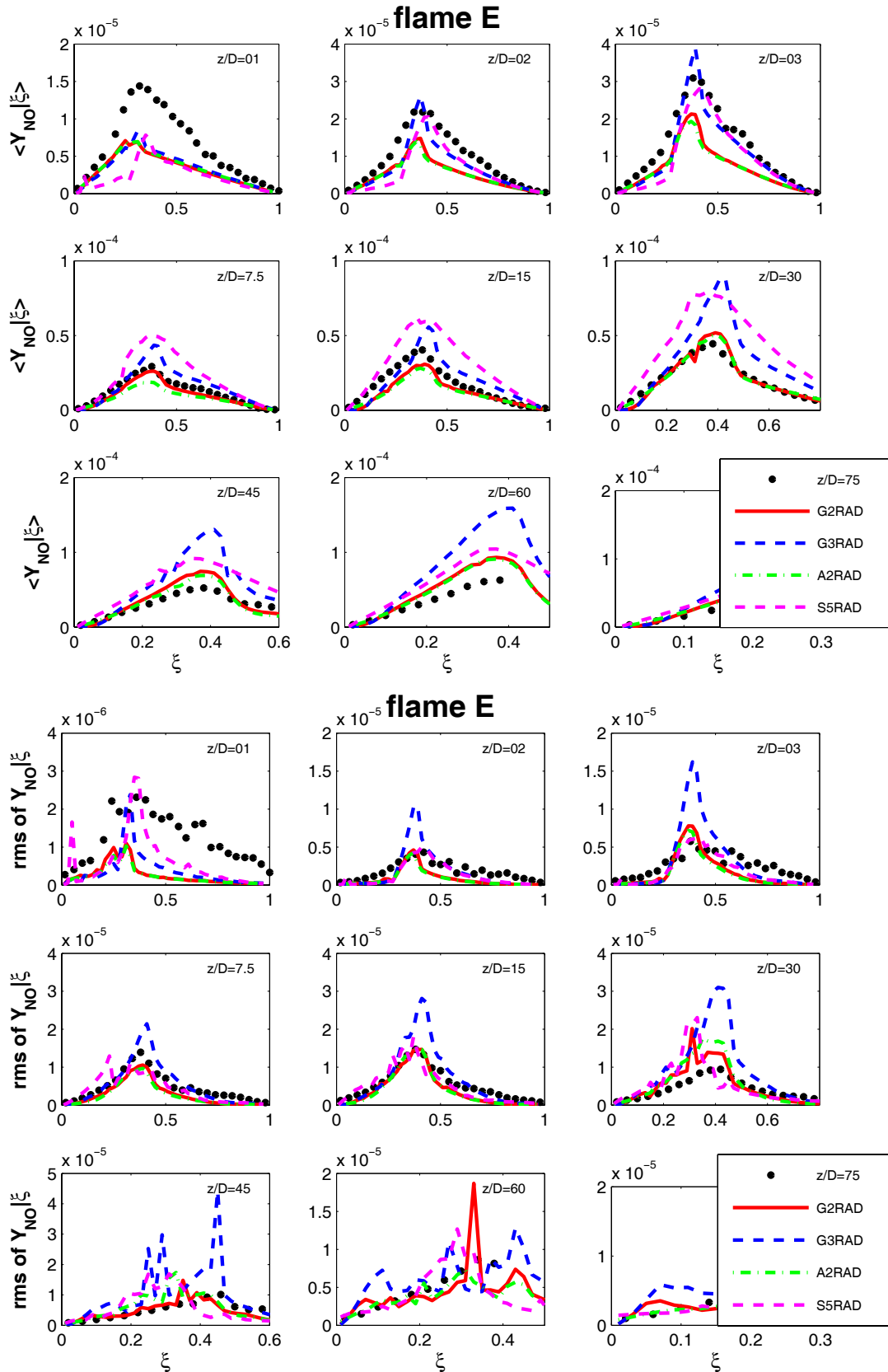




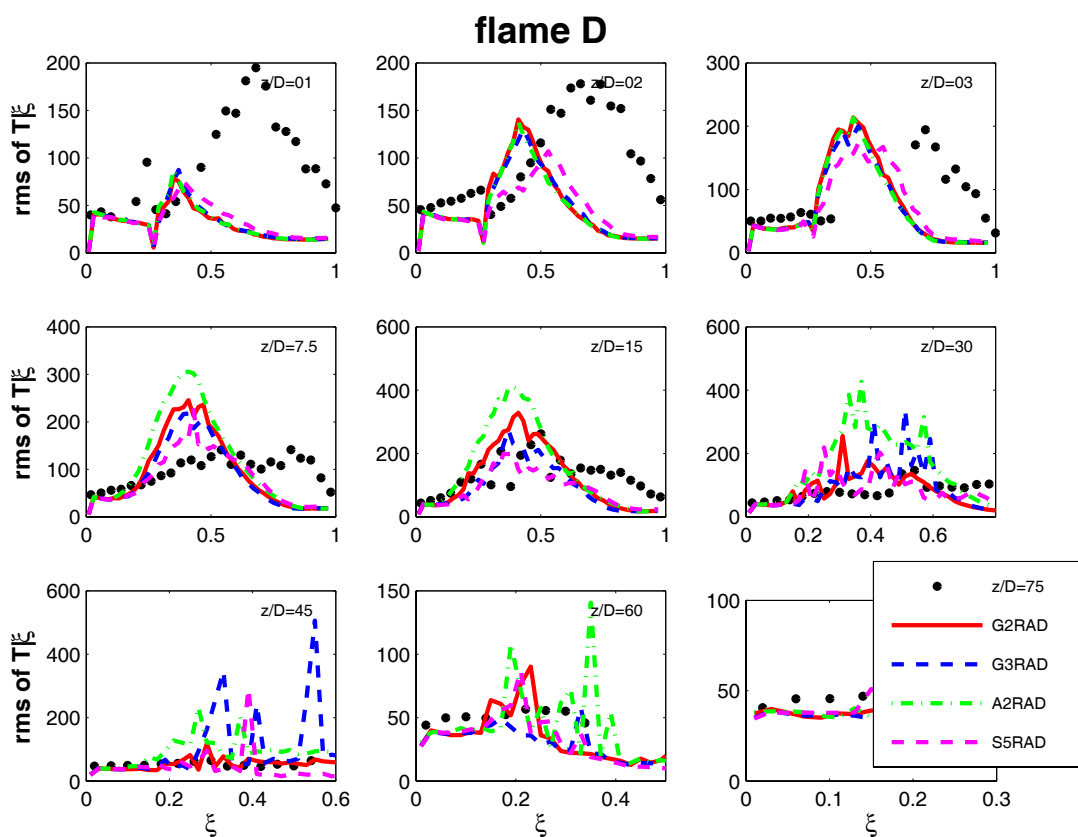
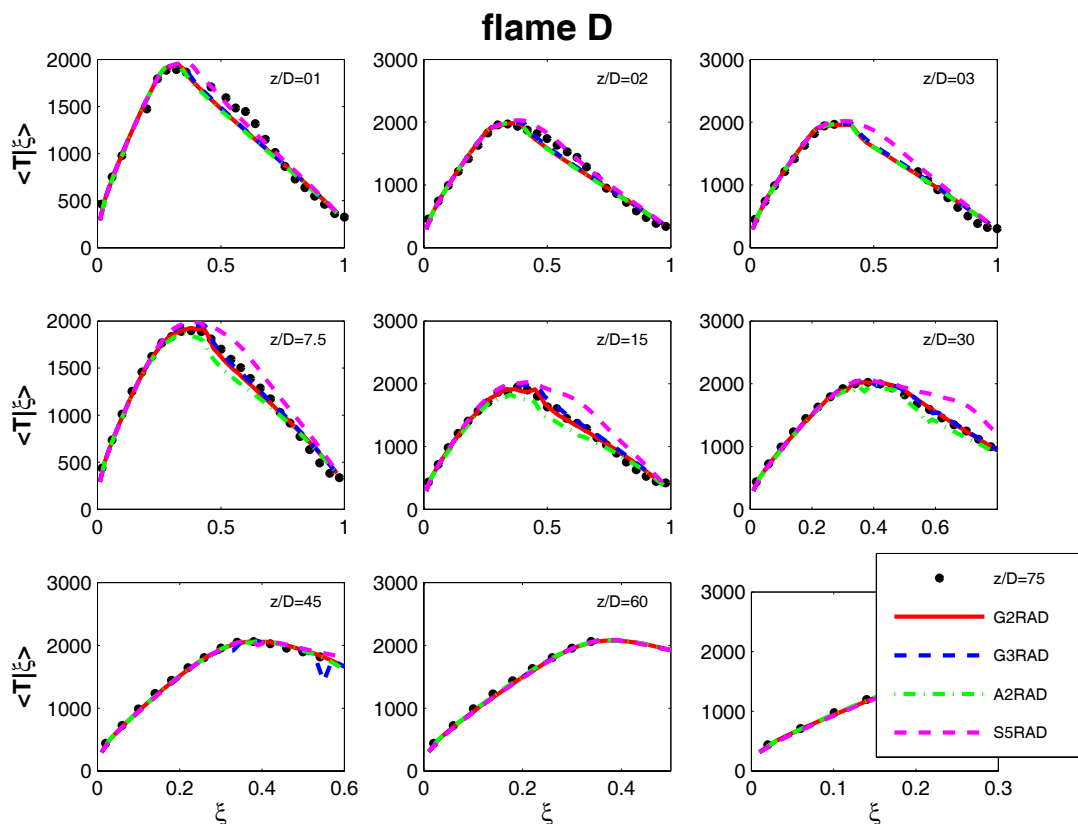


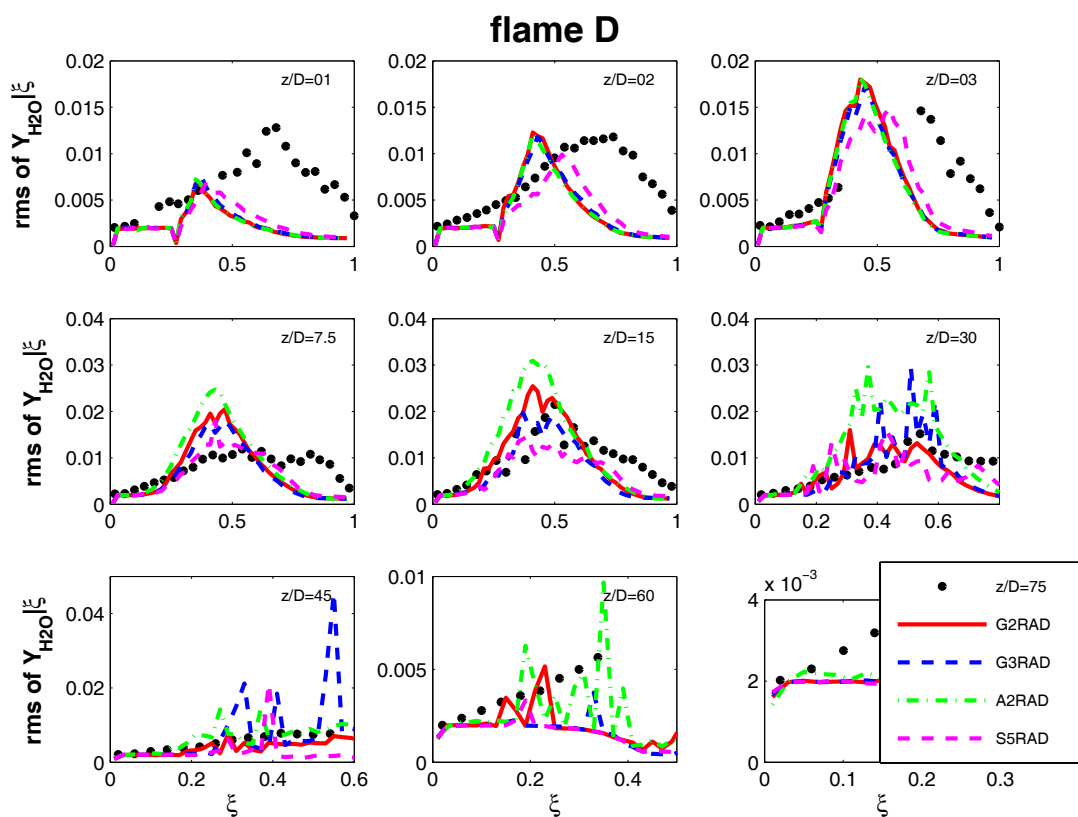
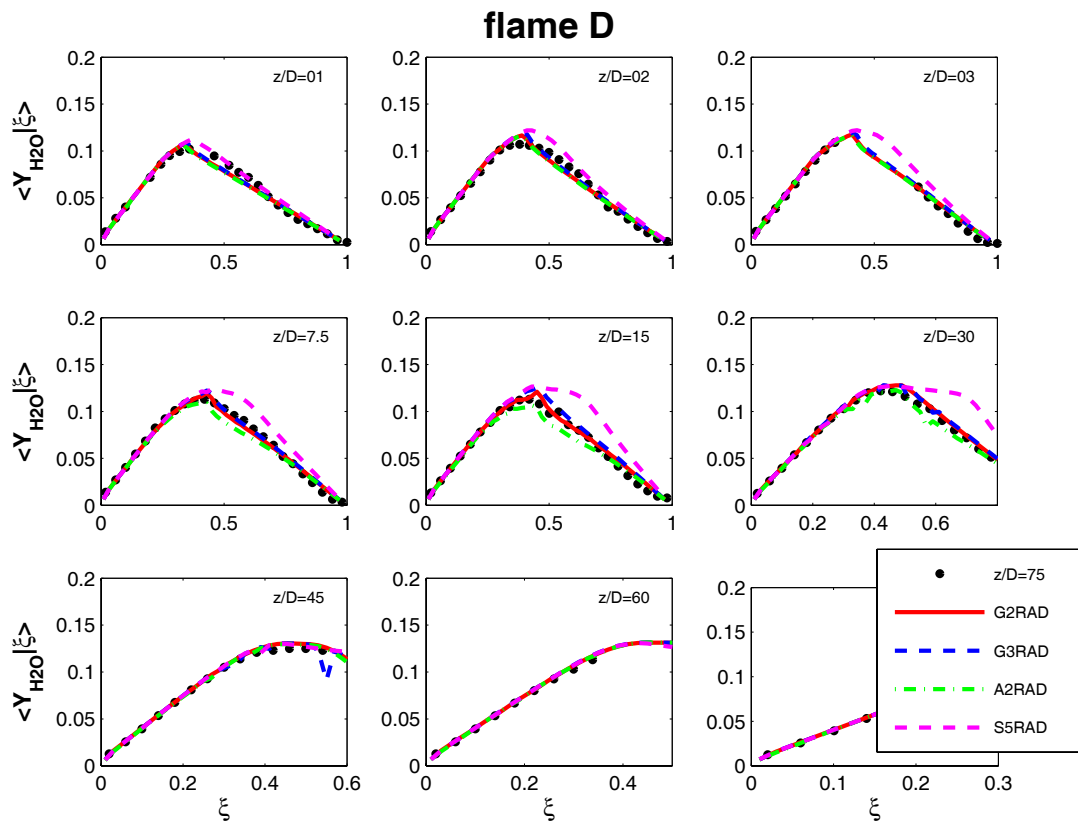


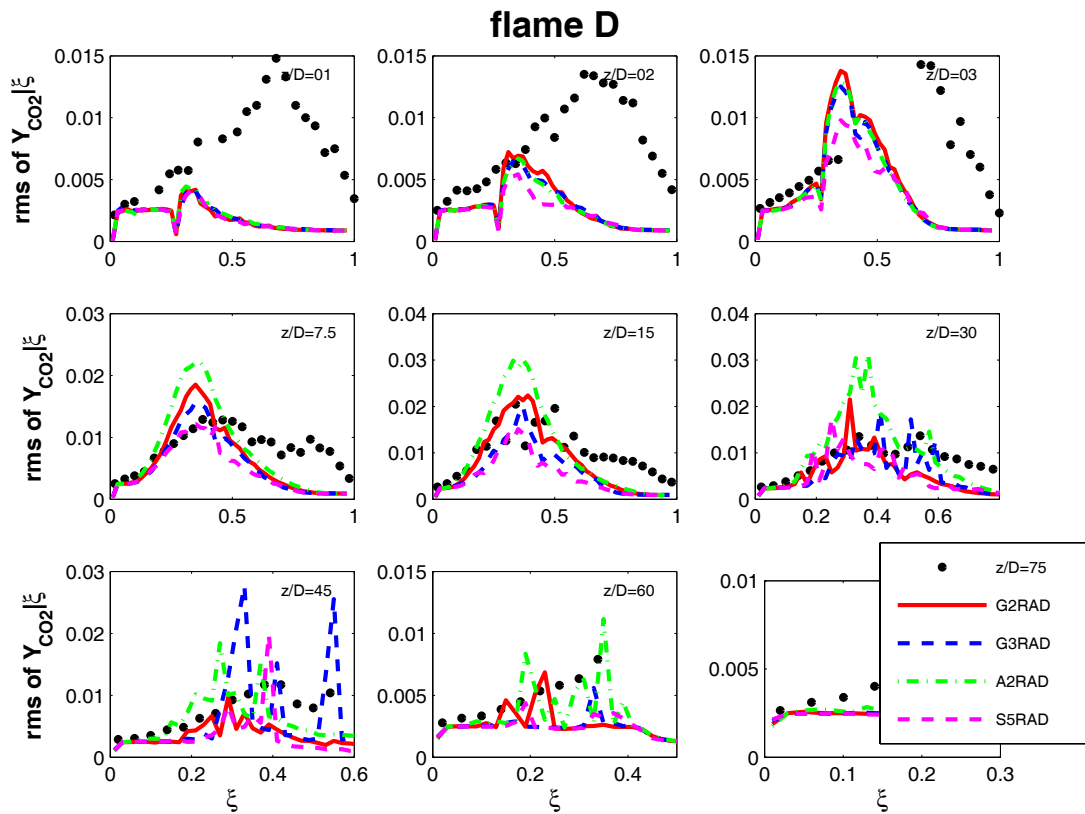
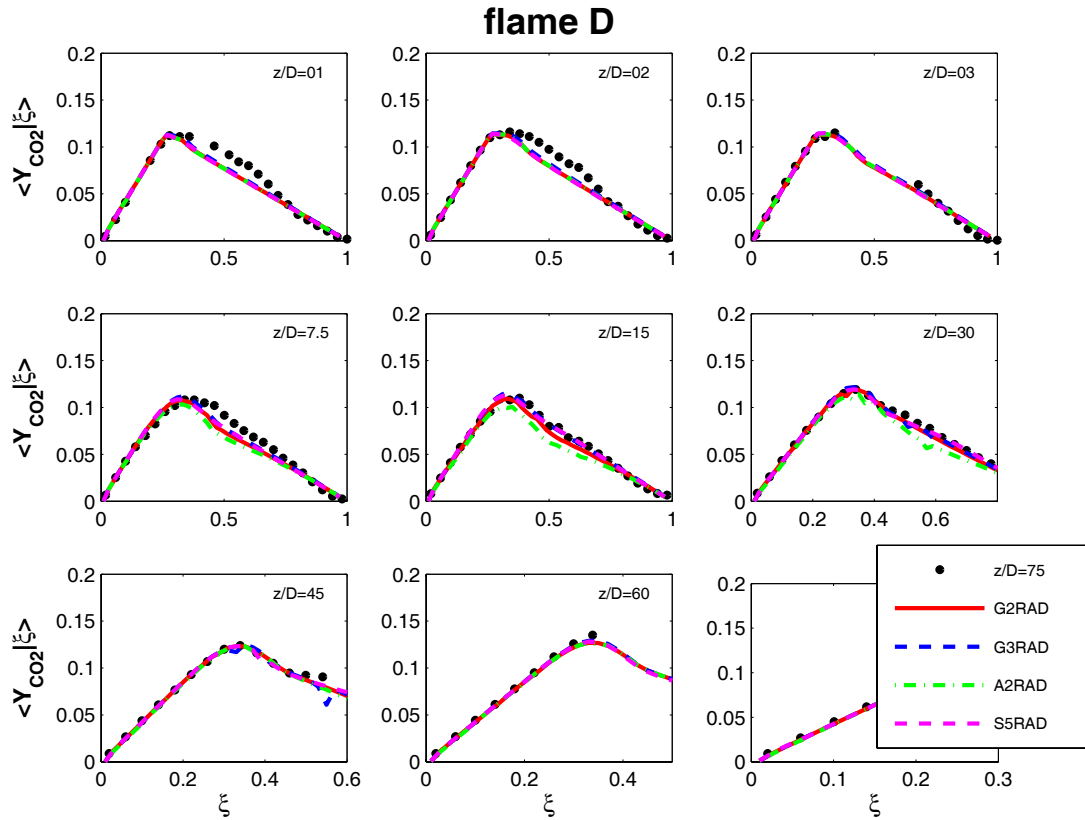


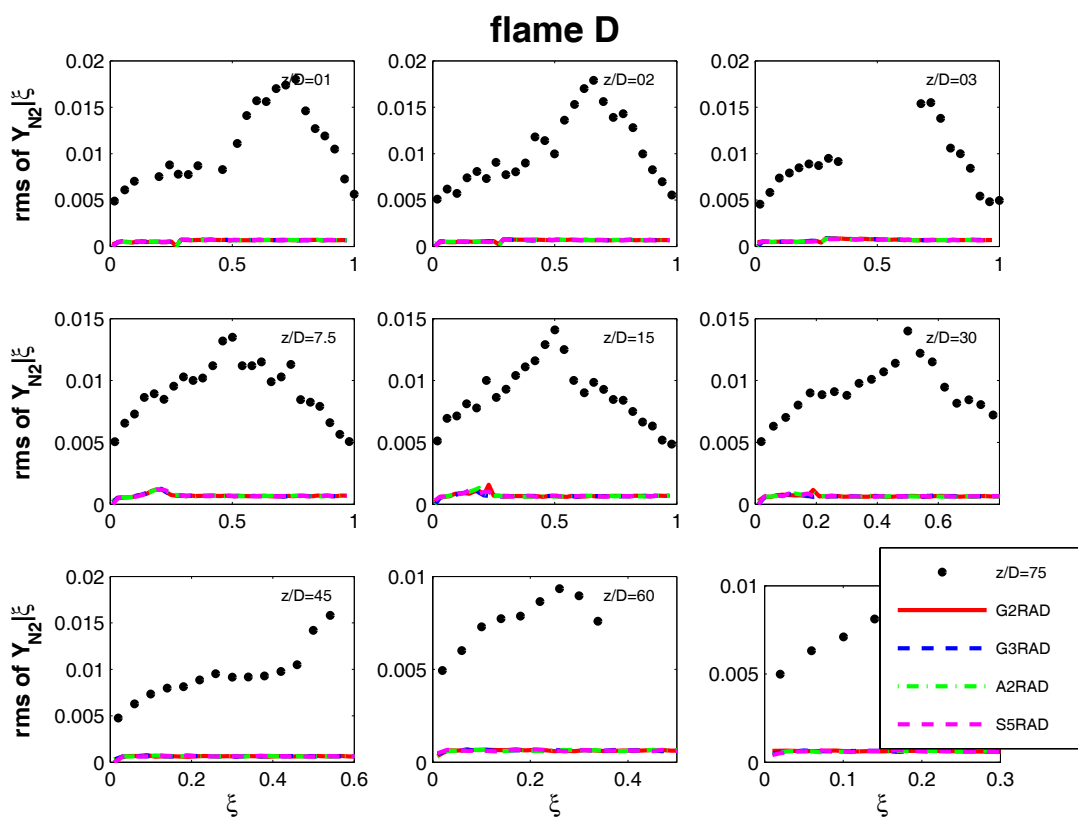
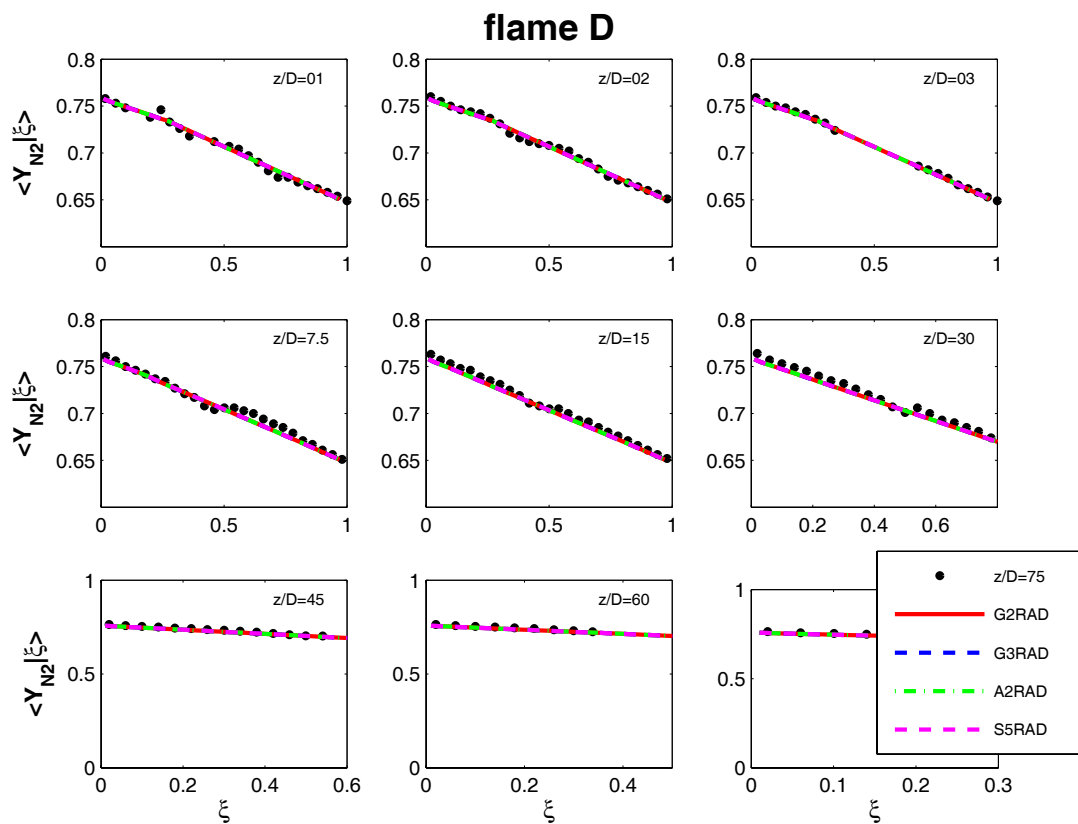


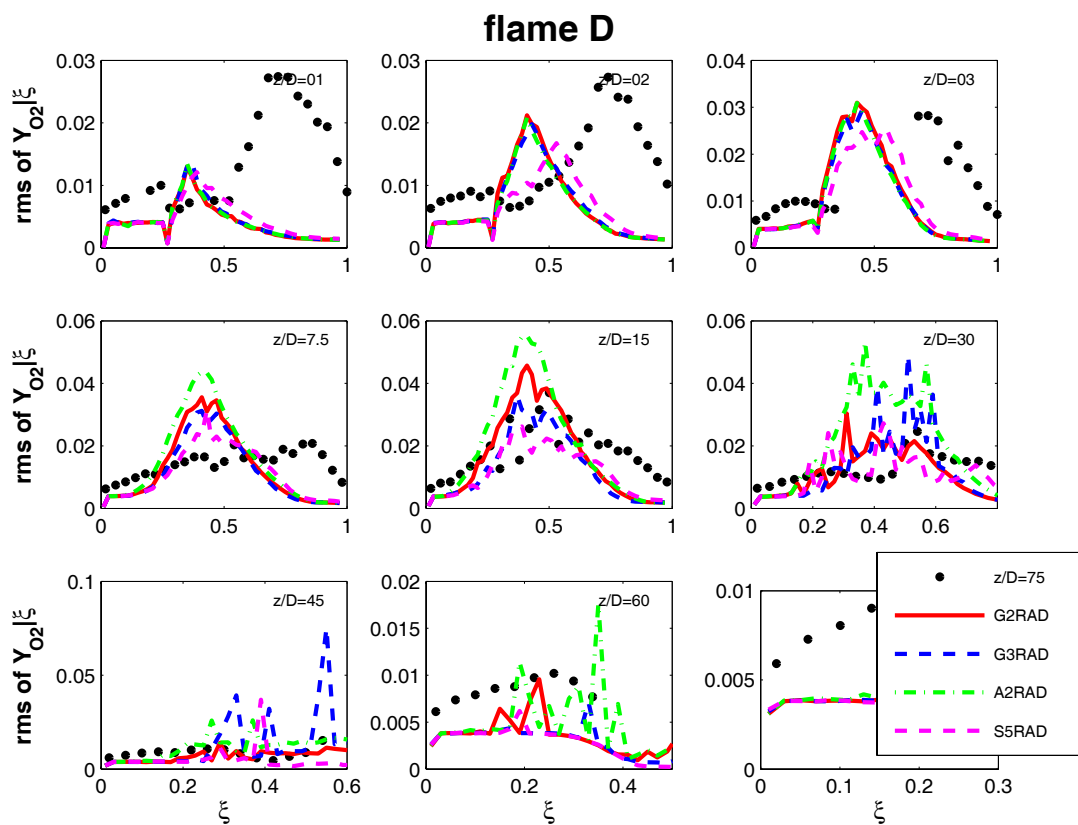
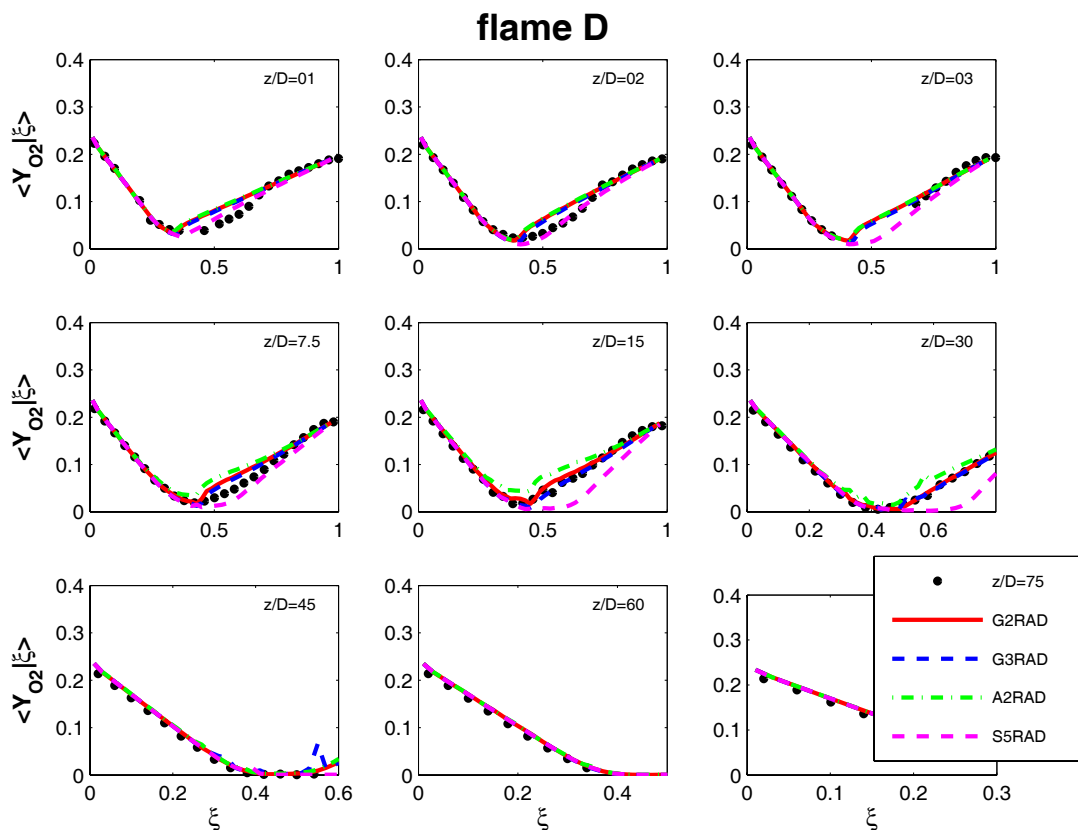
(4) Flame D with radiation (G2, G3, A2, S5)

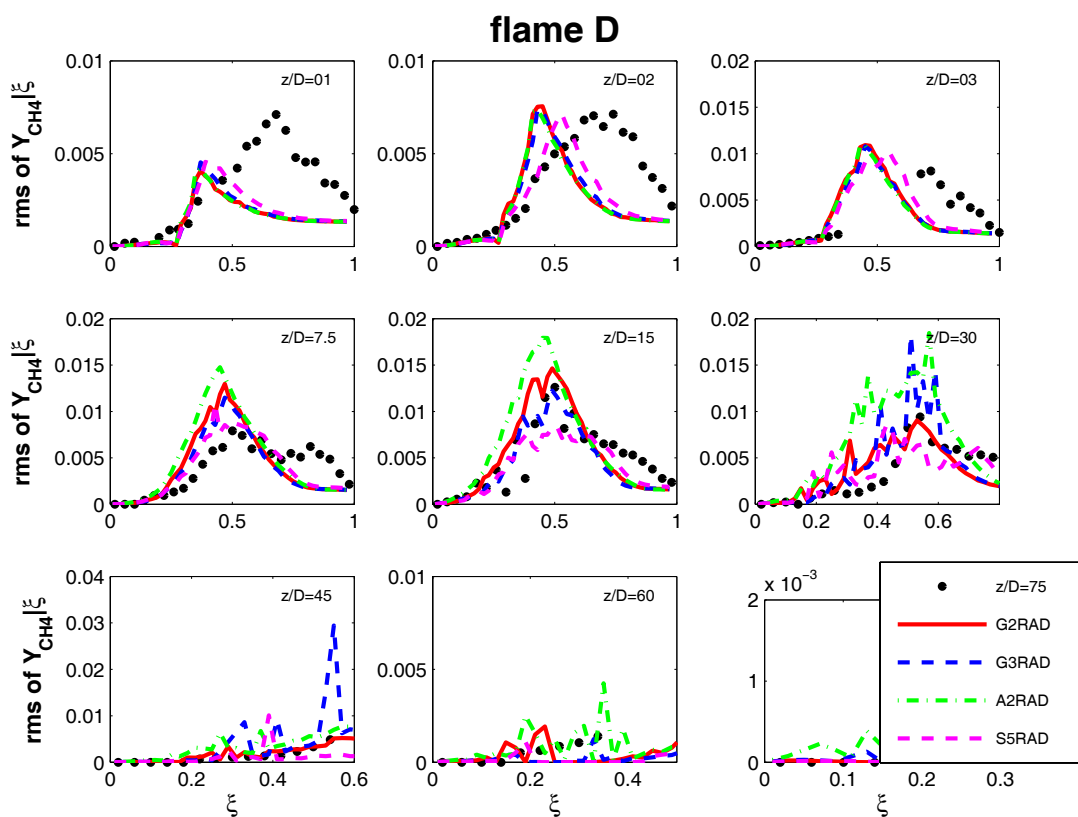
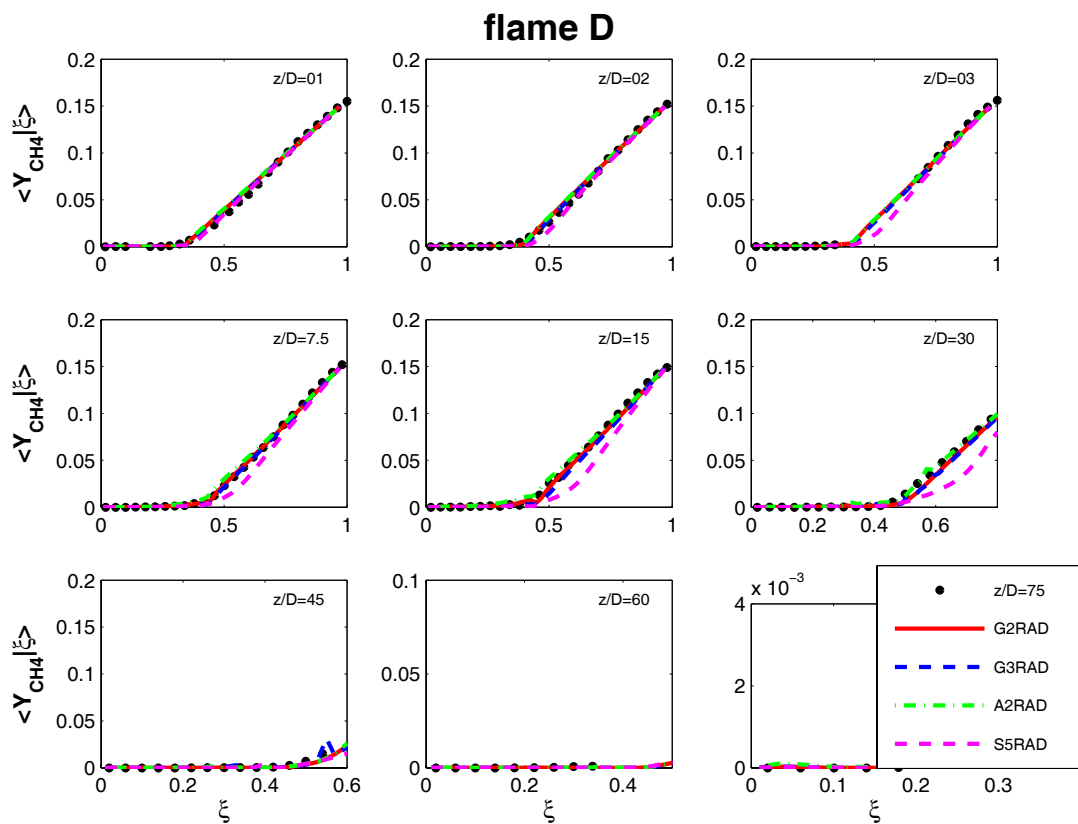


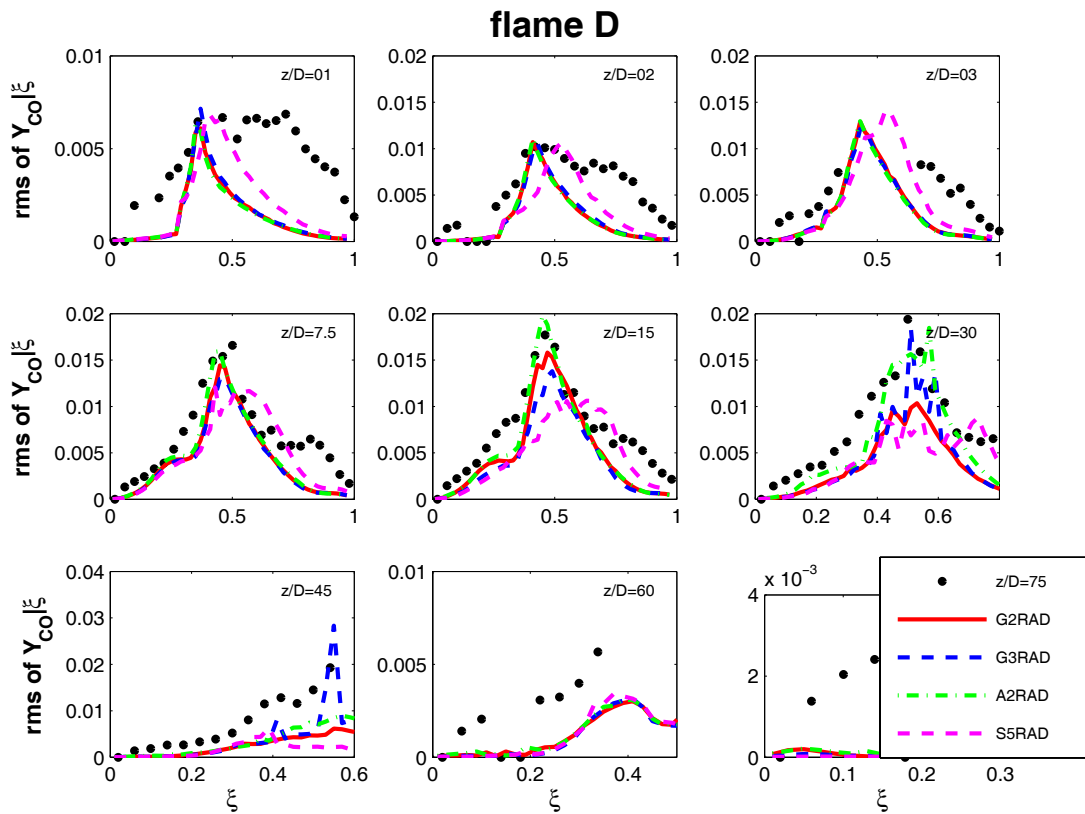
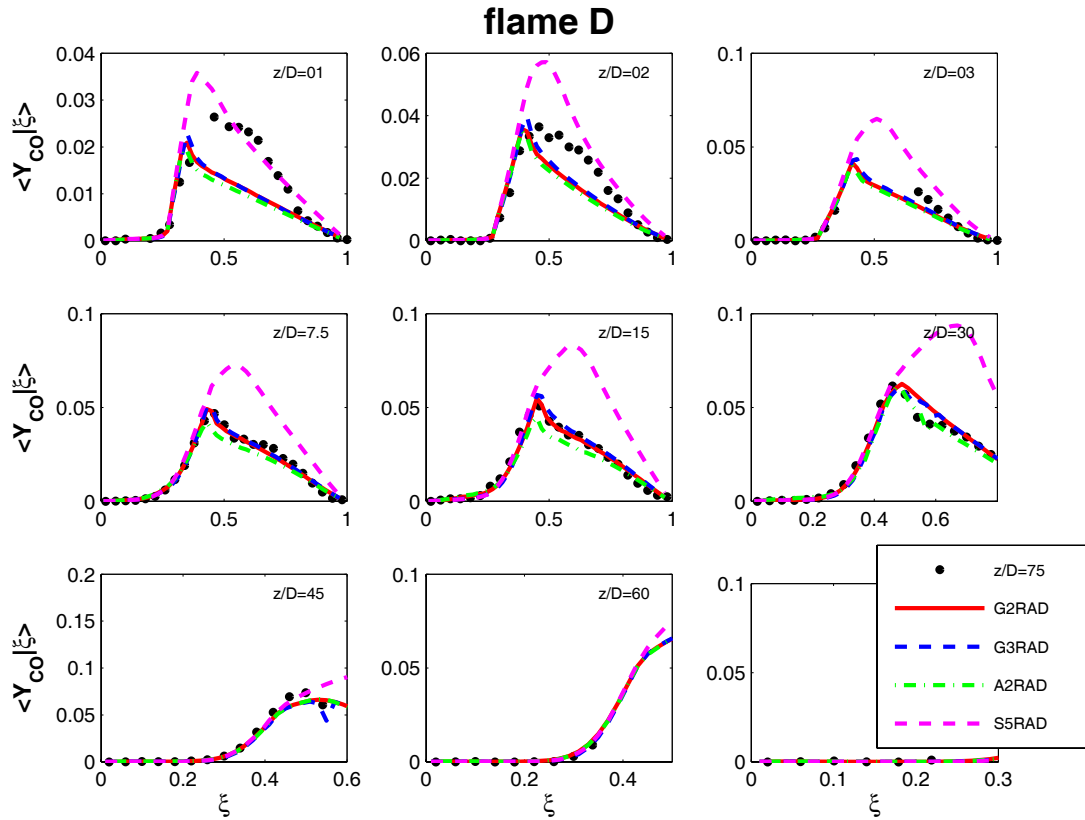


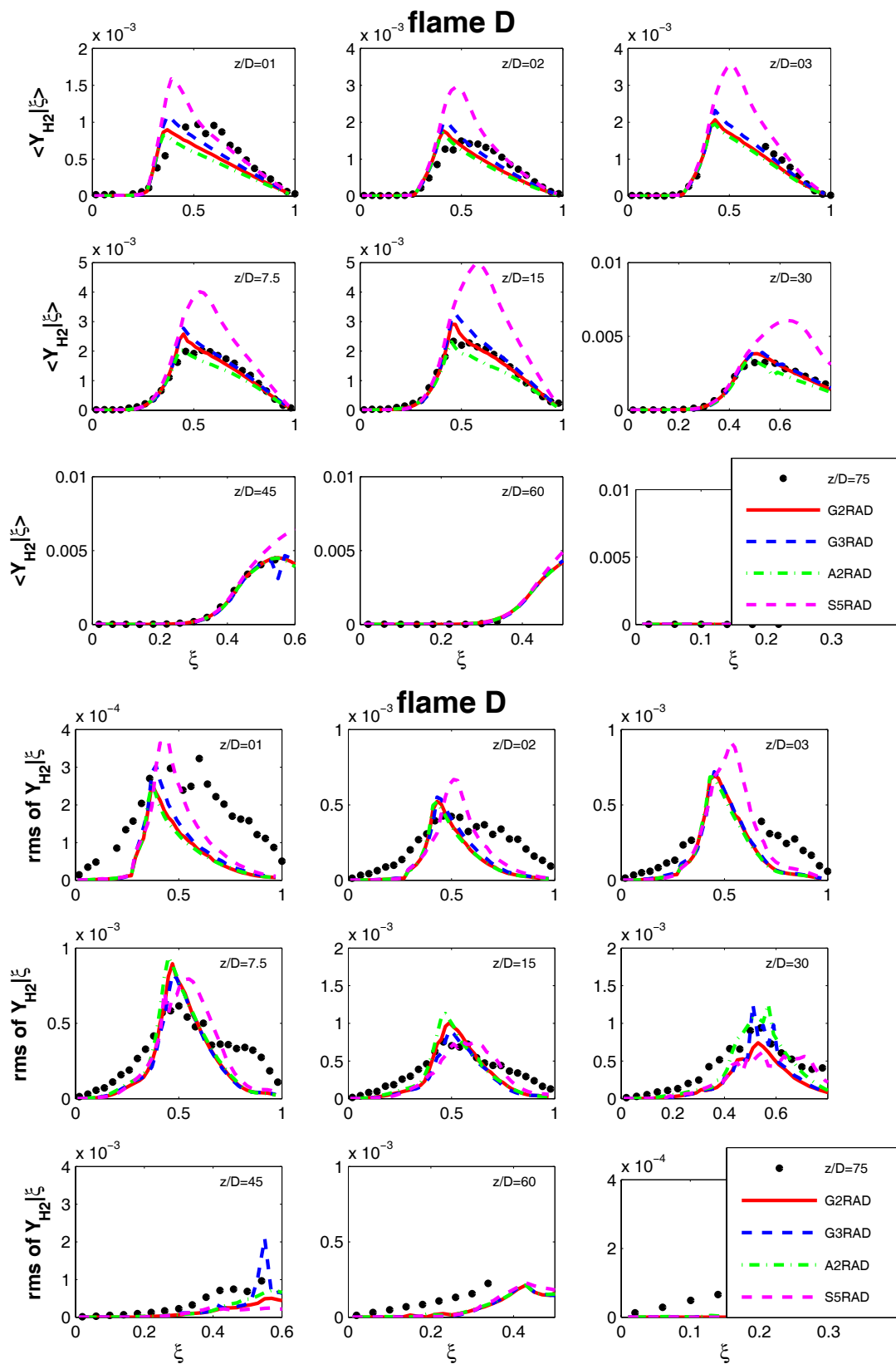


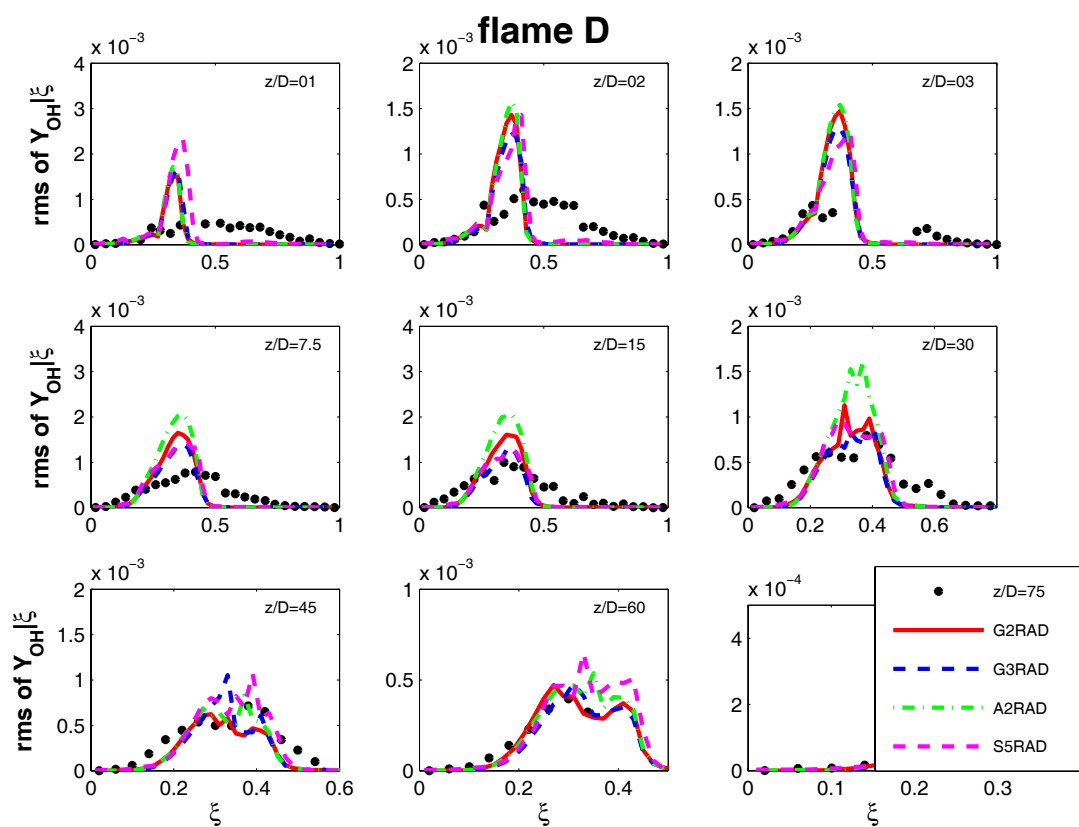
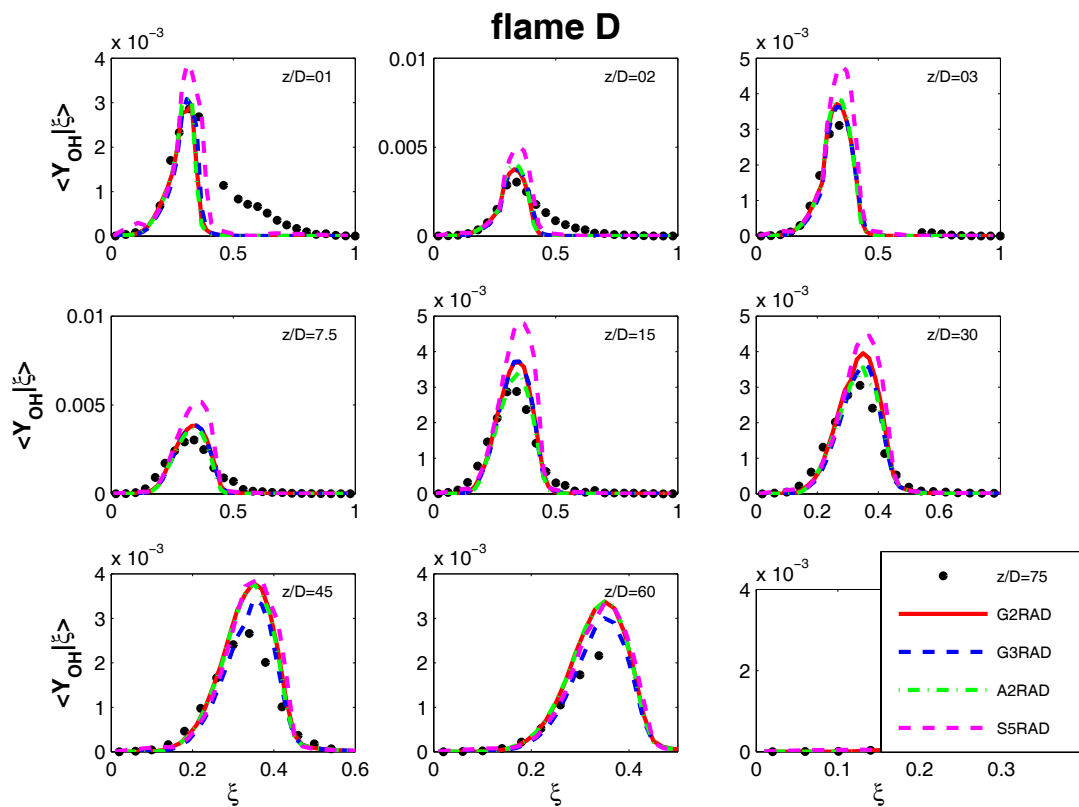


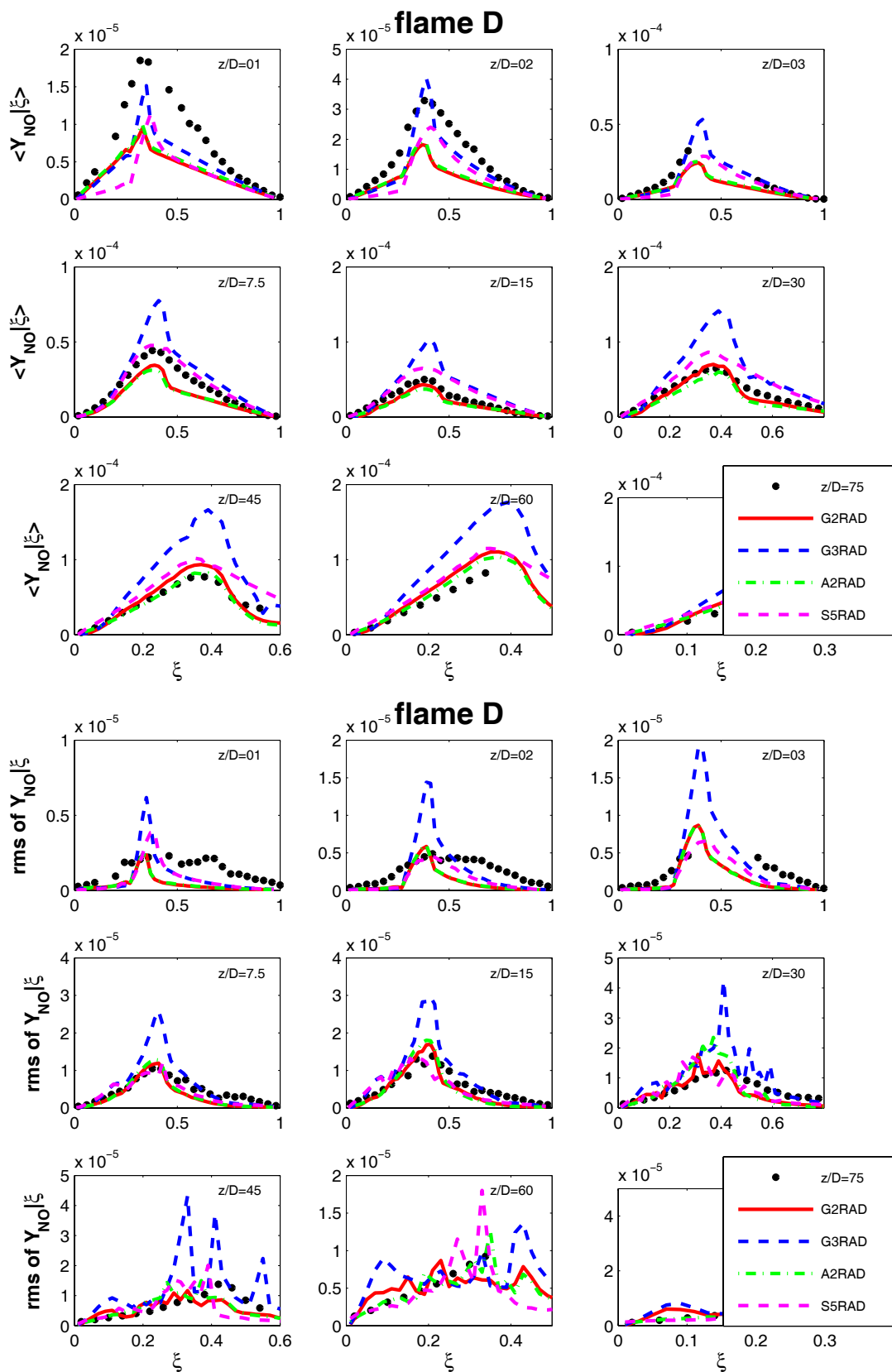




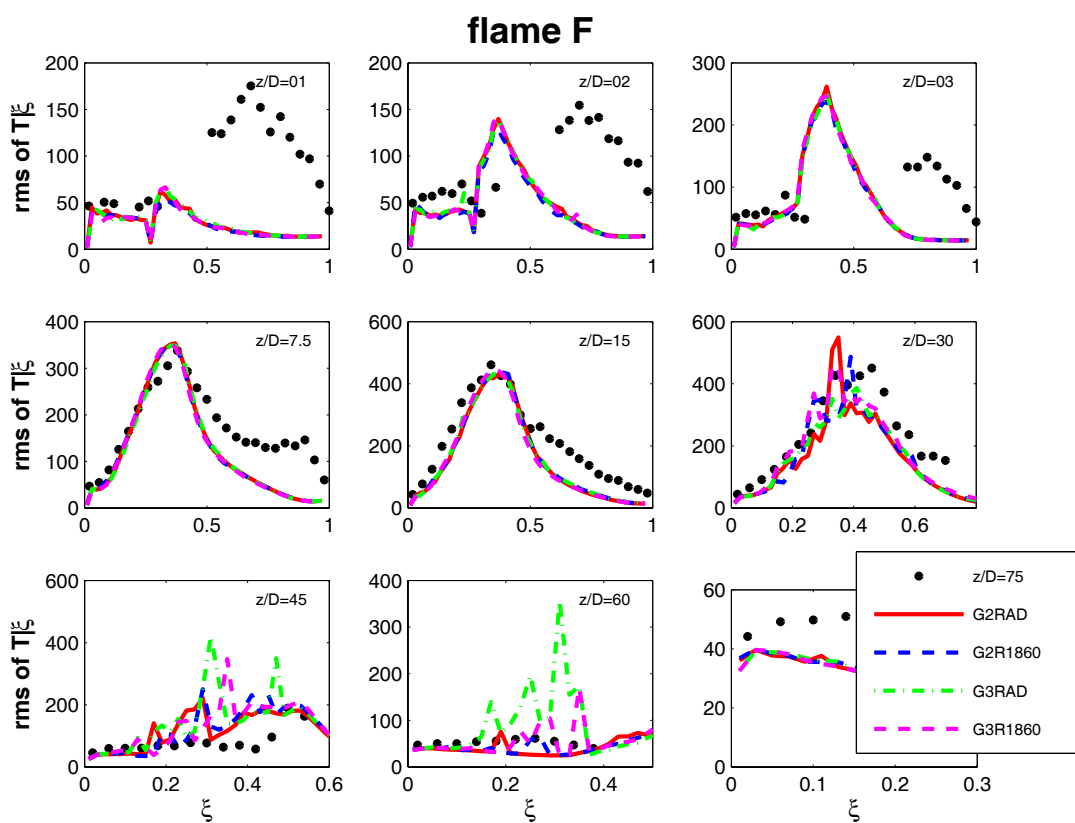
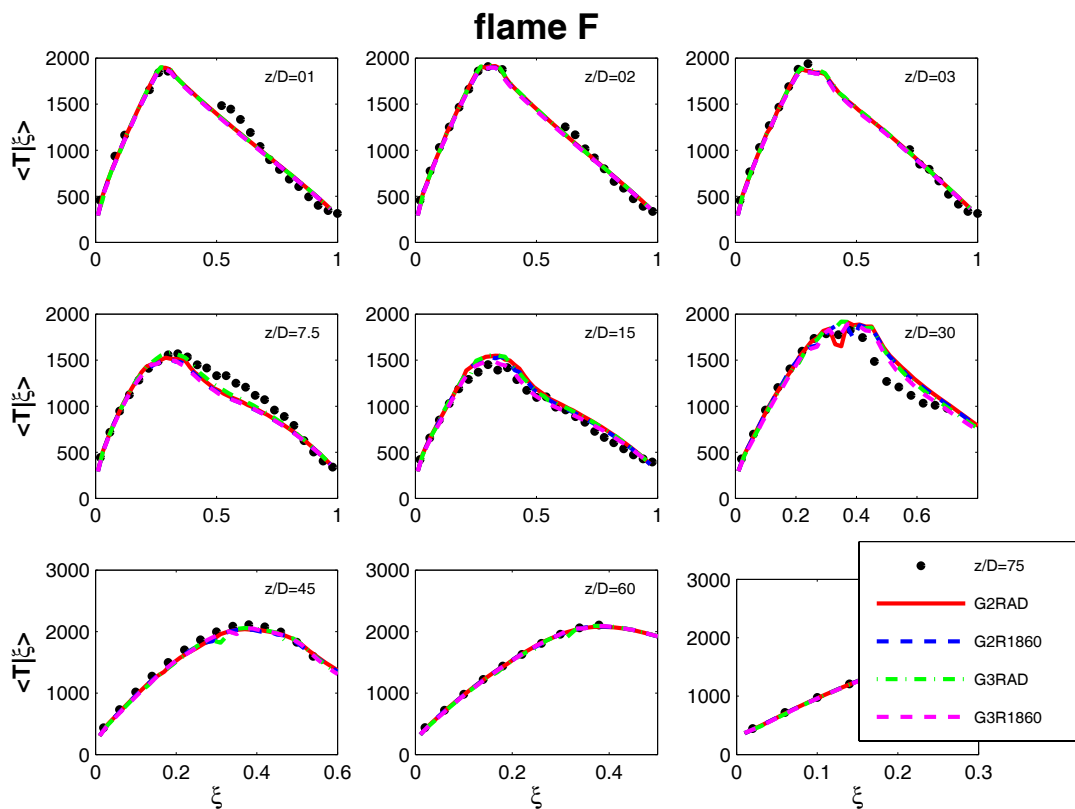


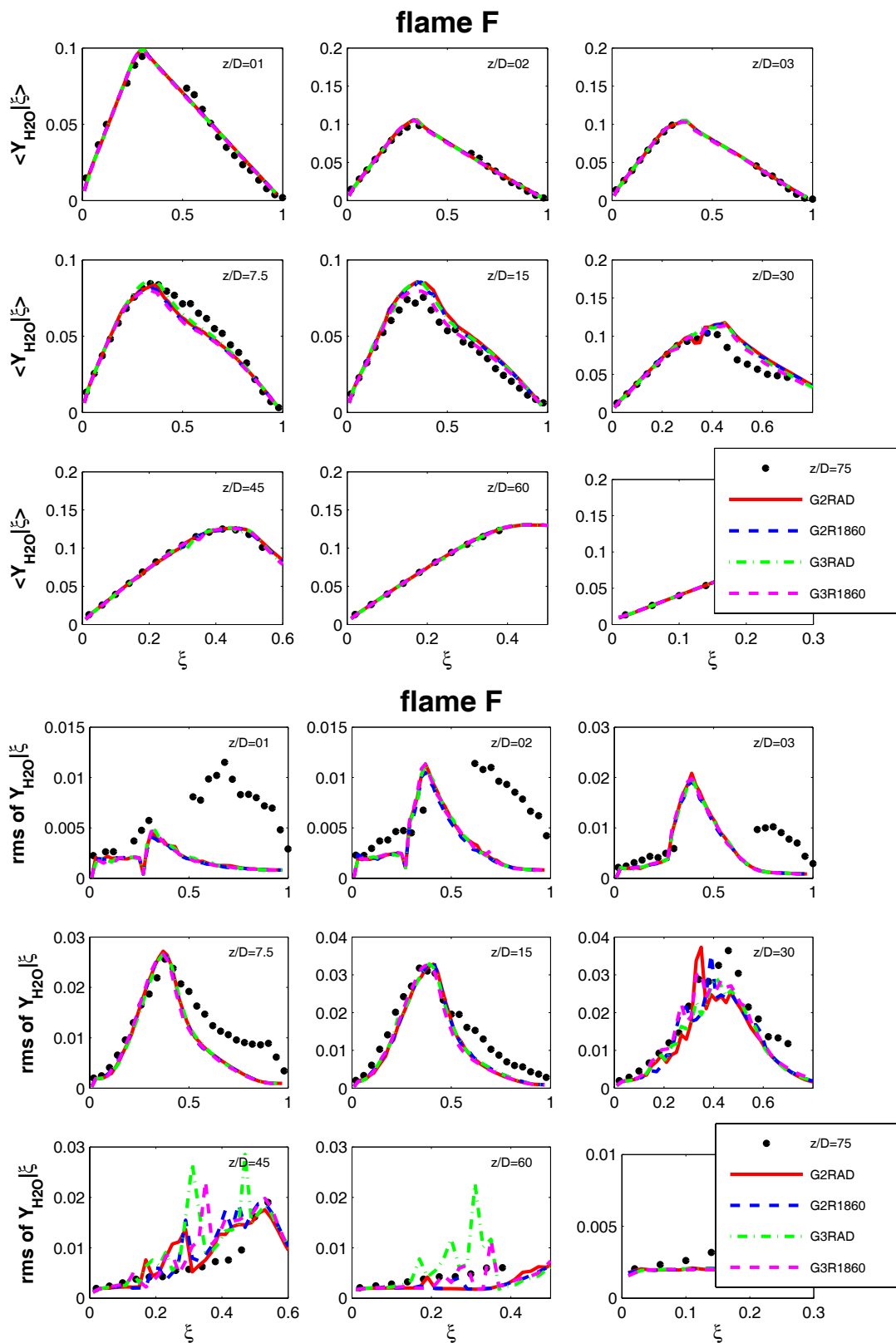


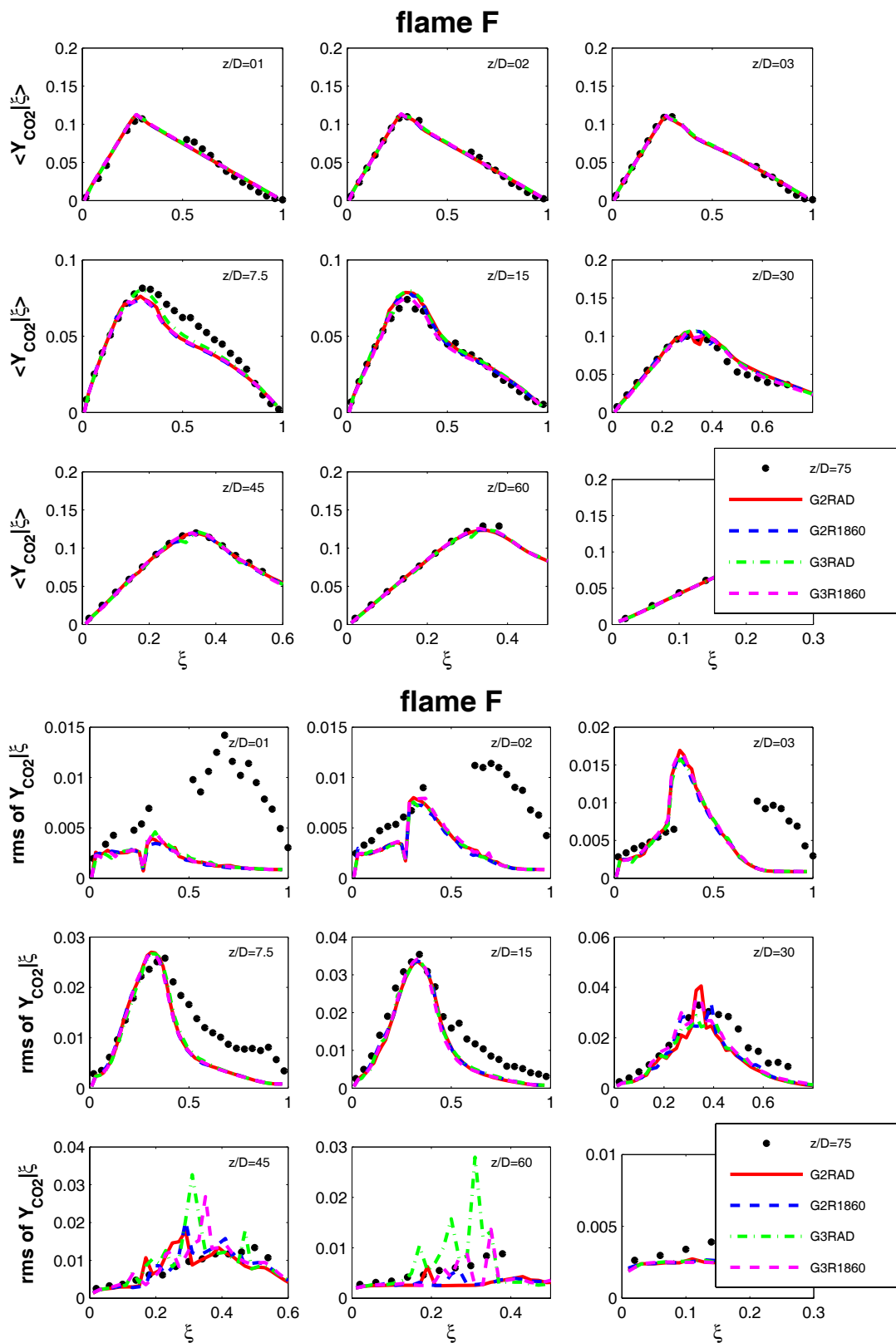


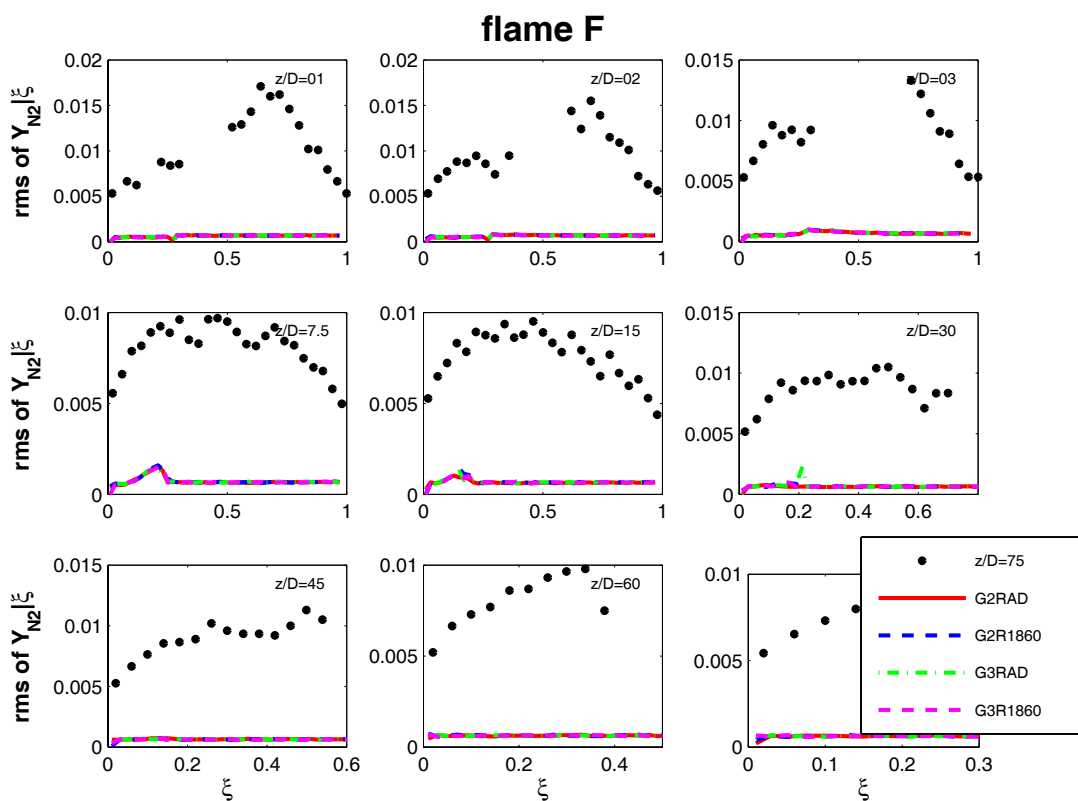
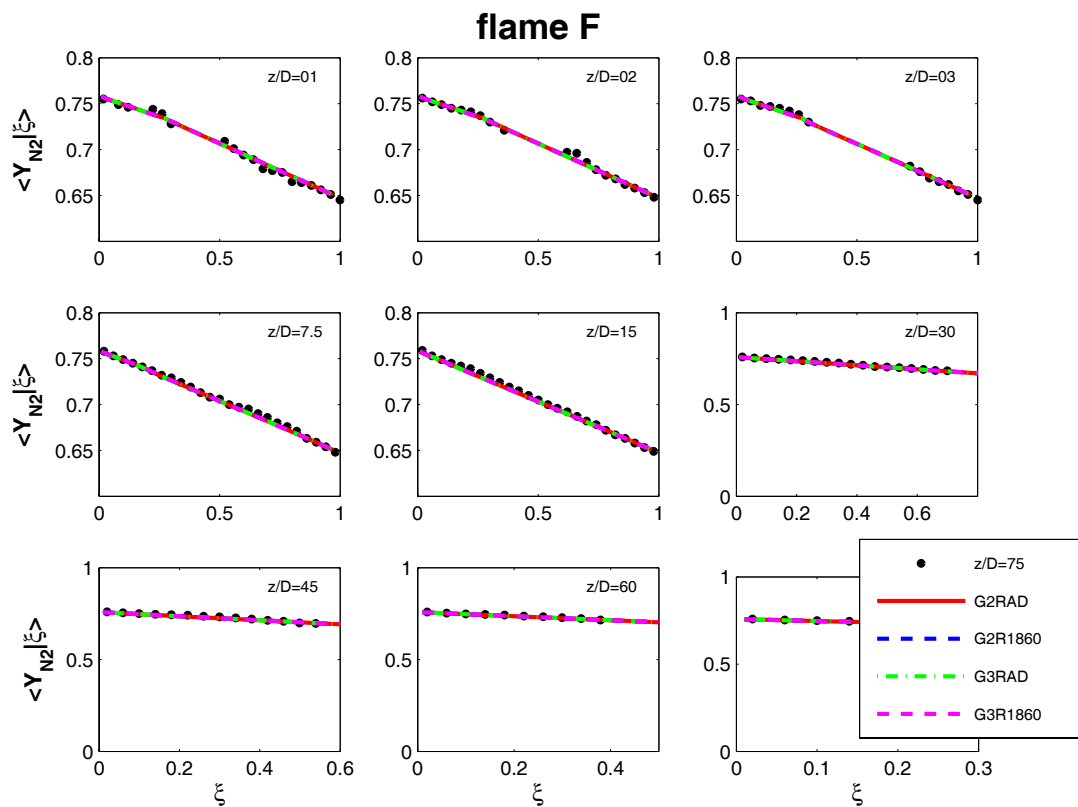


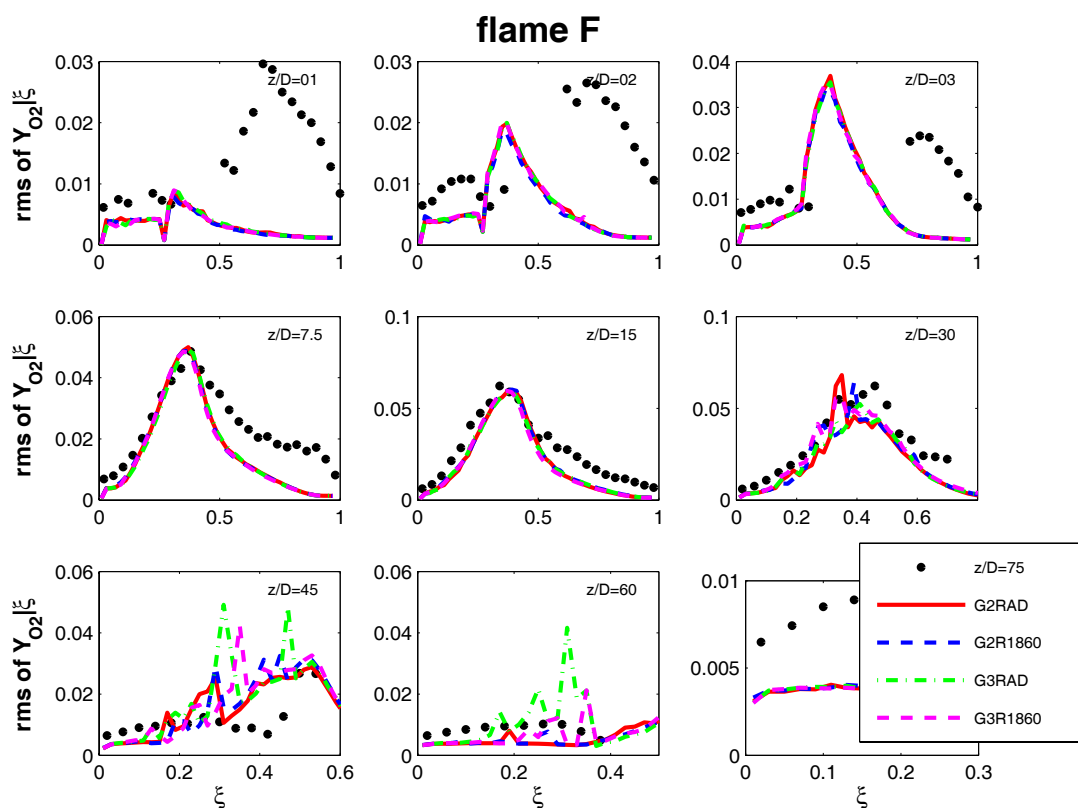
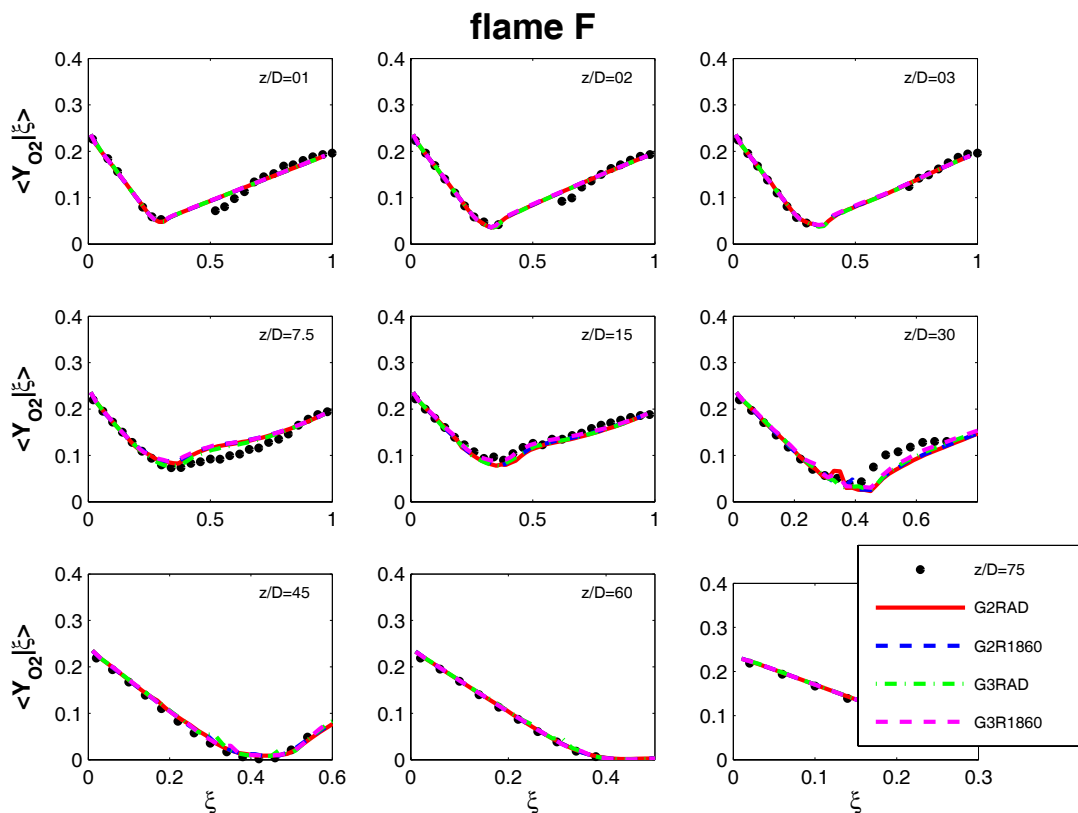
(5) Flame F, effect of piloted jet temperature on NO

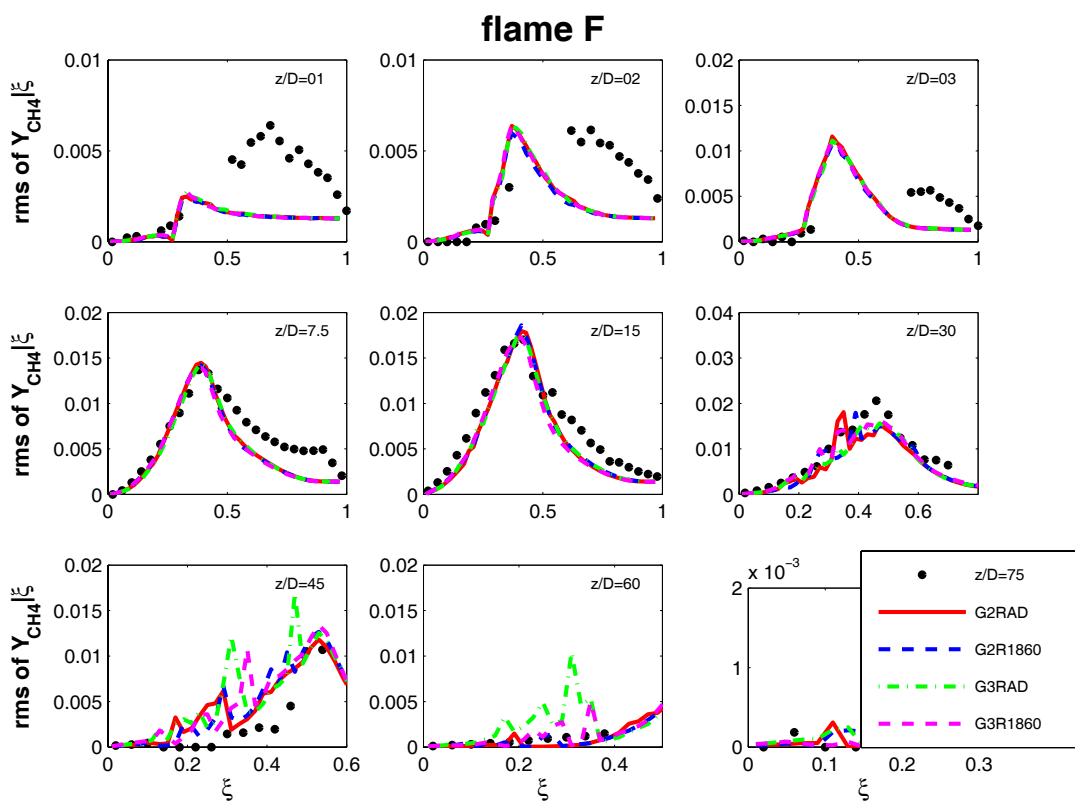
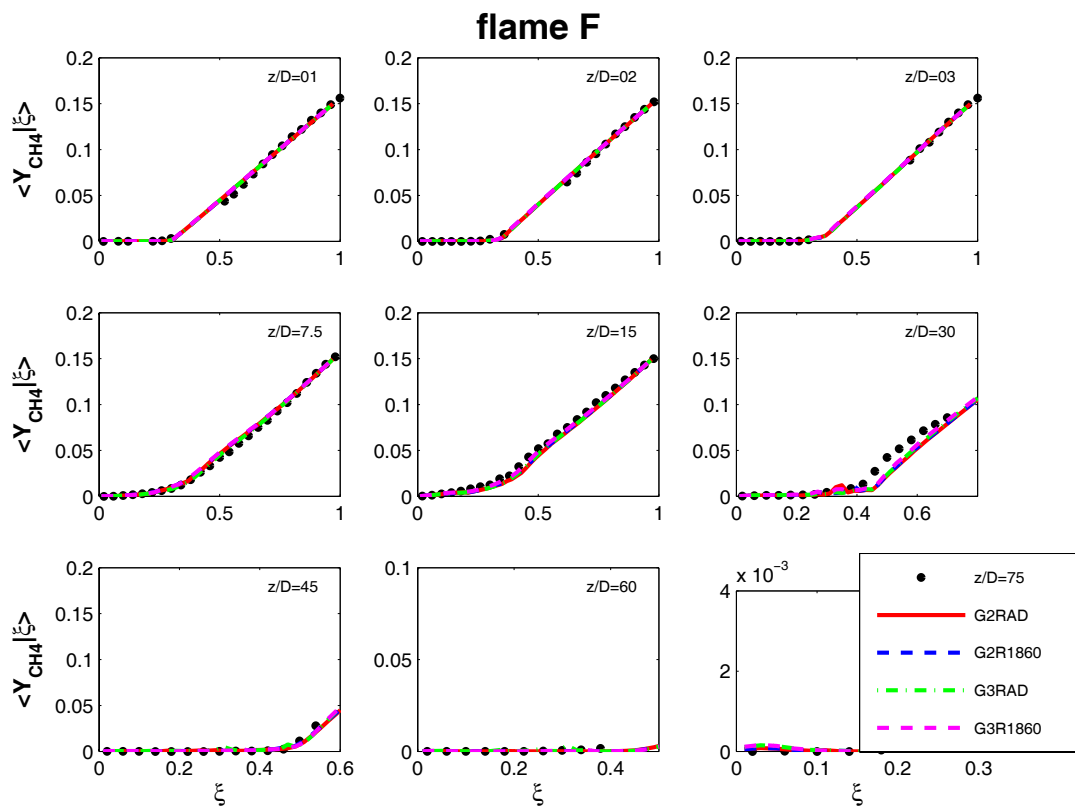


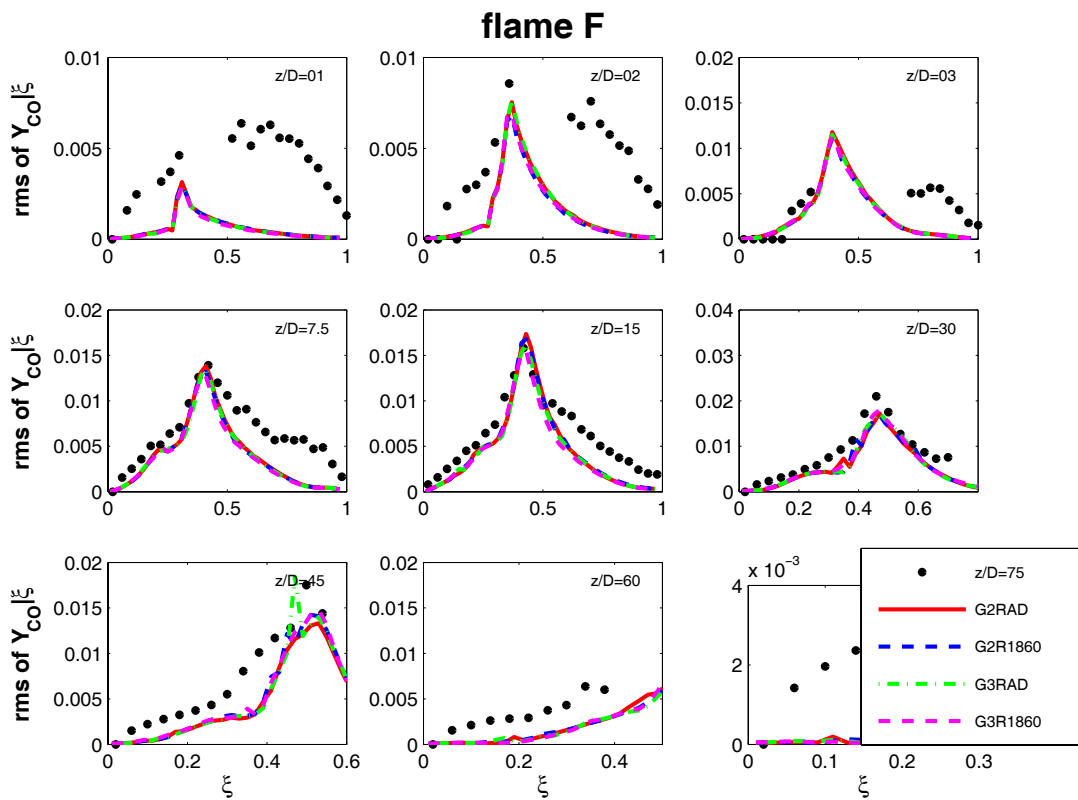
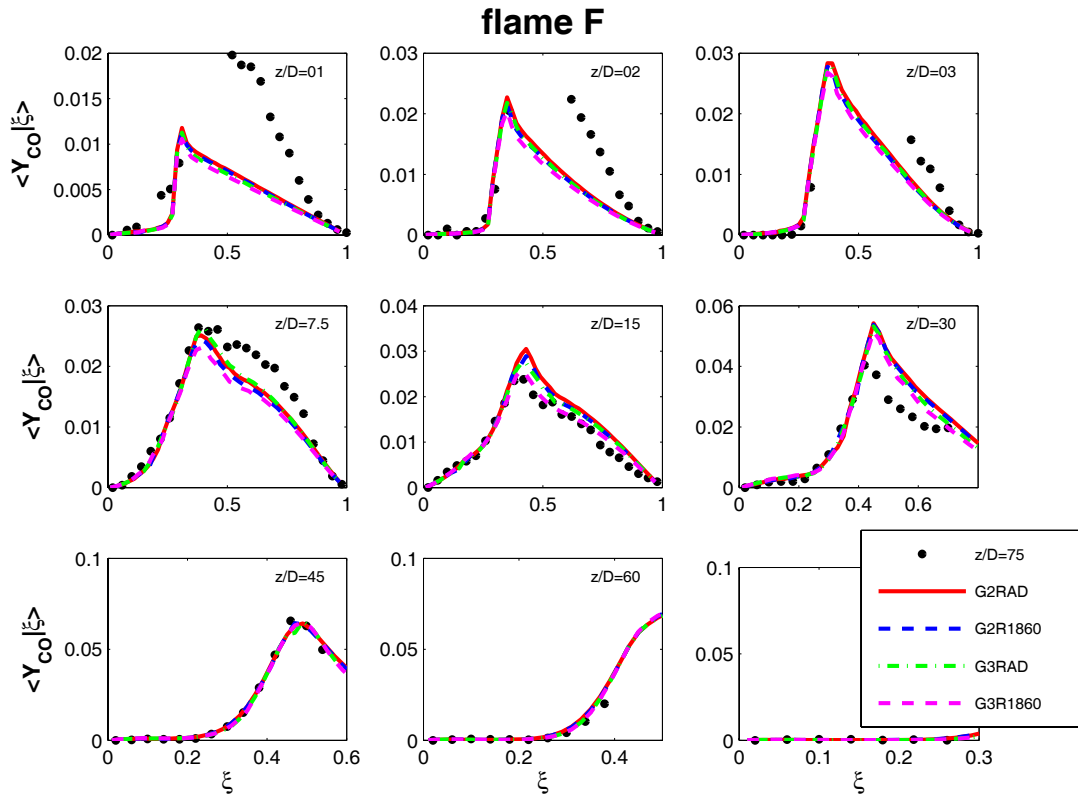


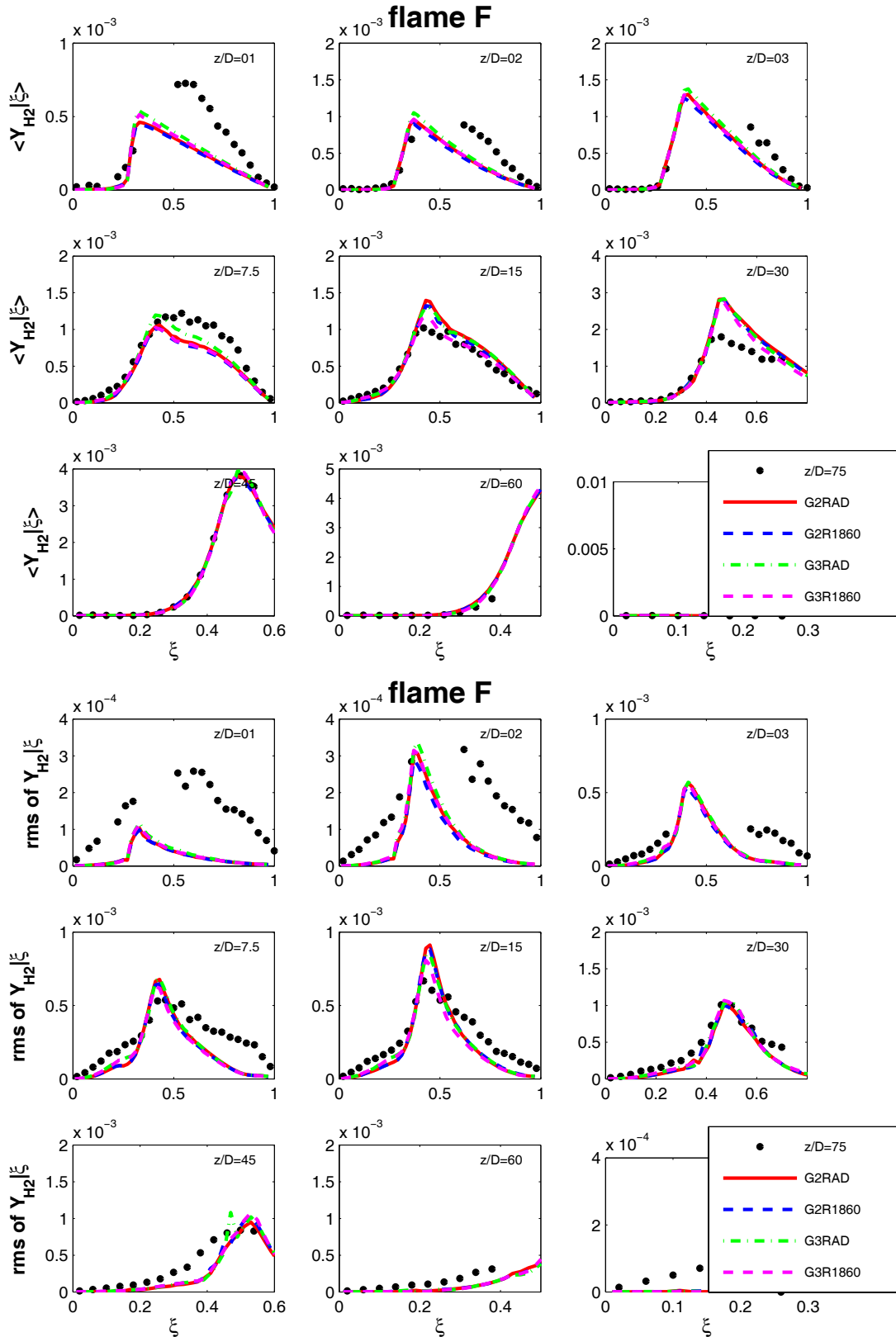


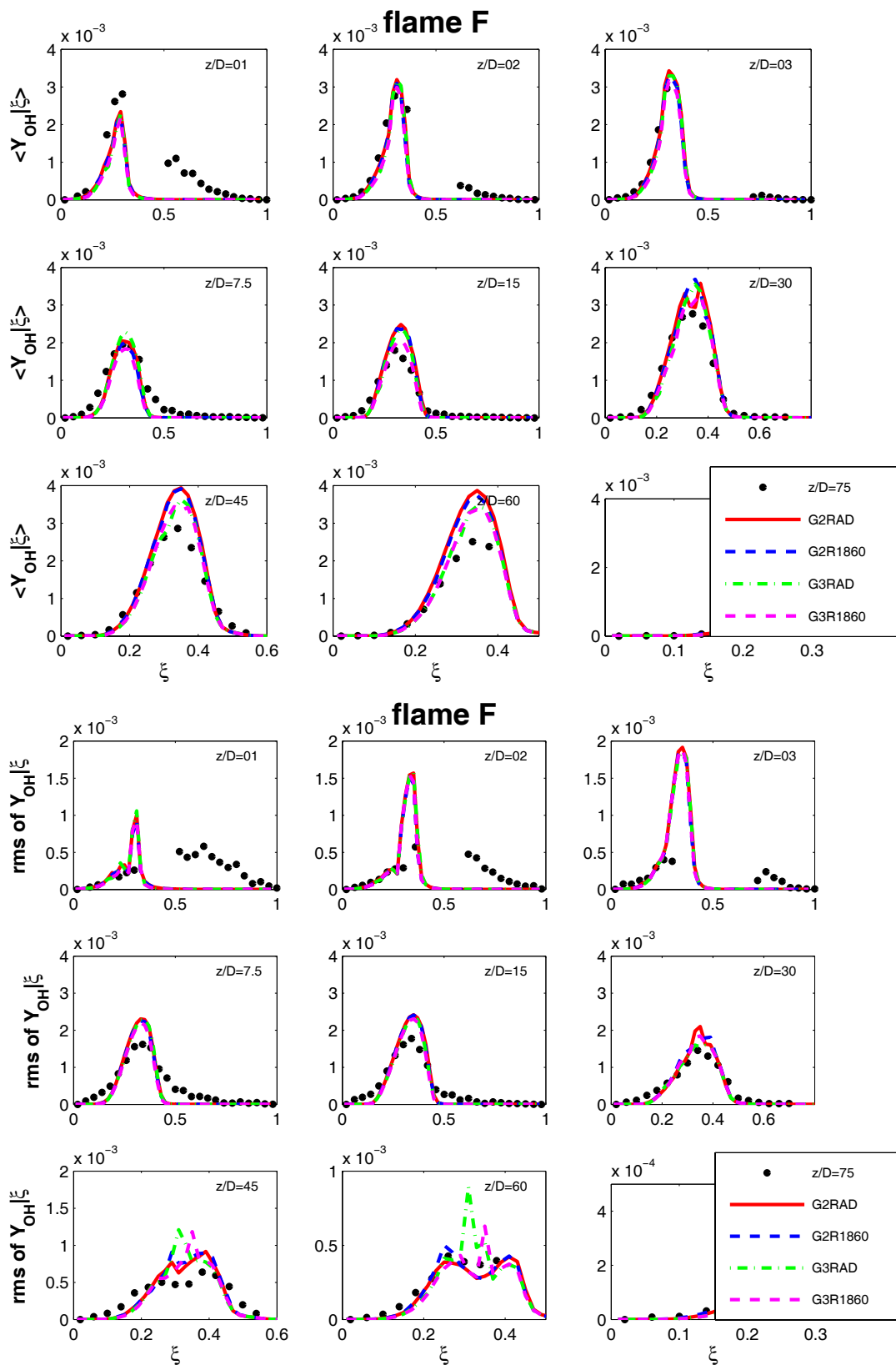


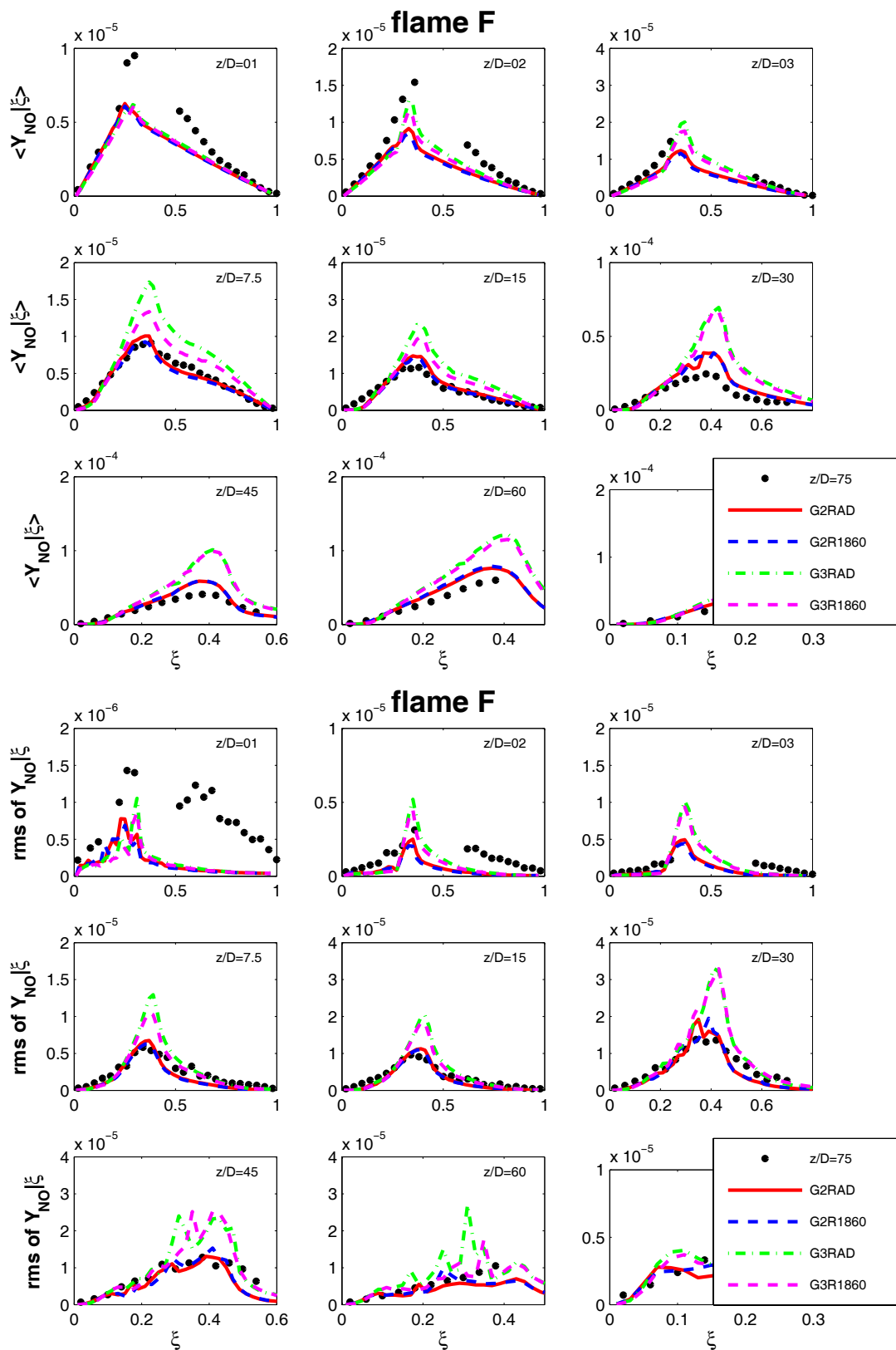




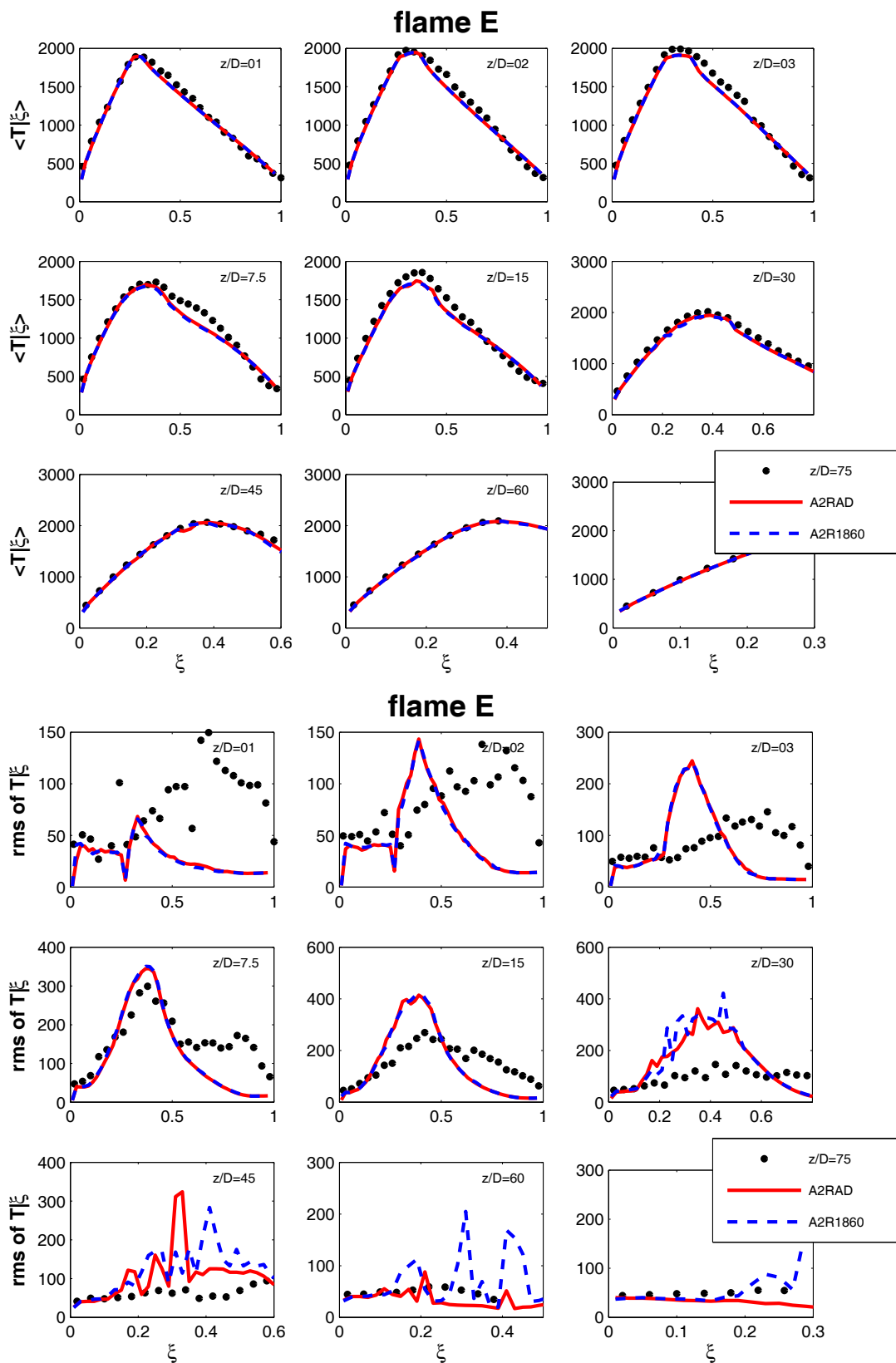


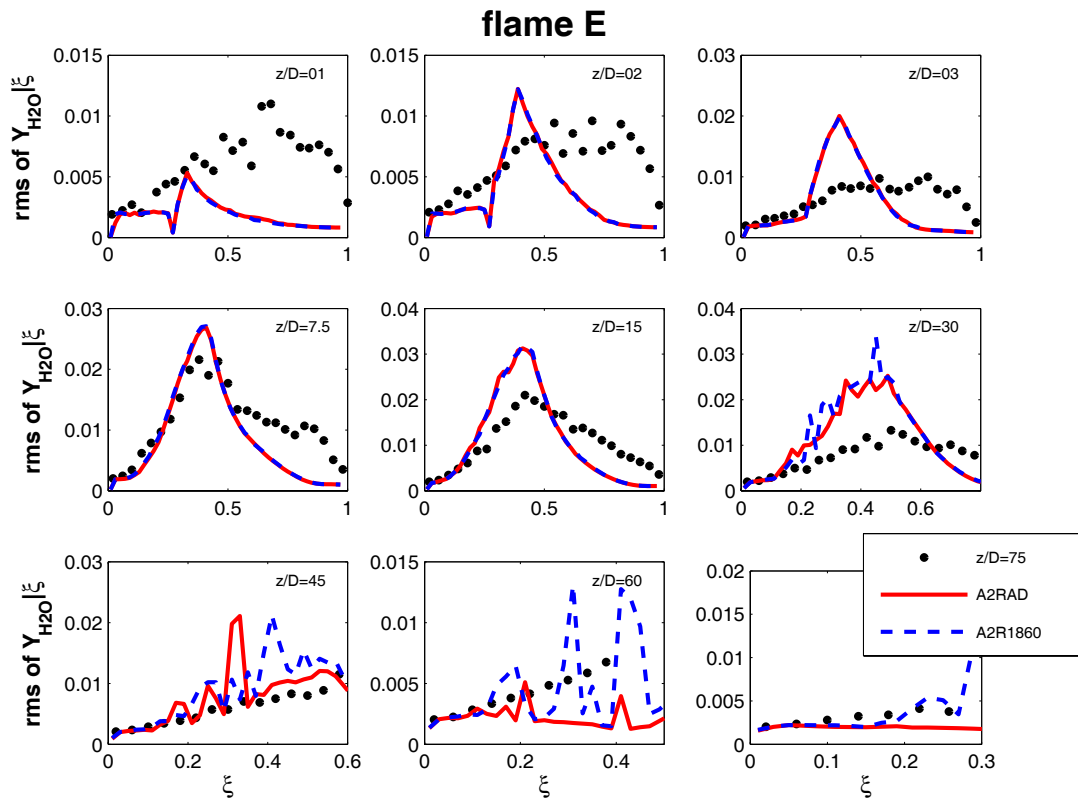
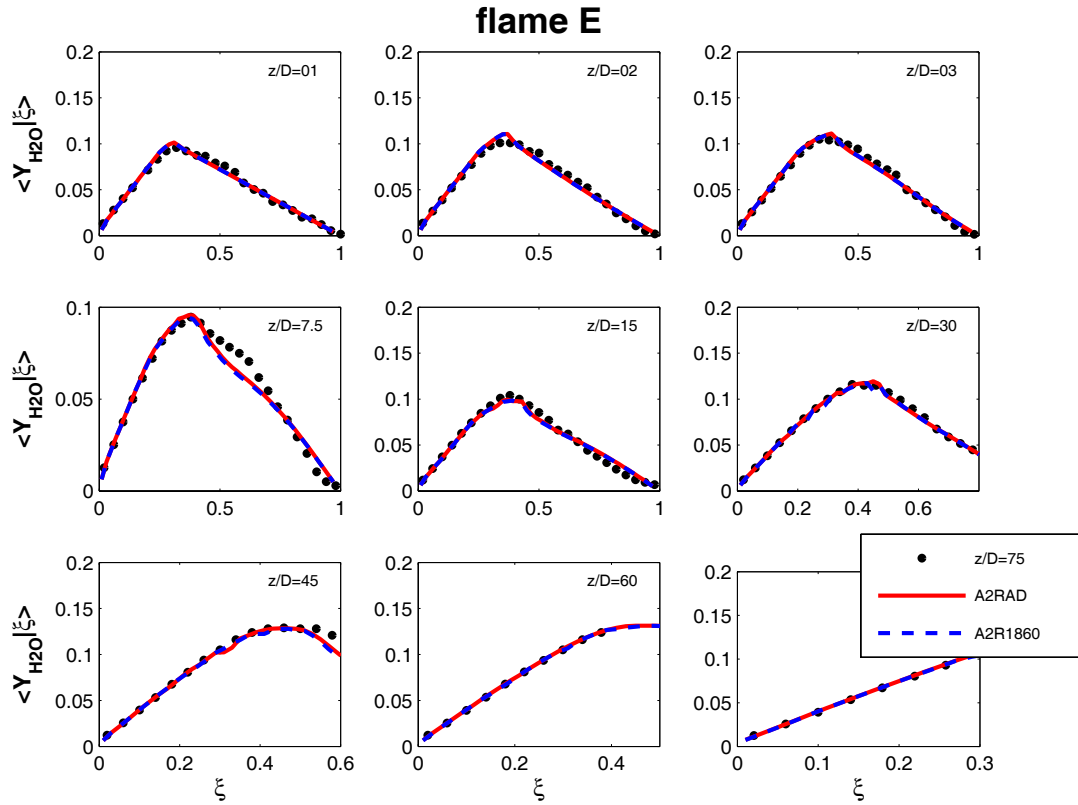


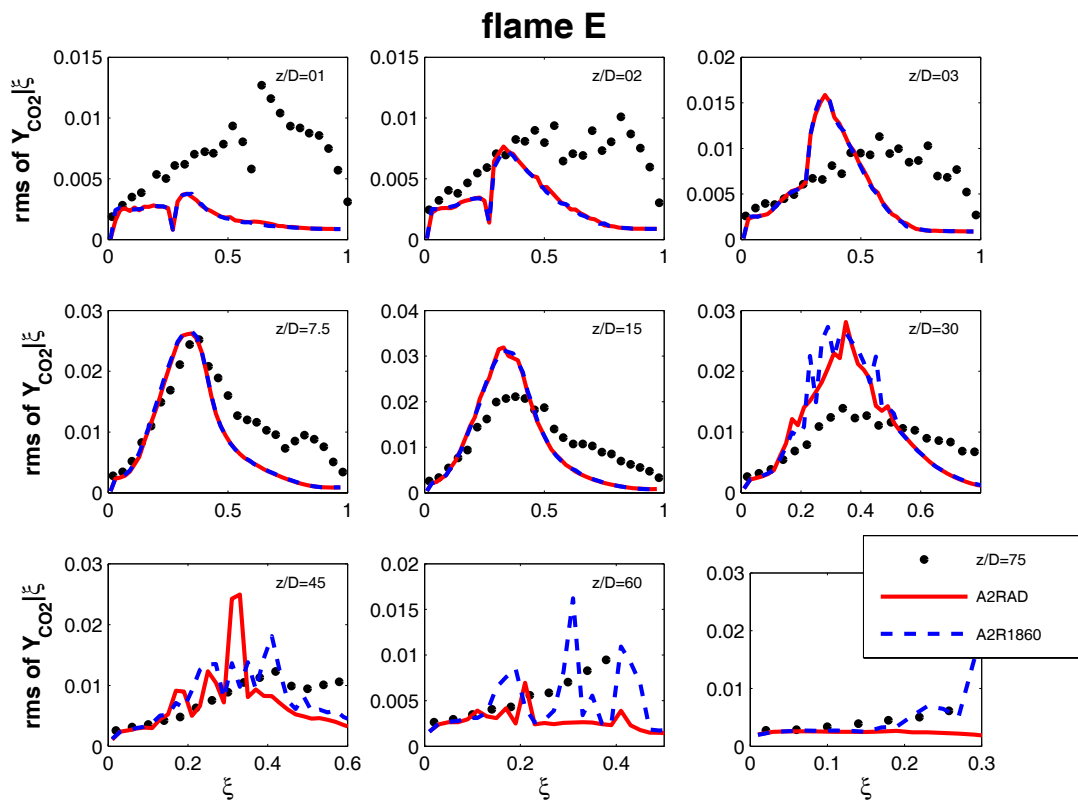
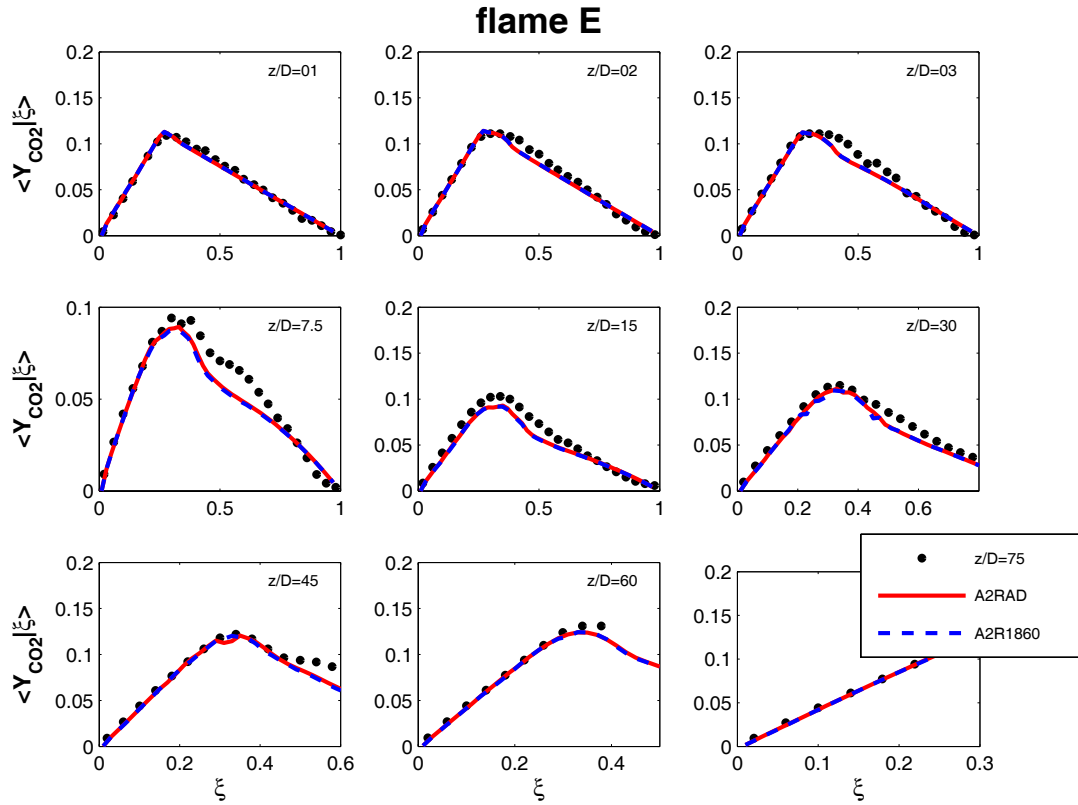


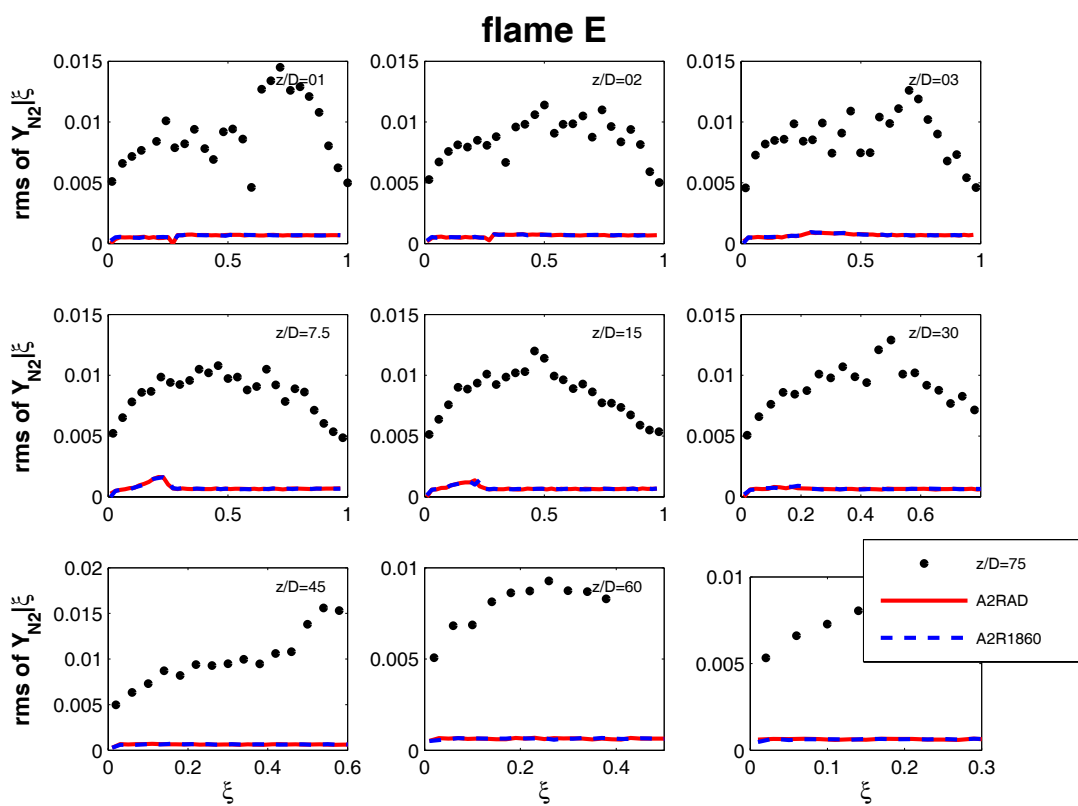
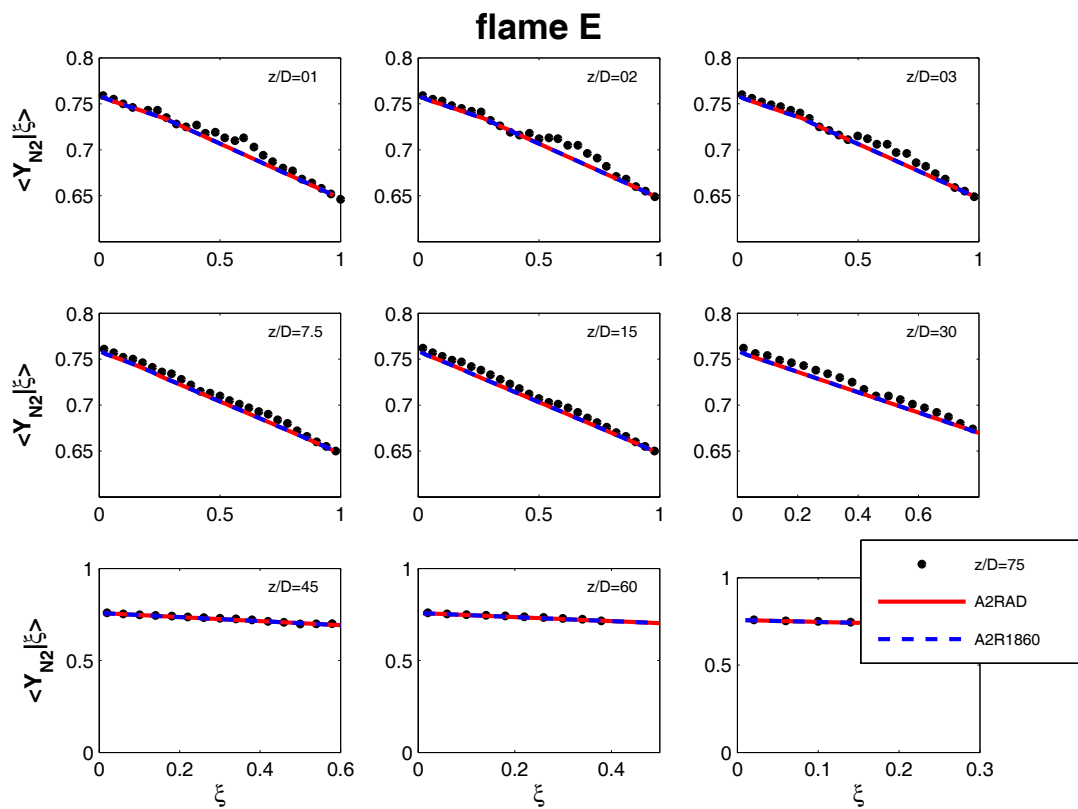


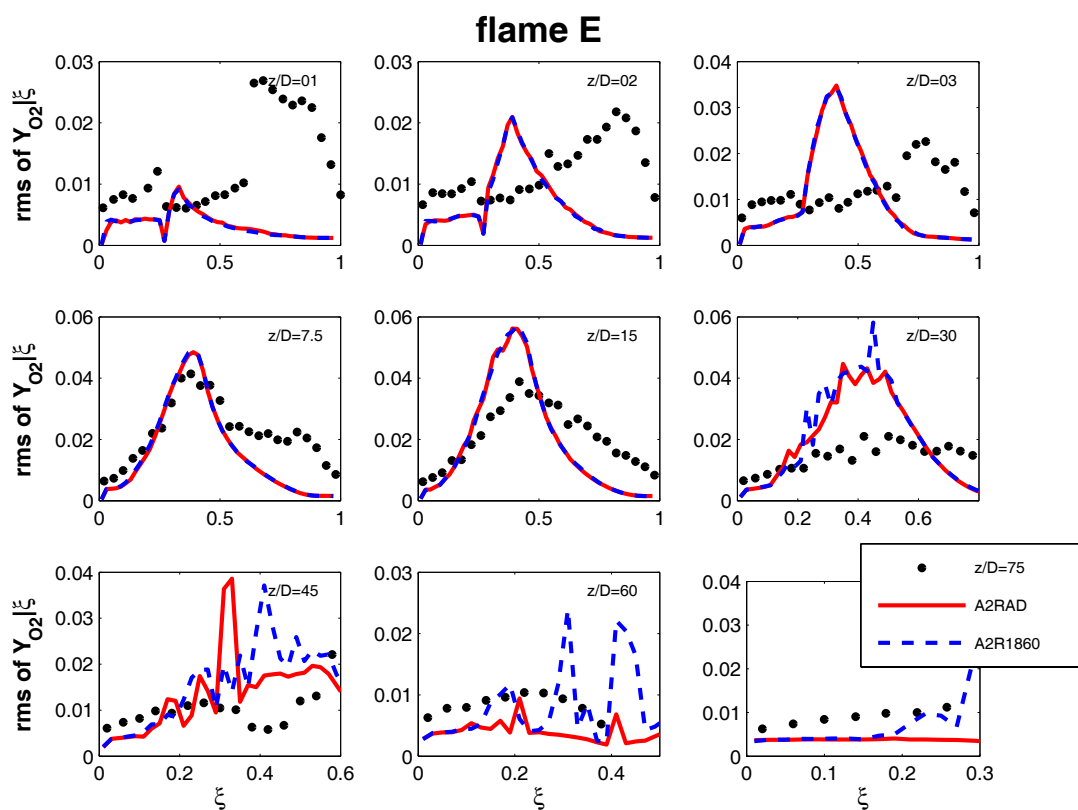
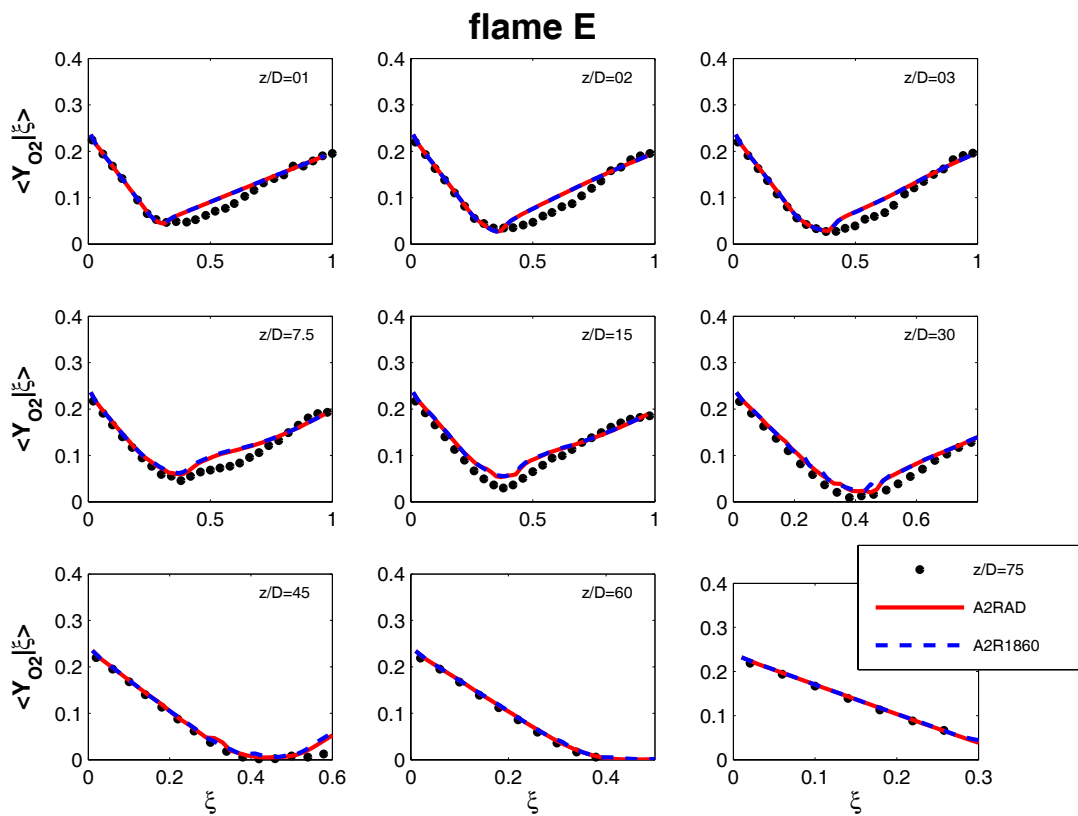
(6) Flame E, effect of piloted jet temperature on NO

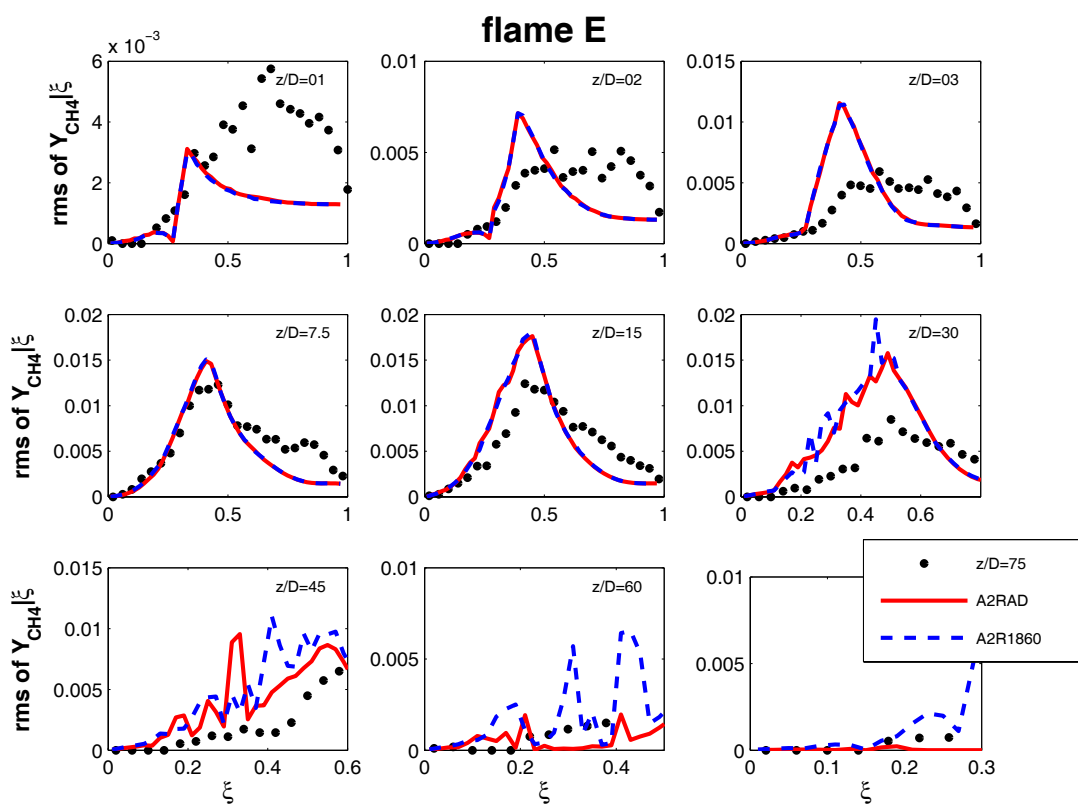
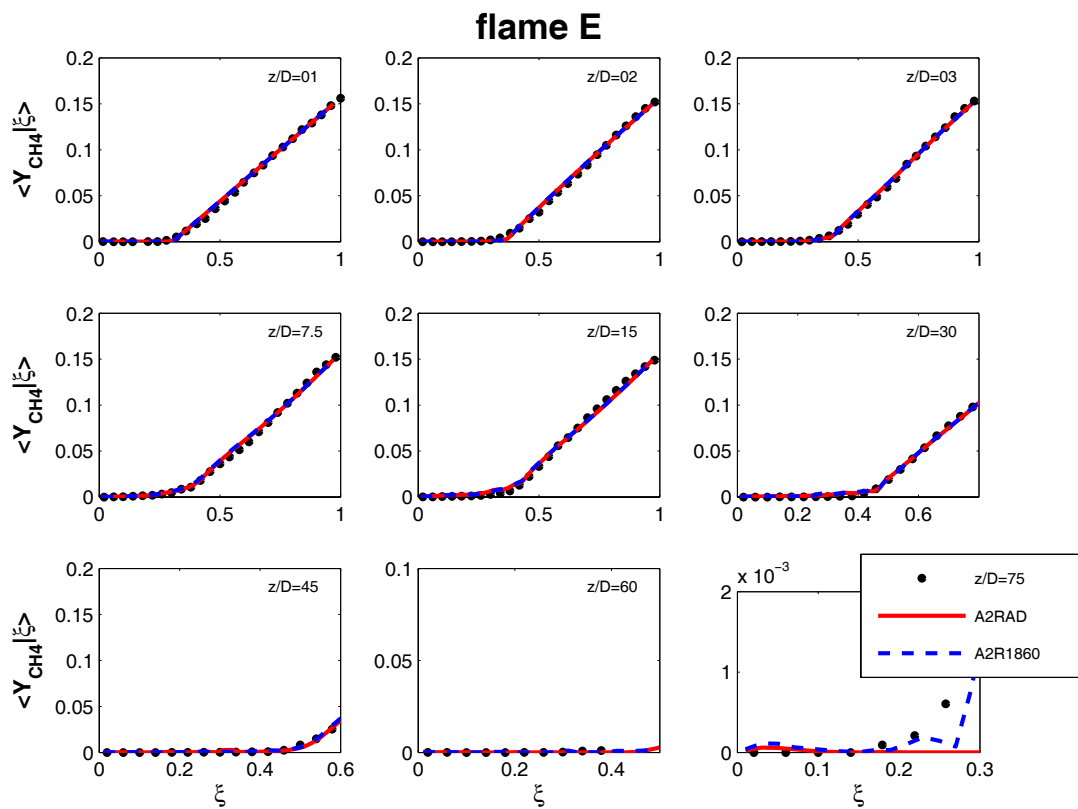


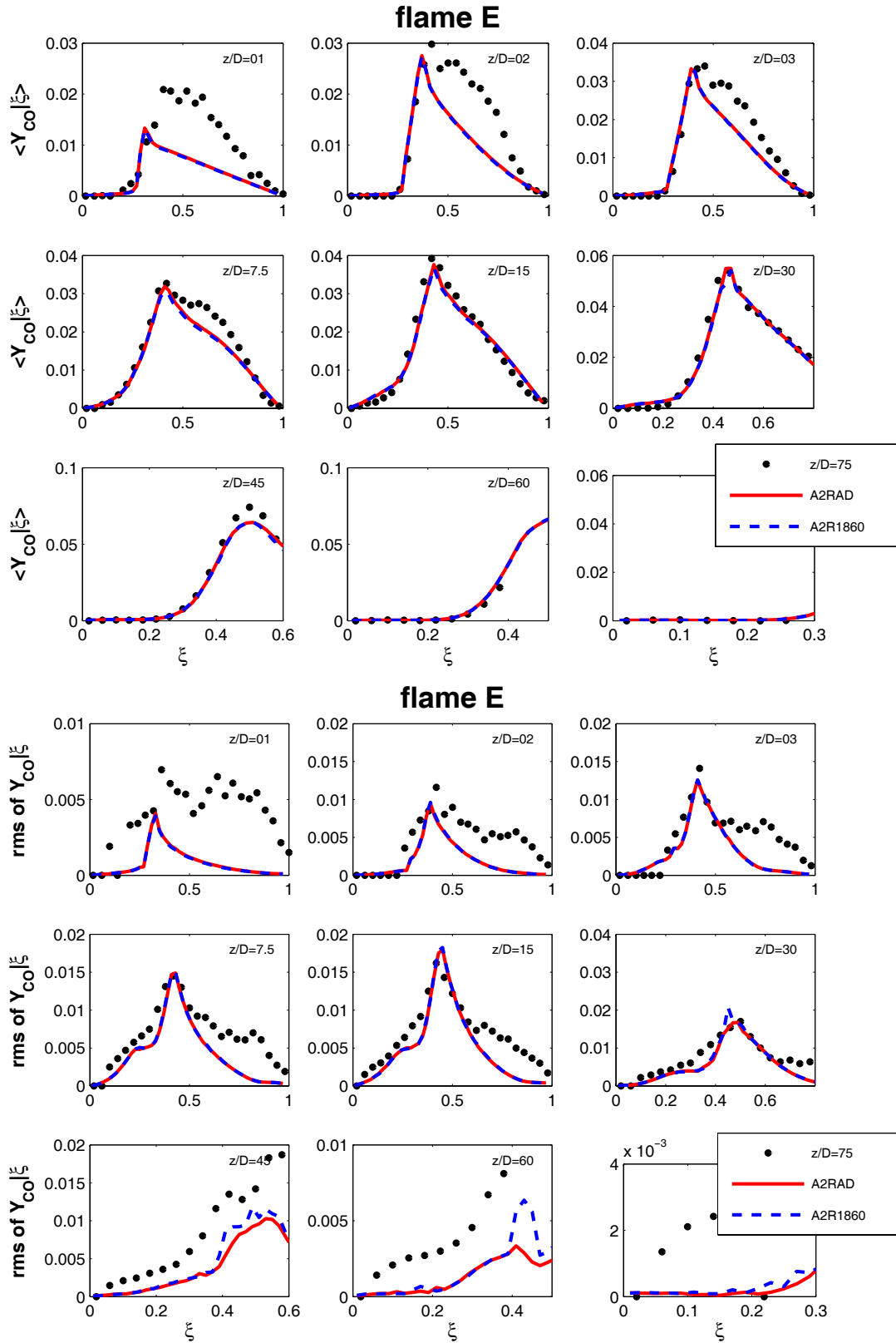


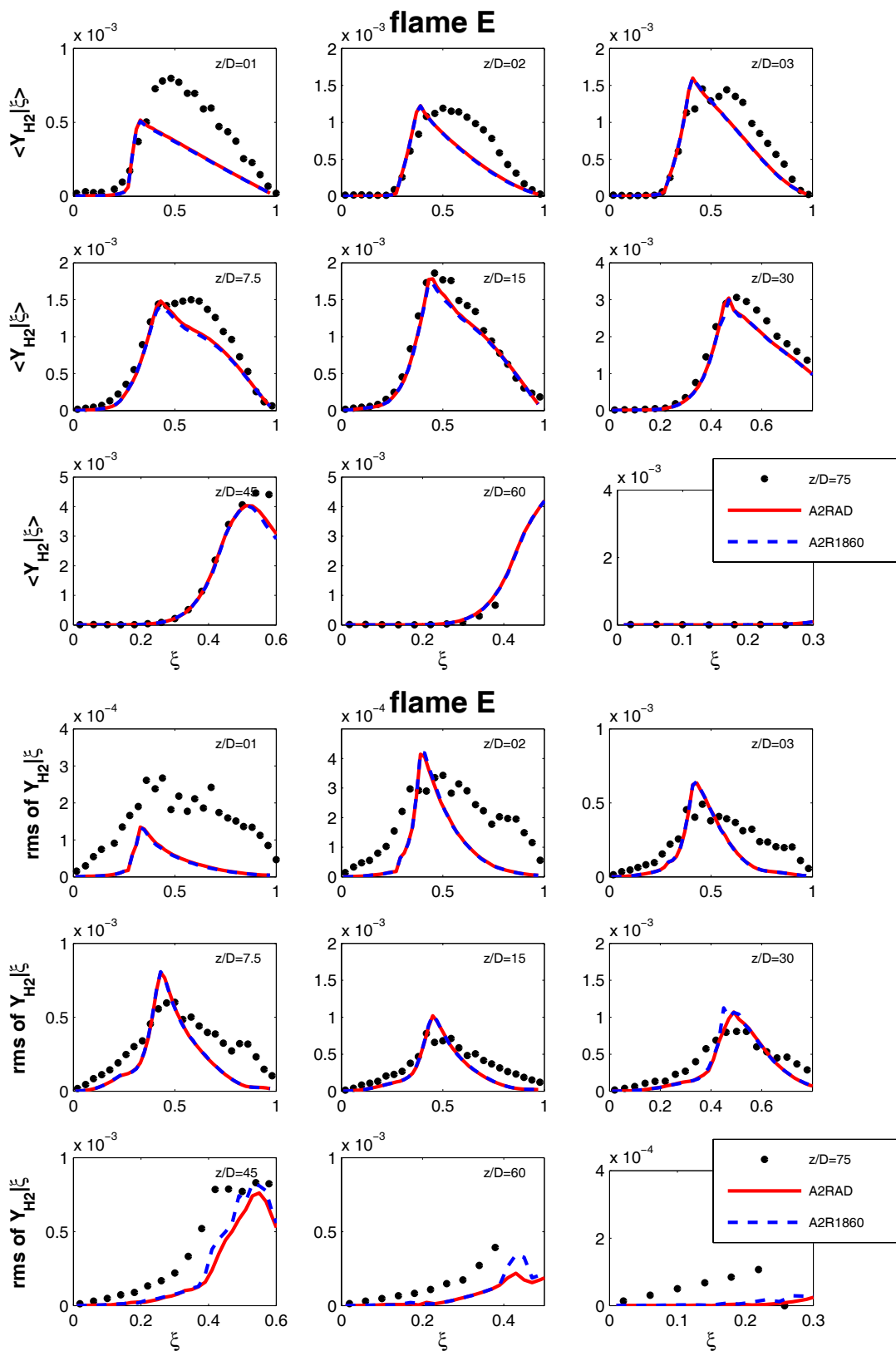


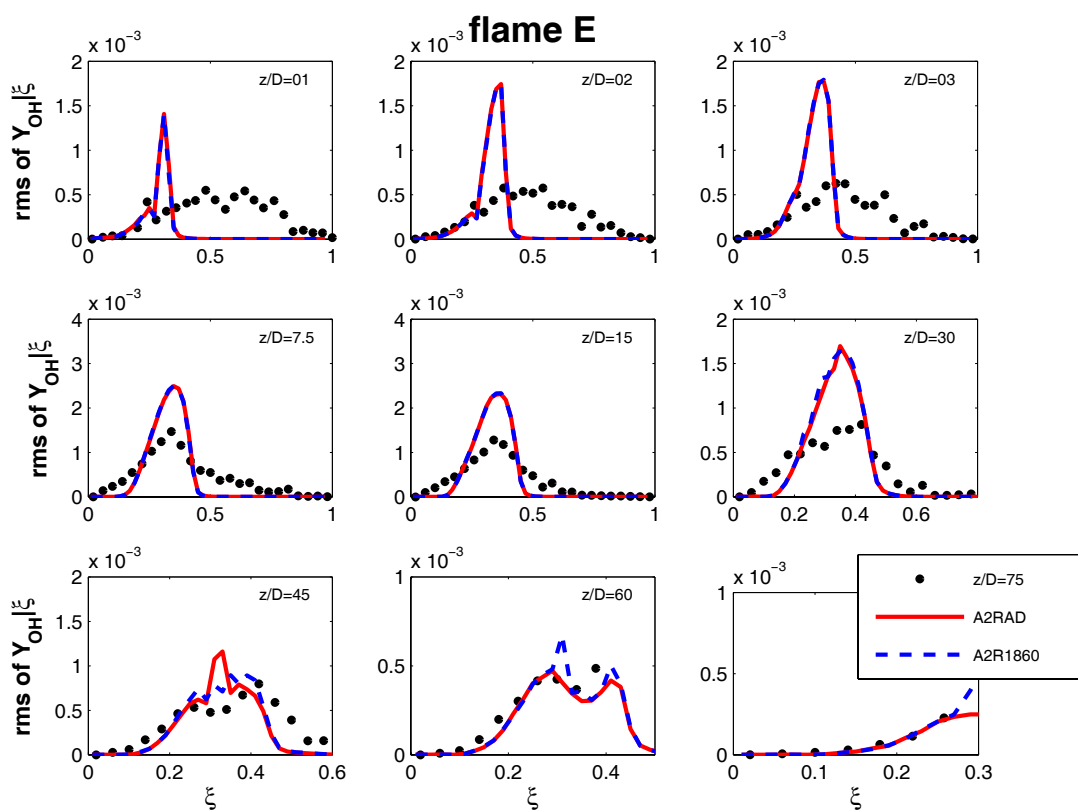
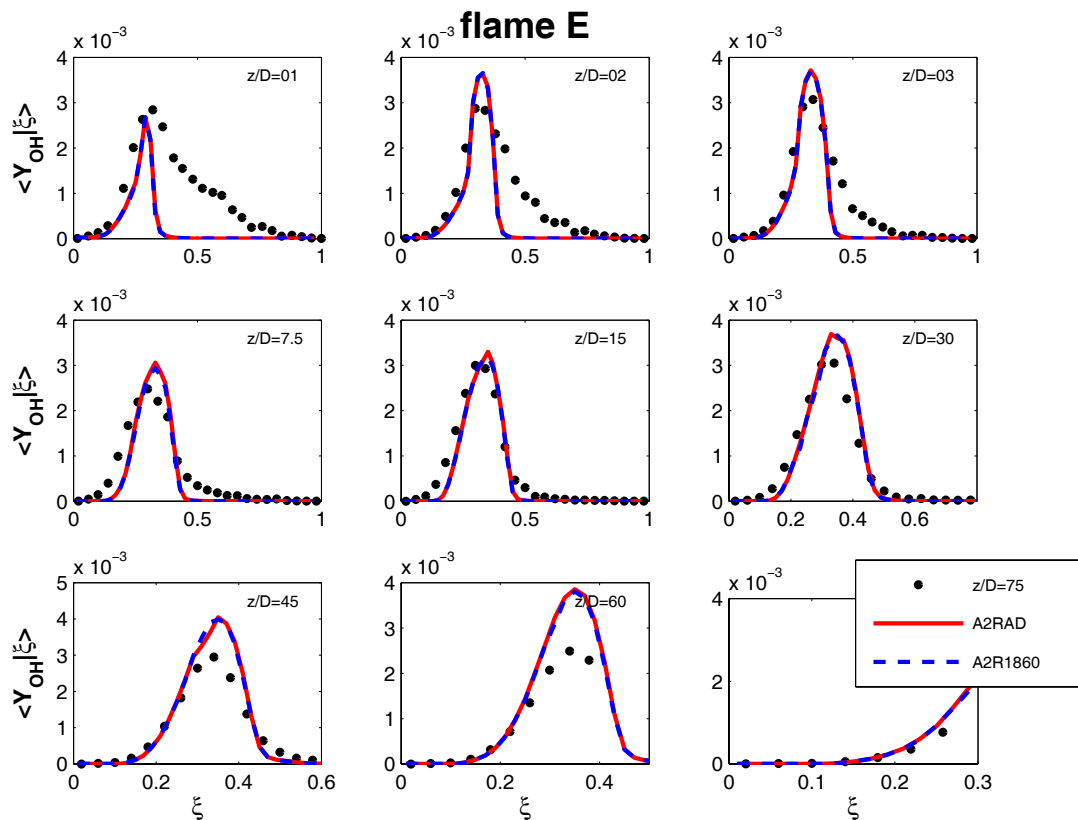


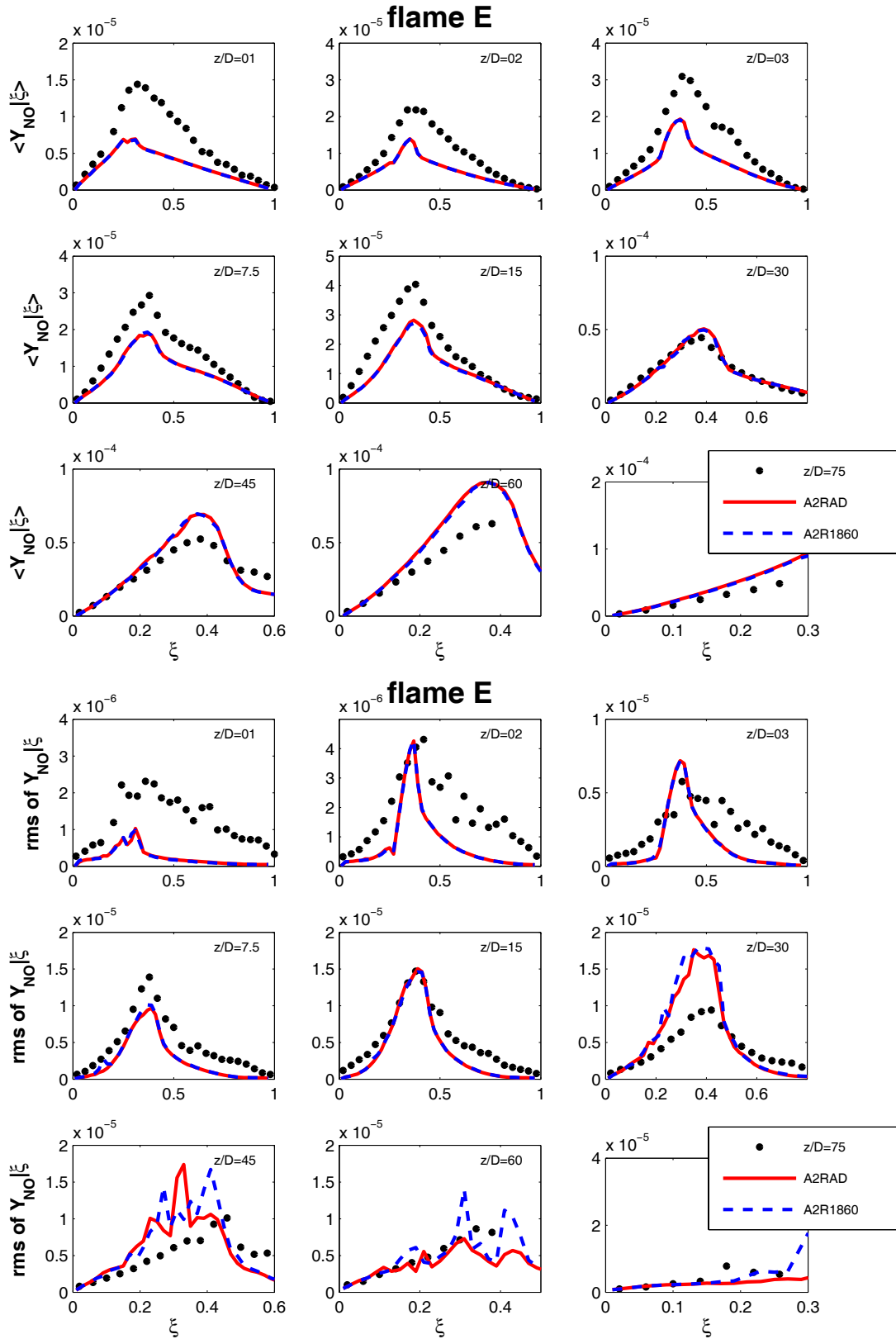




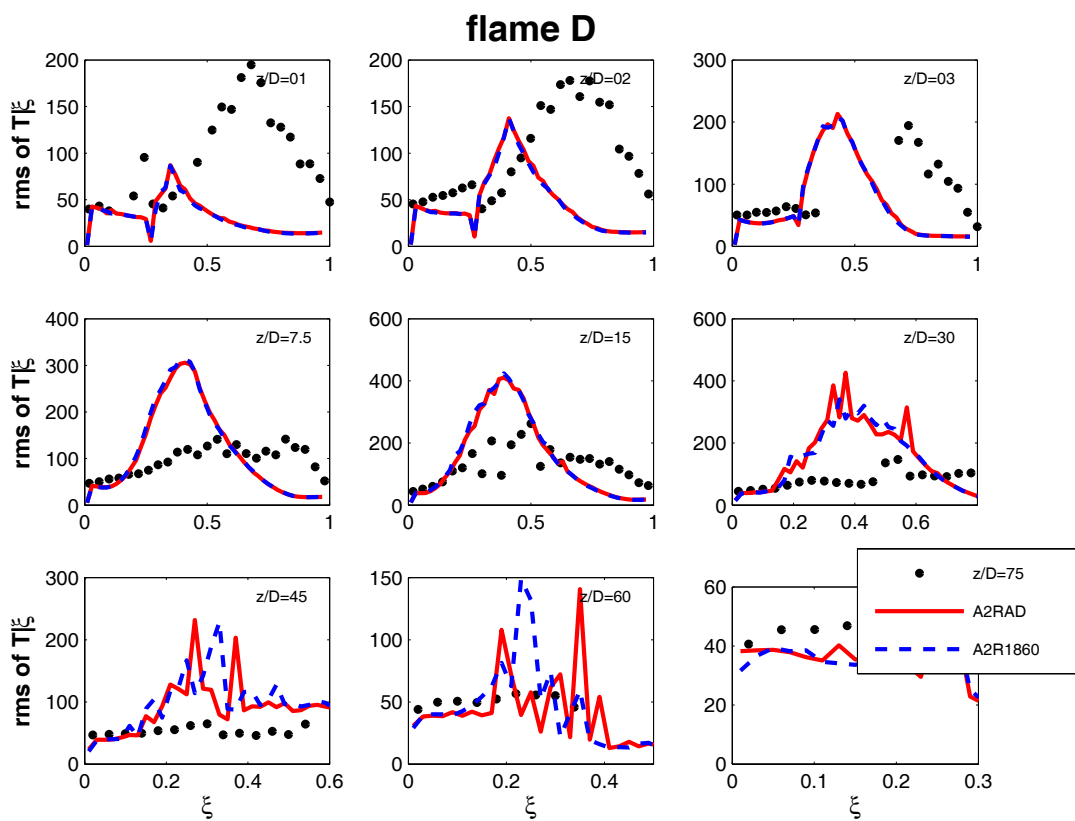
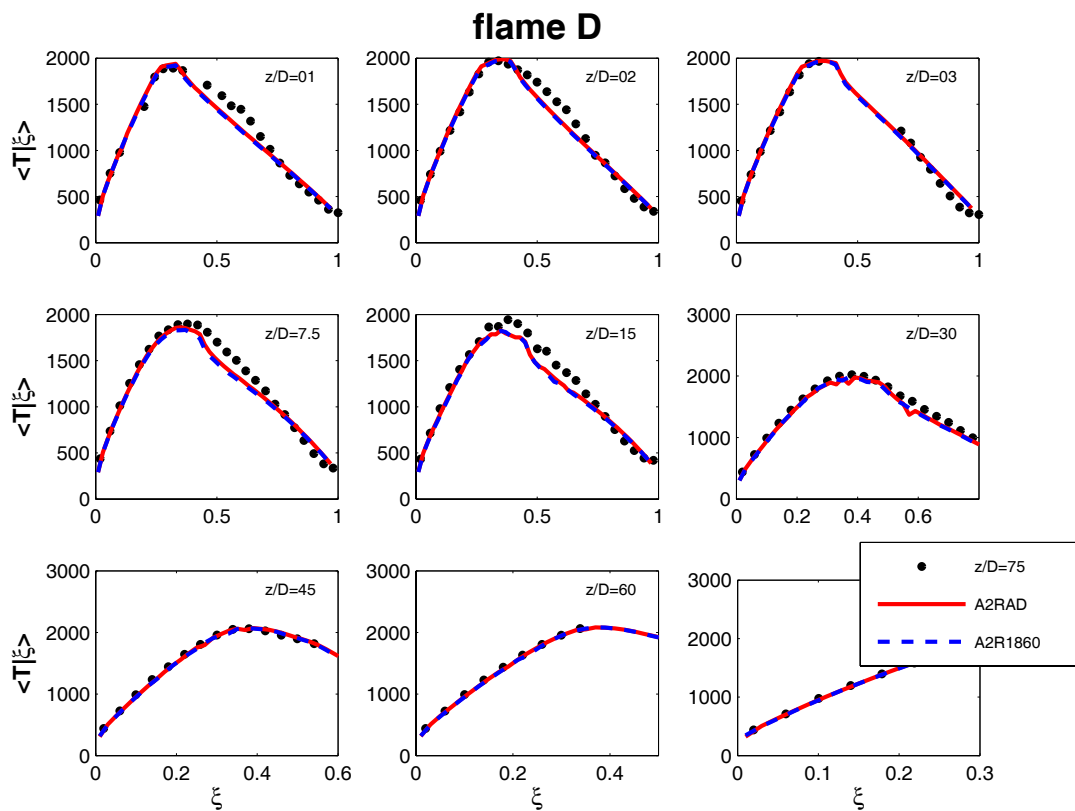


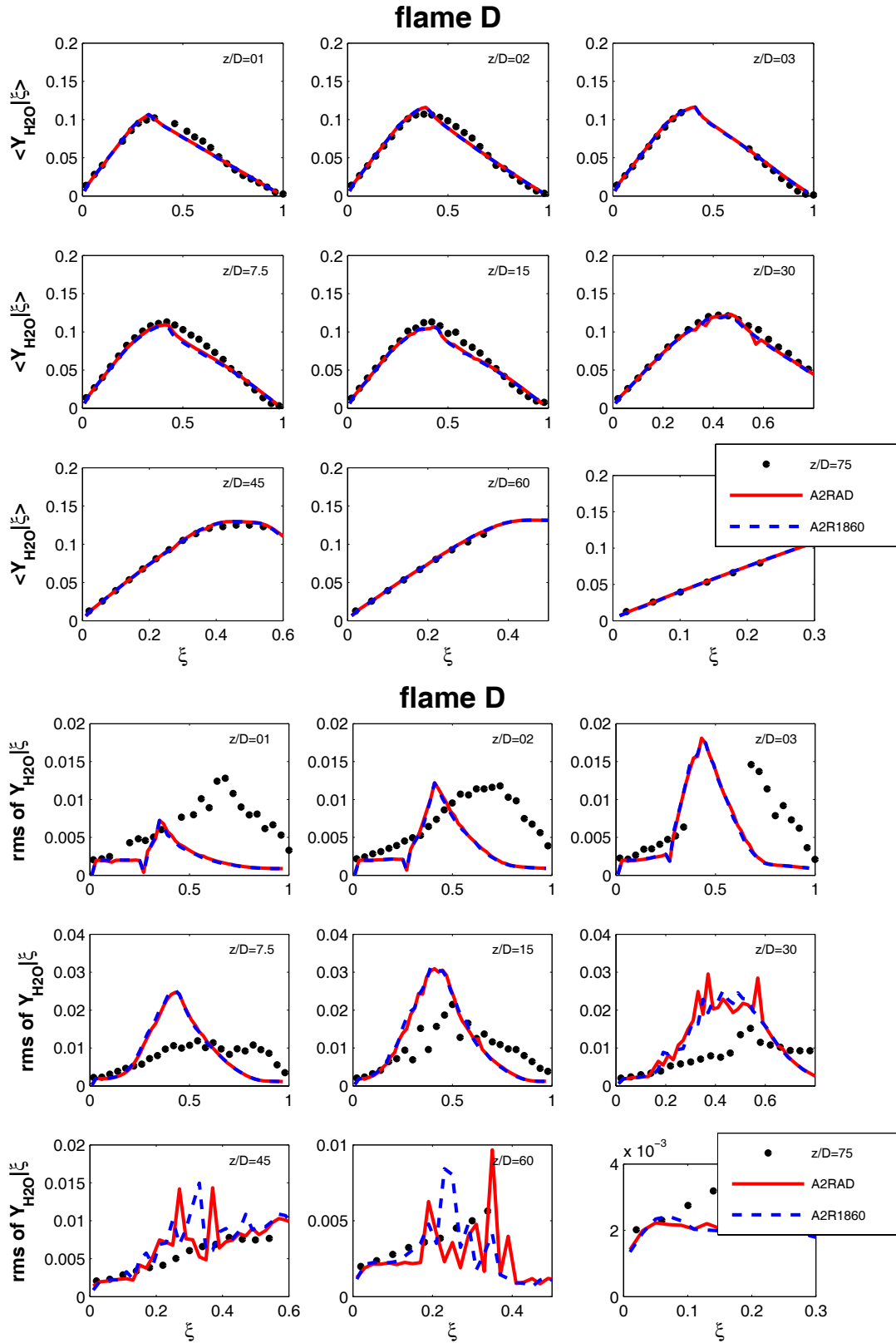


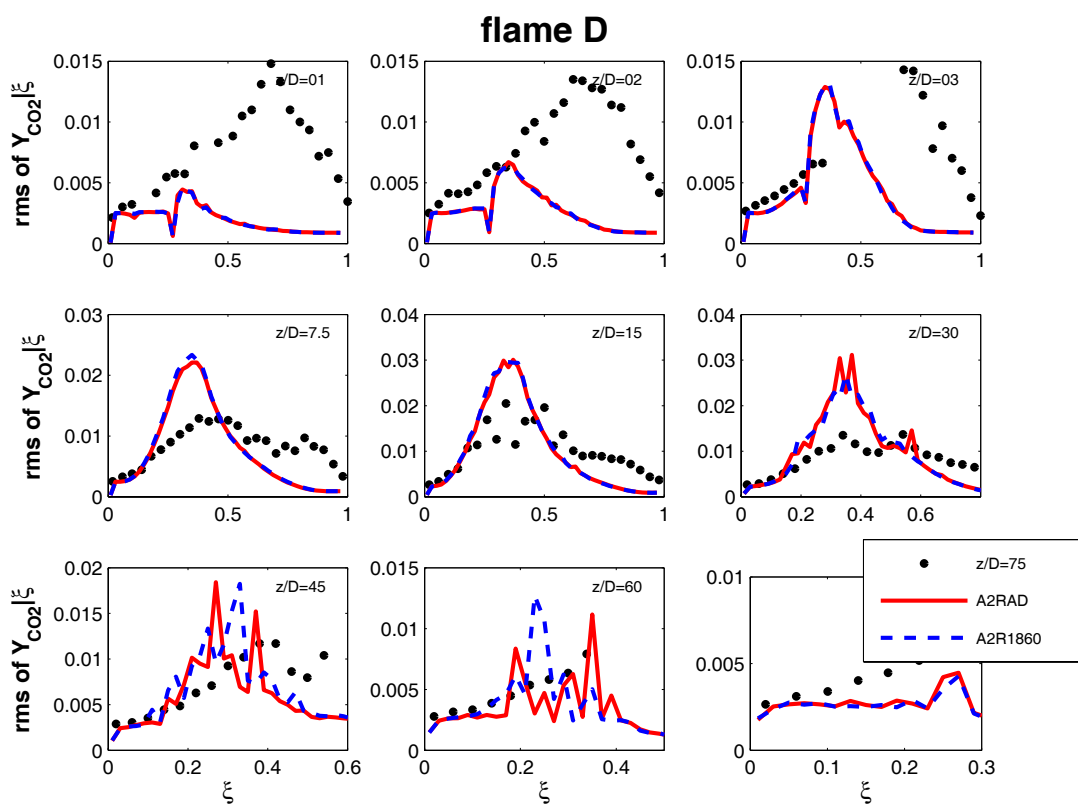
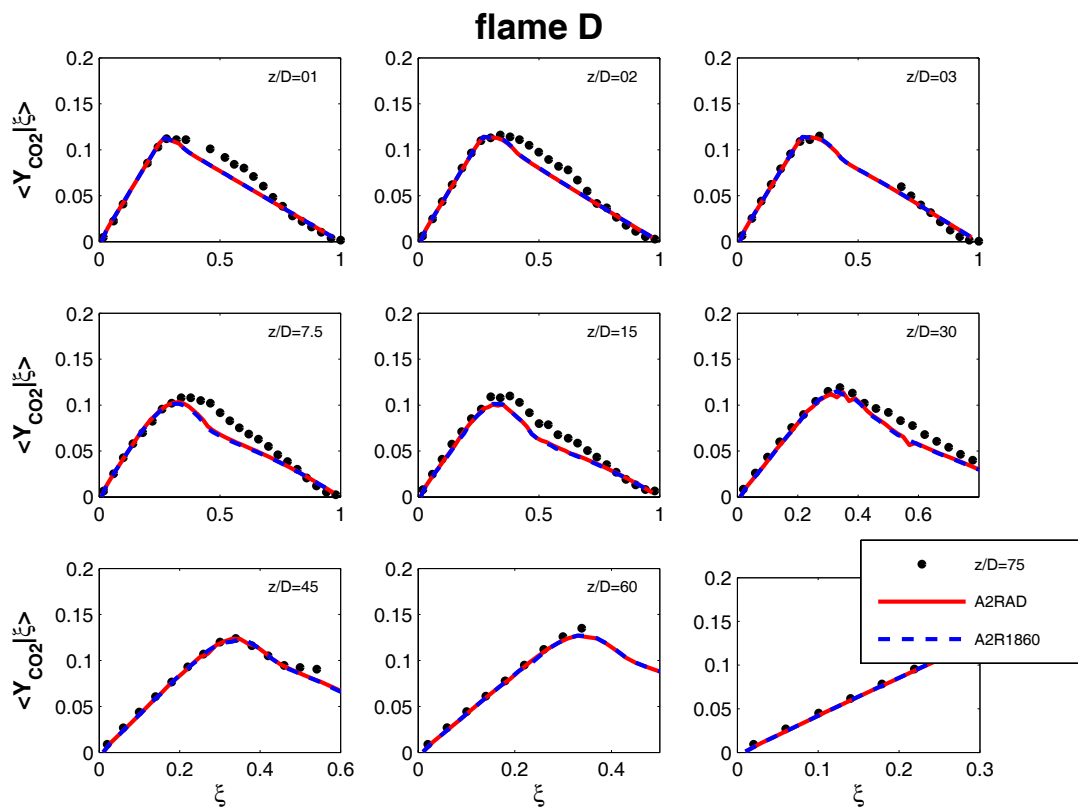


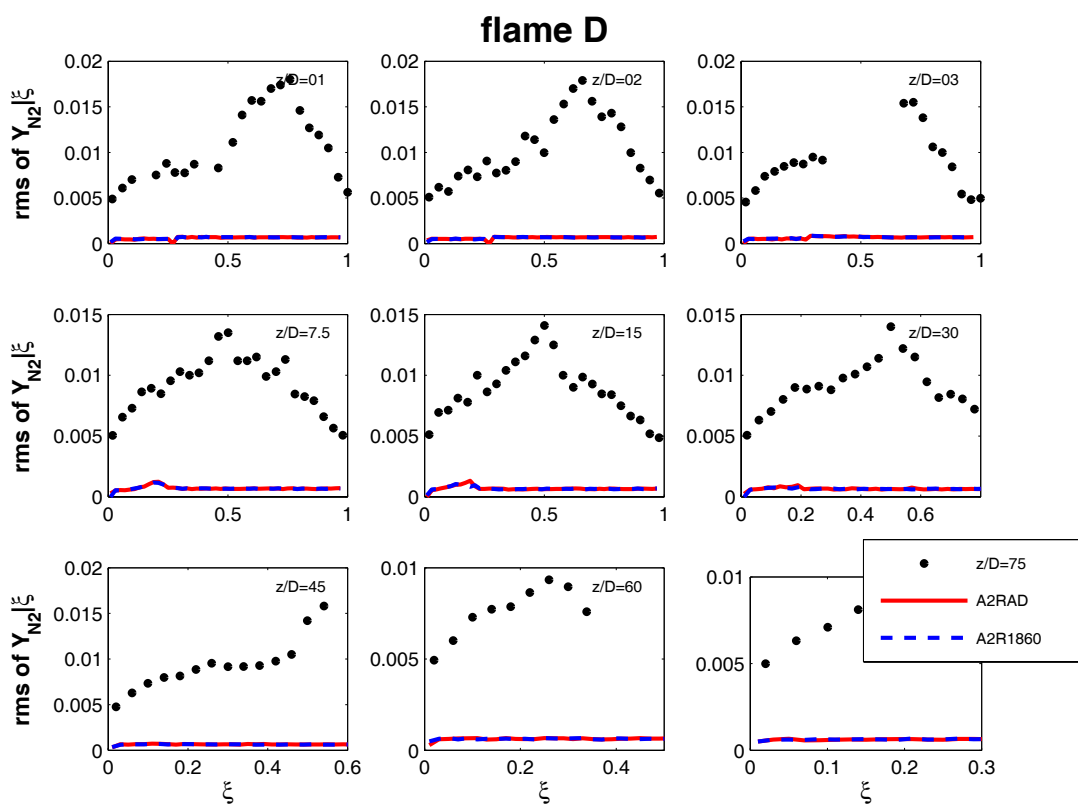
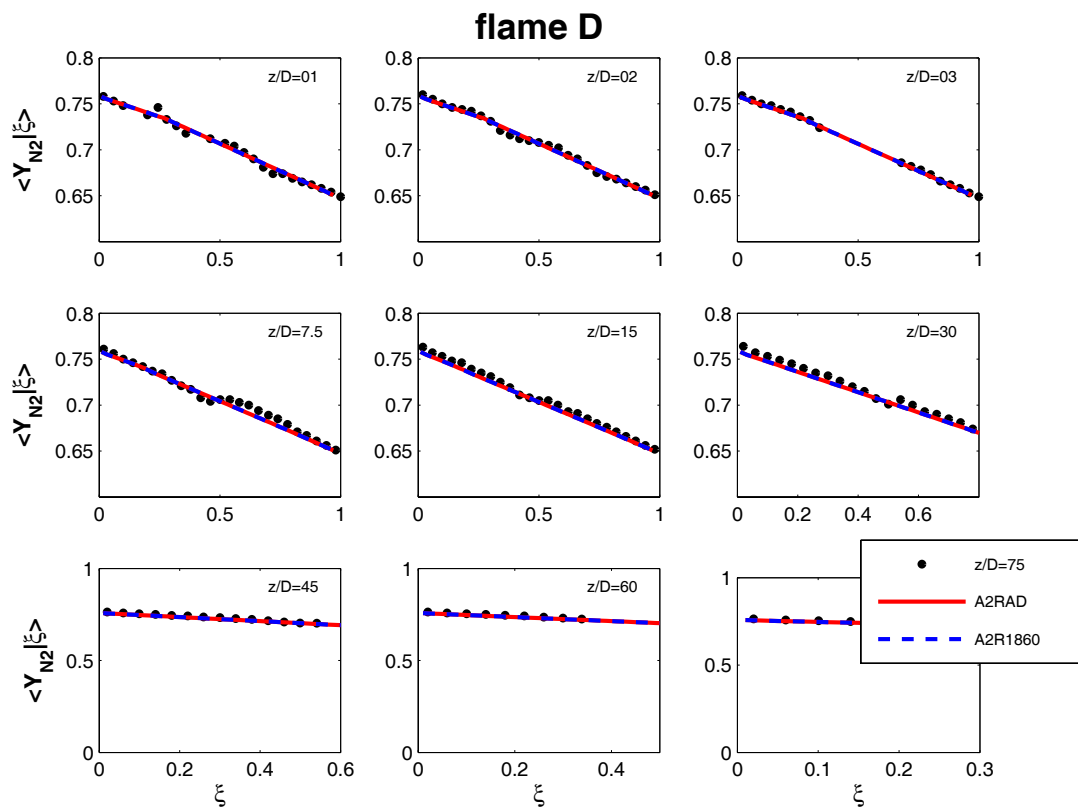


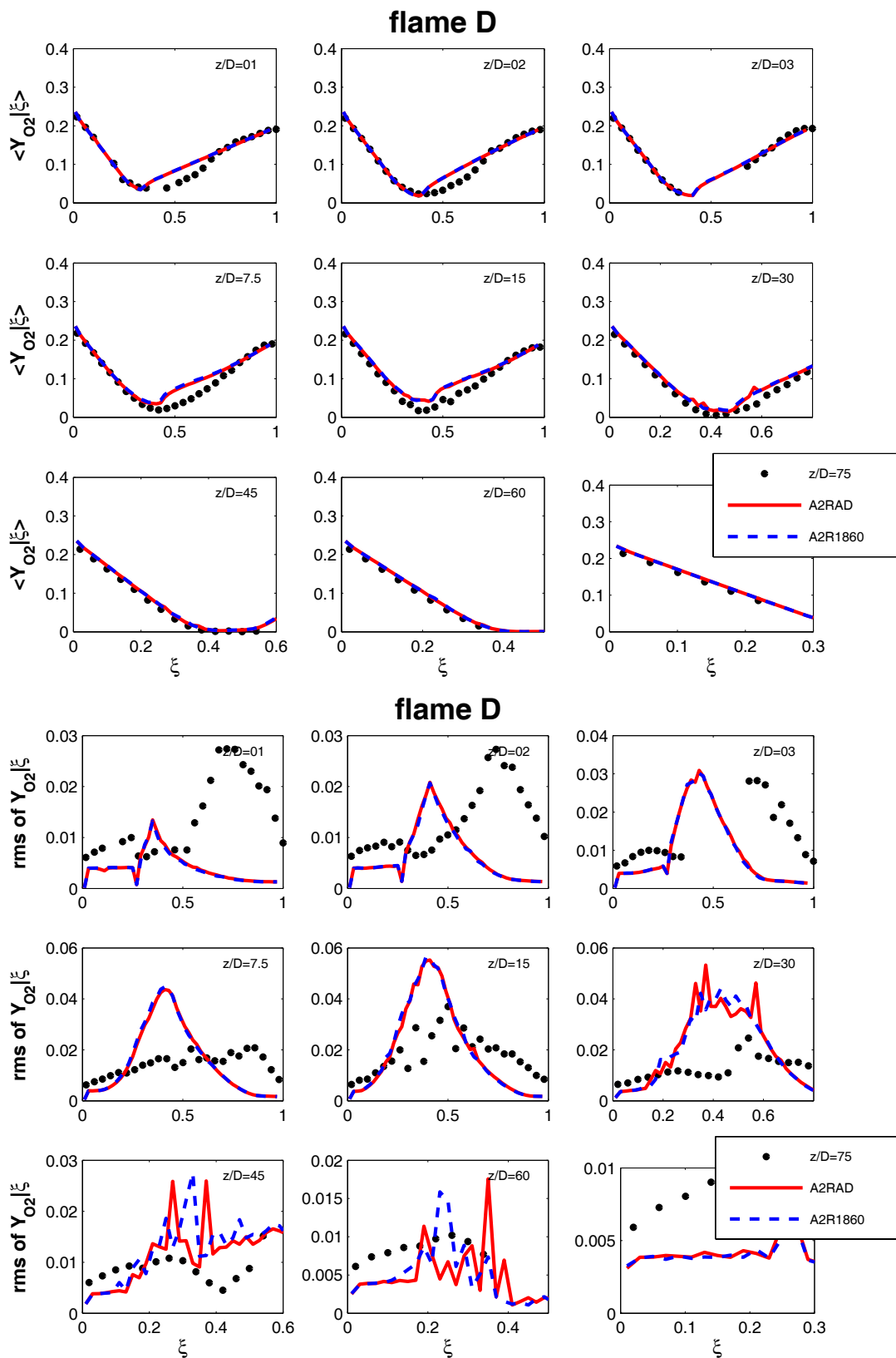
(7) Flame D, effect of piloted jet temperature on NO

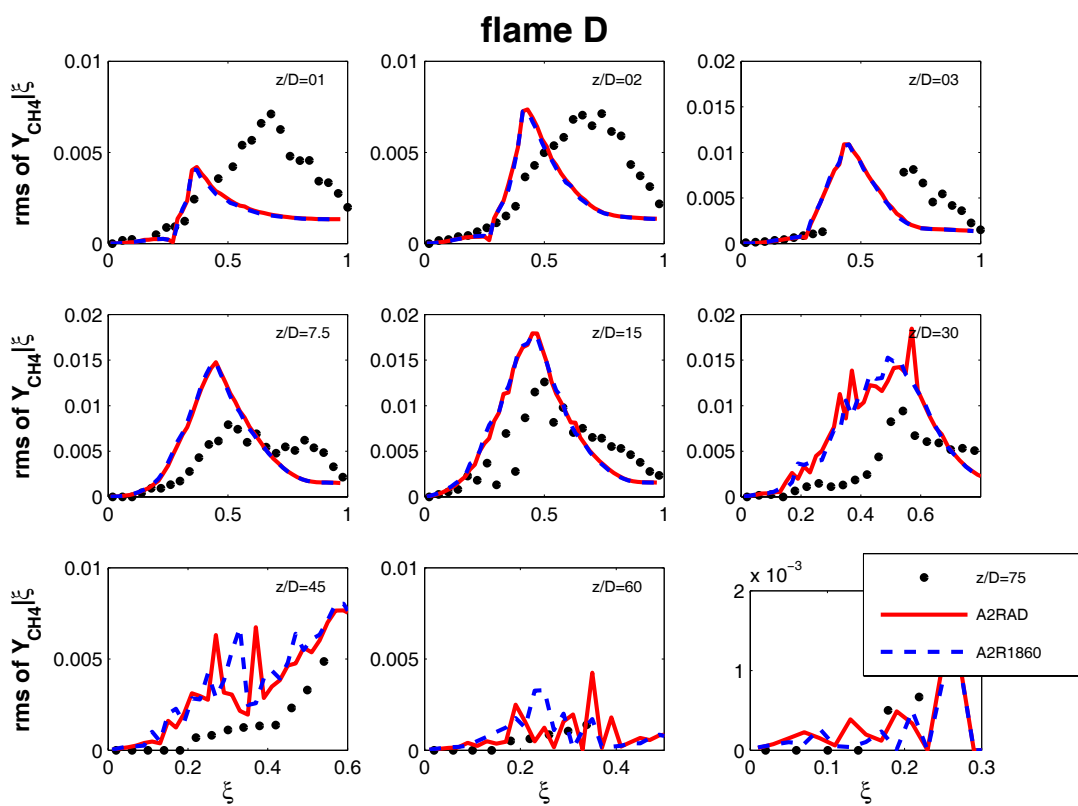
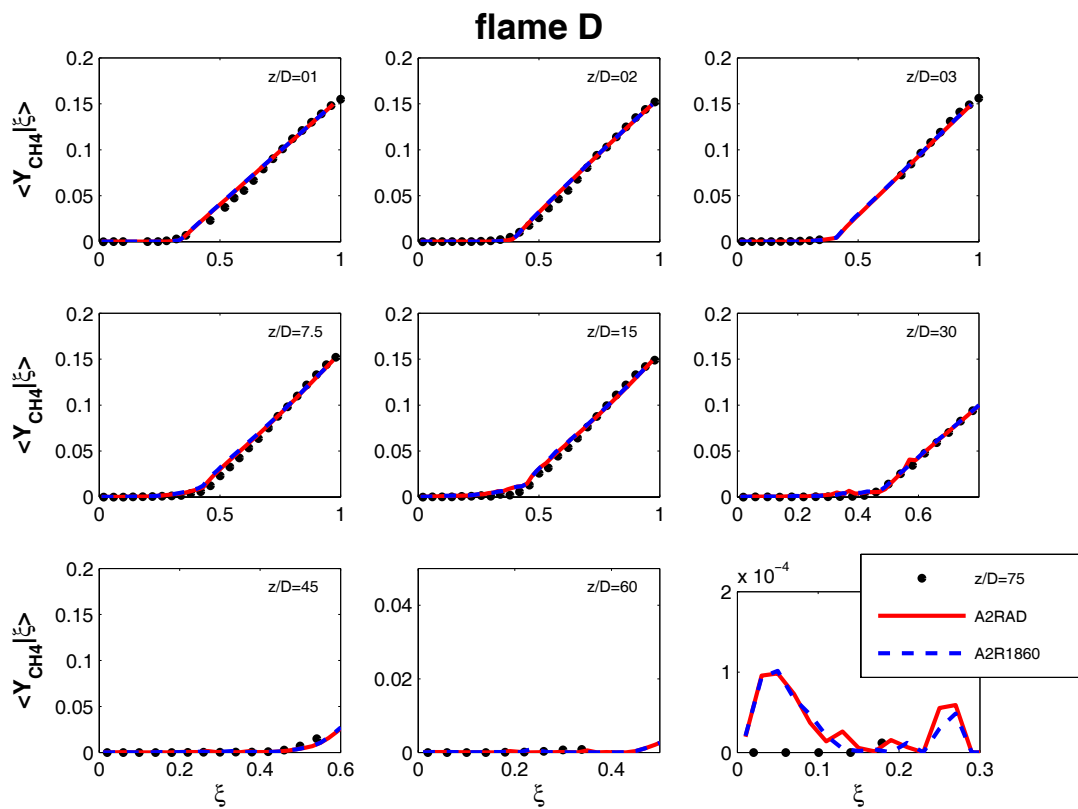


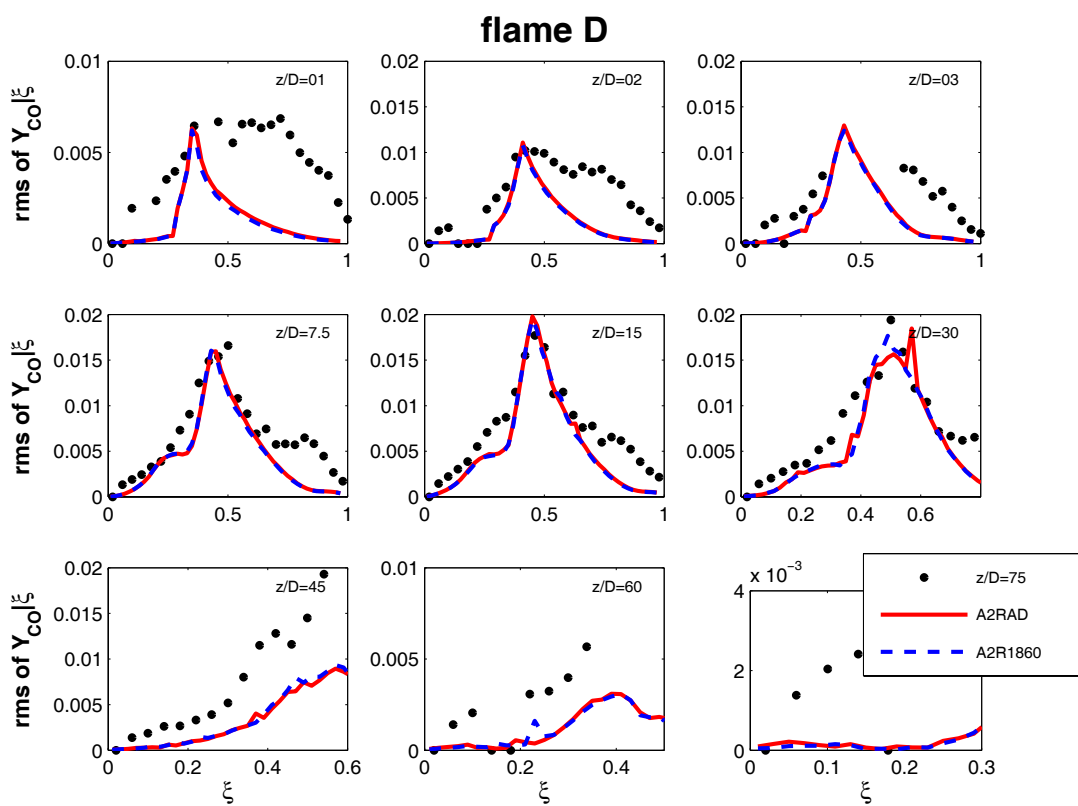
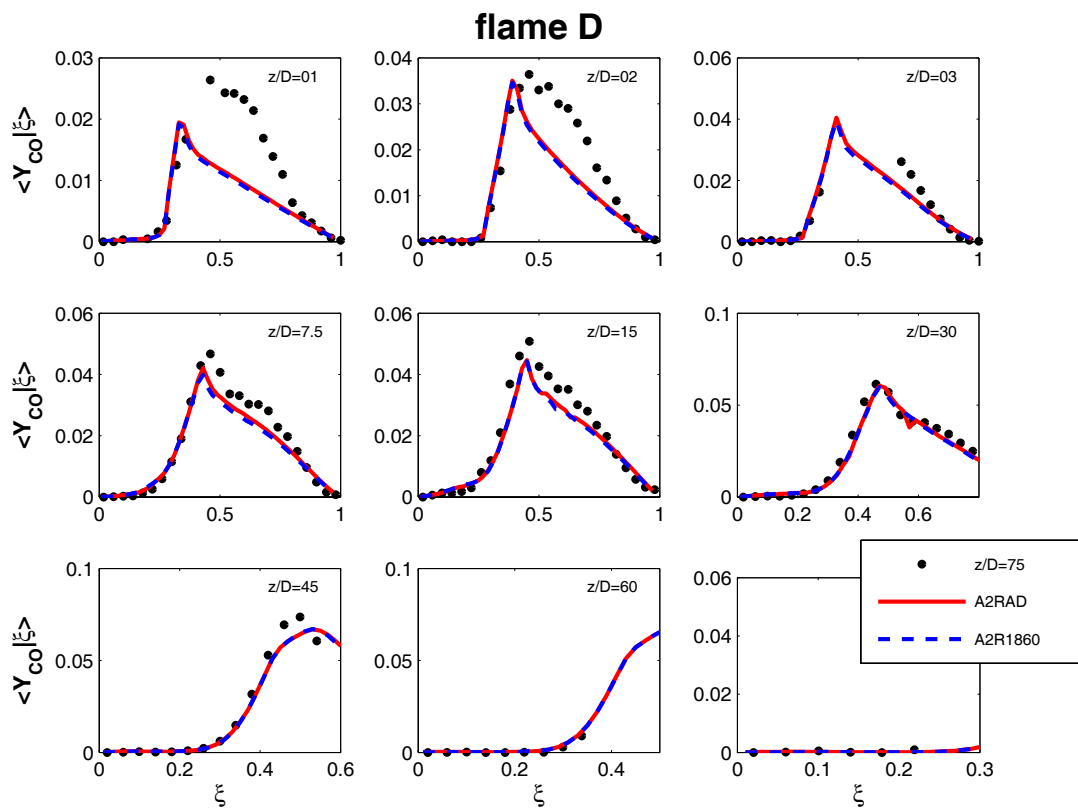


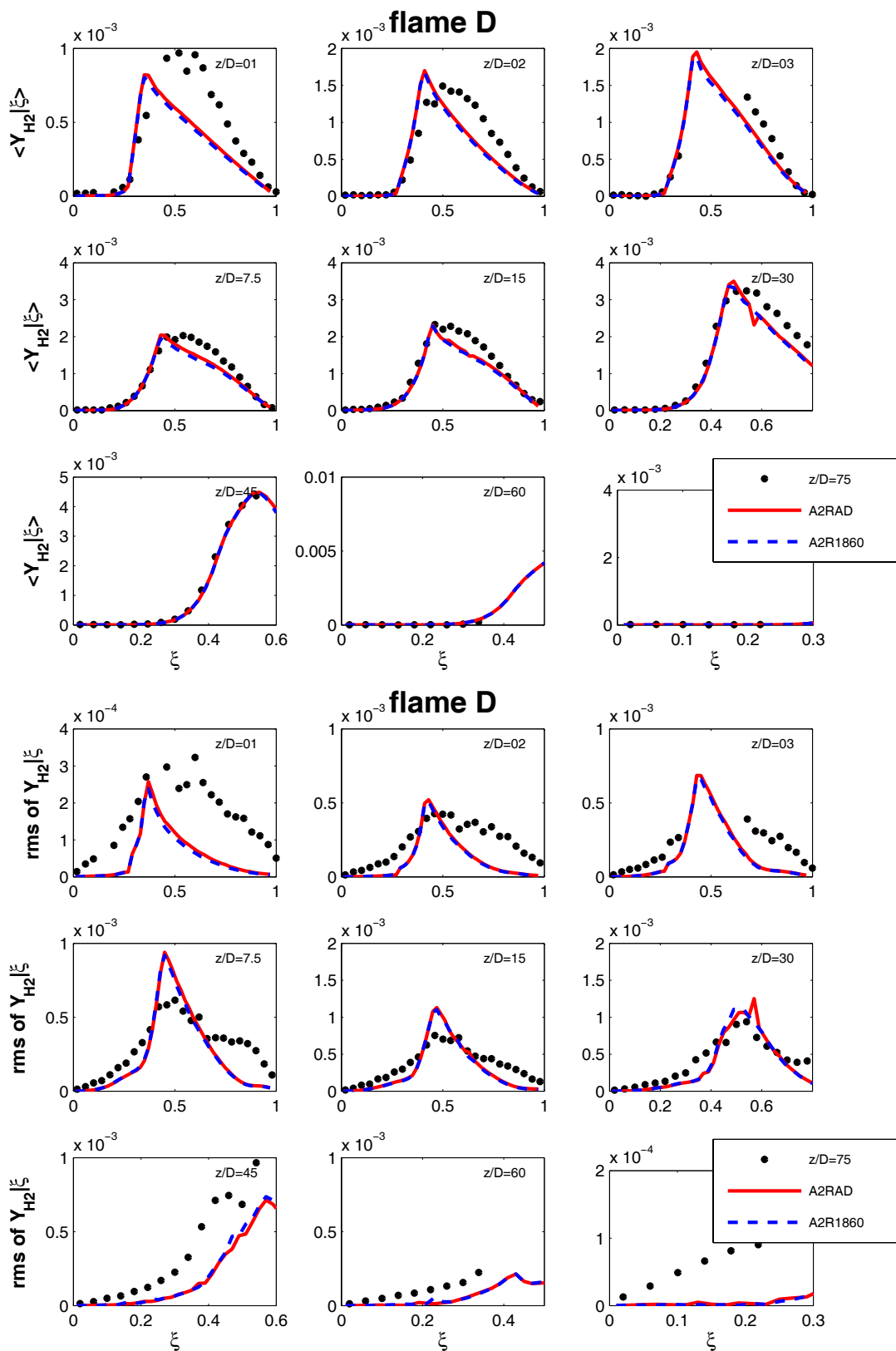


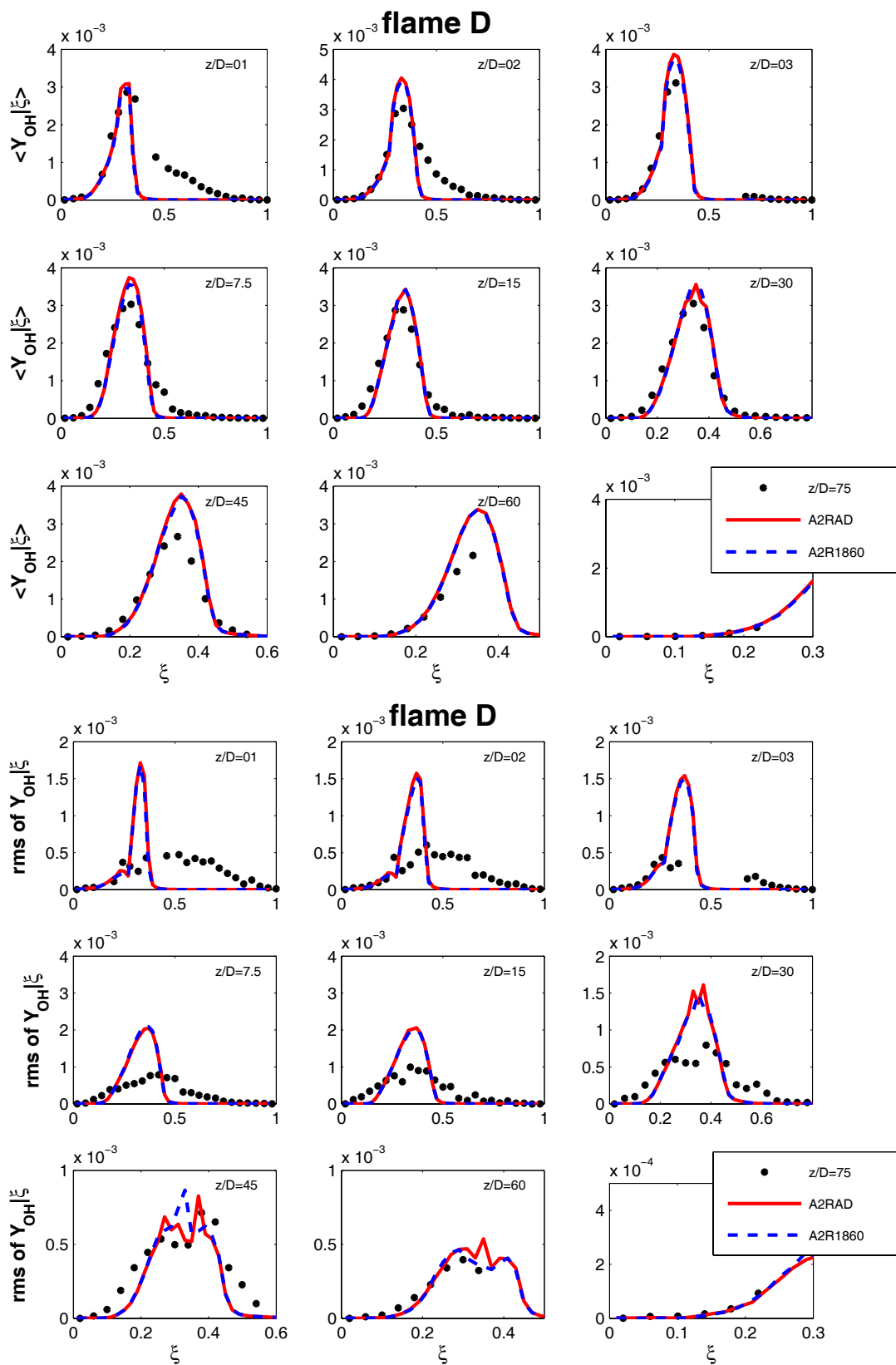


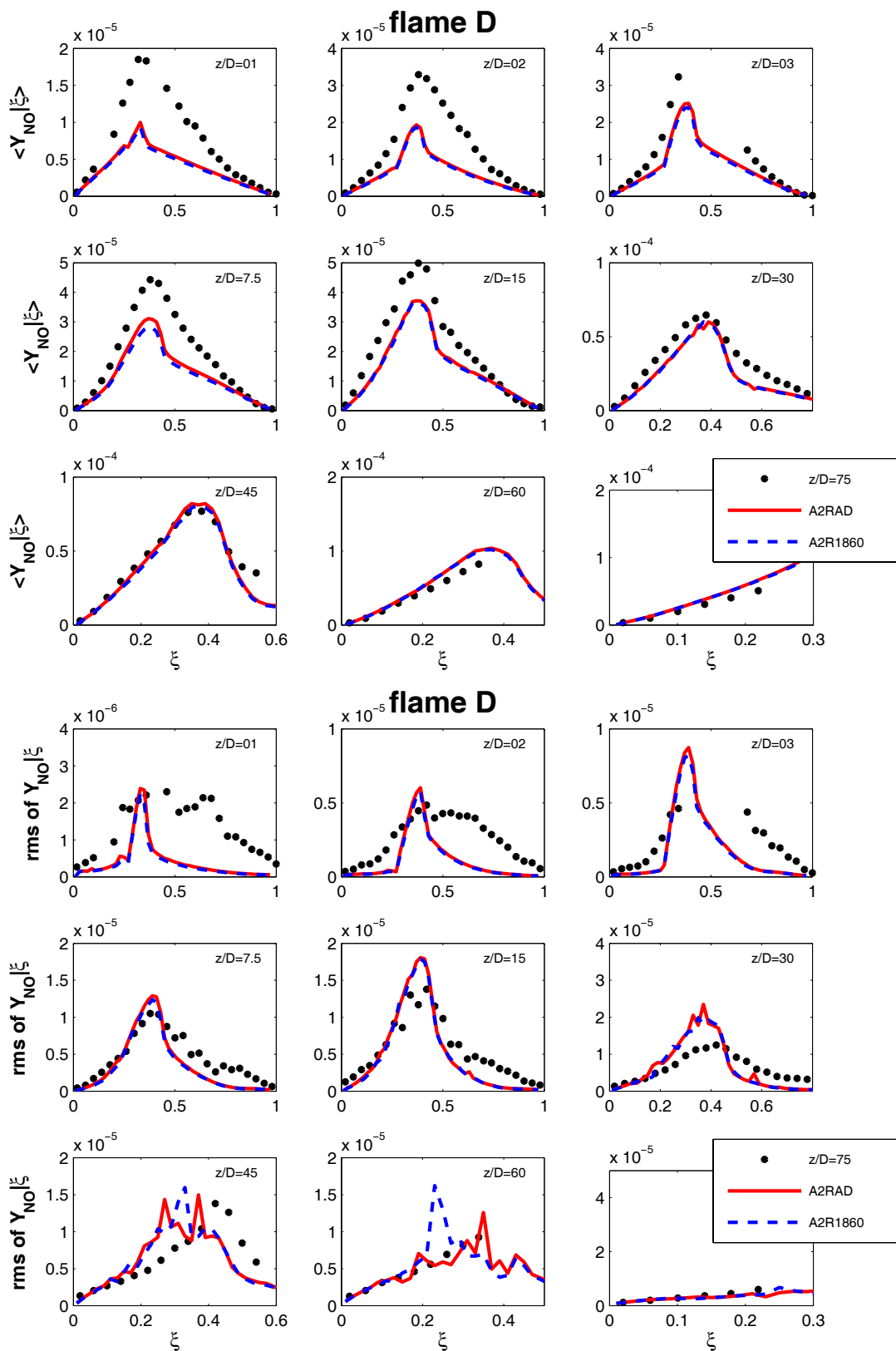








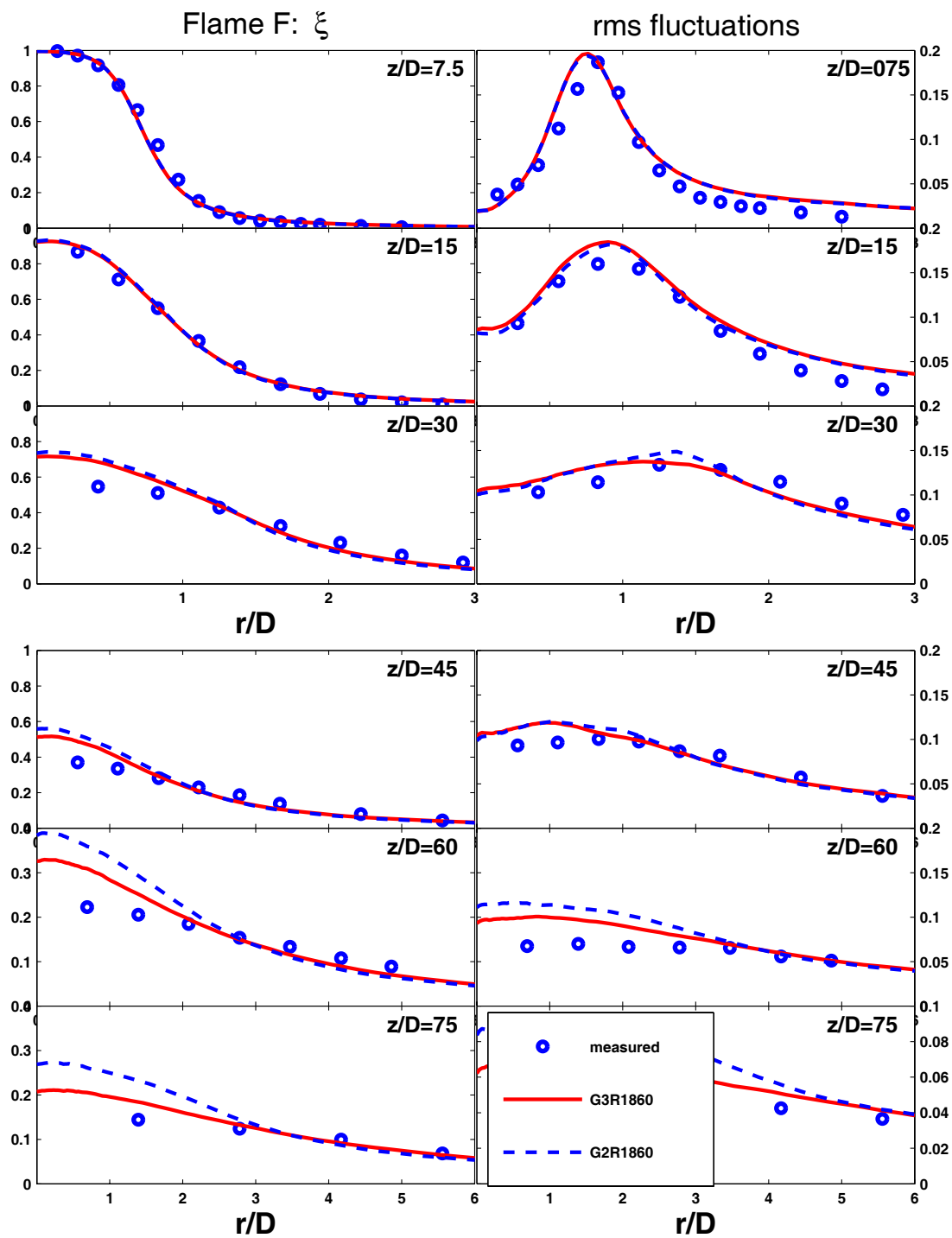


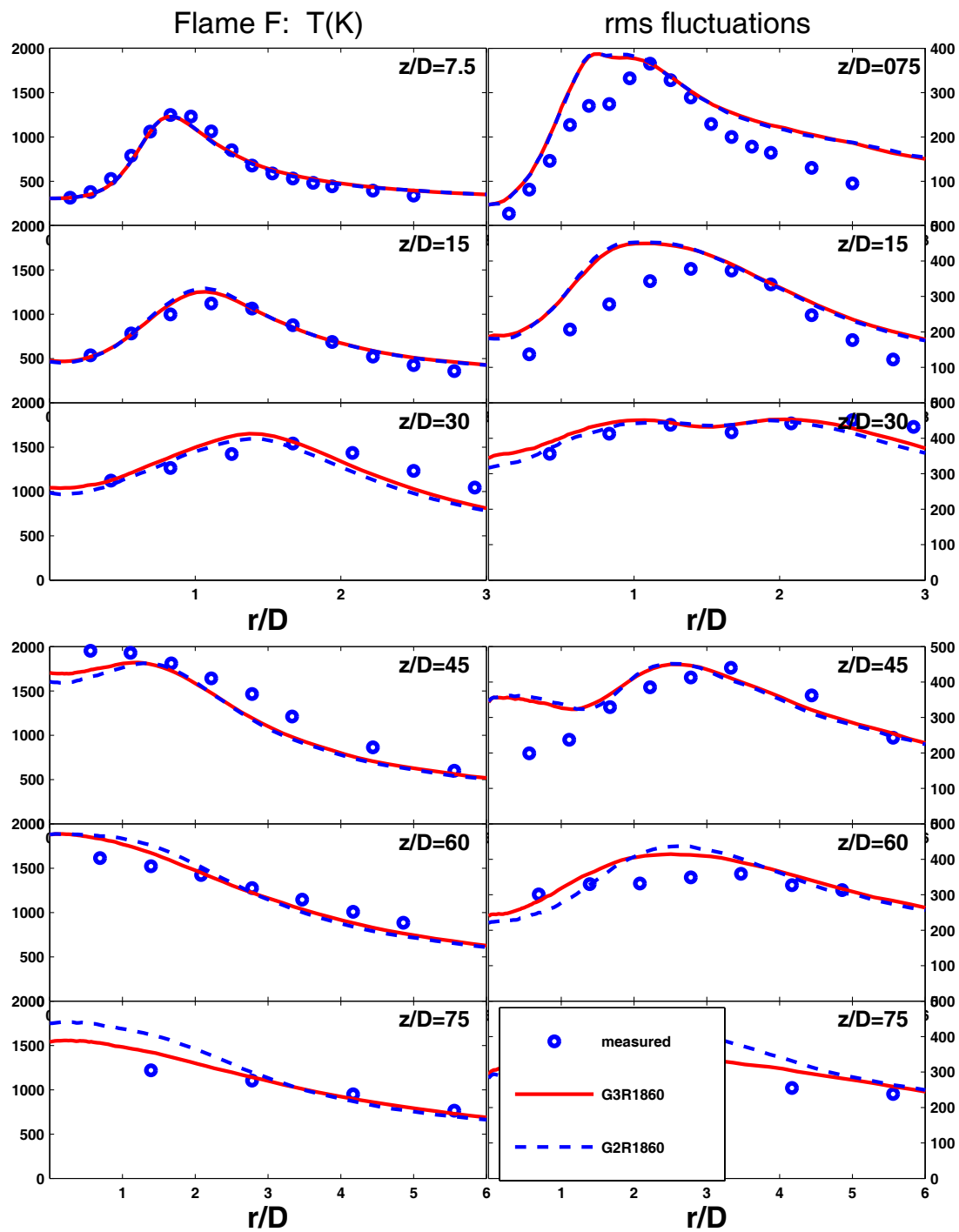


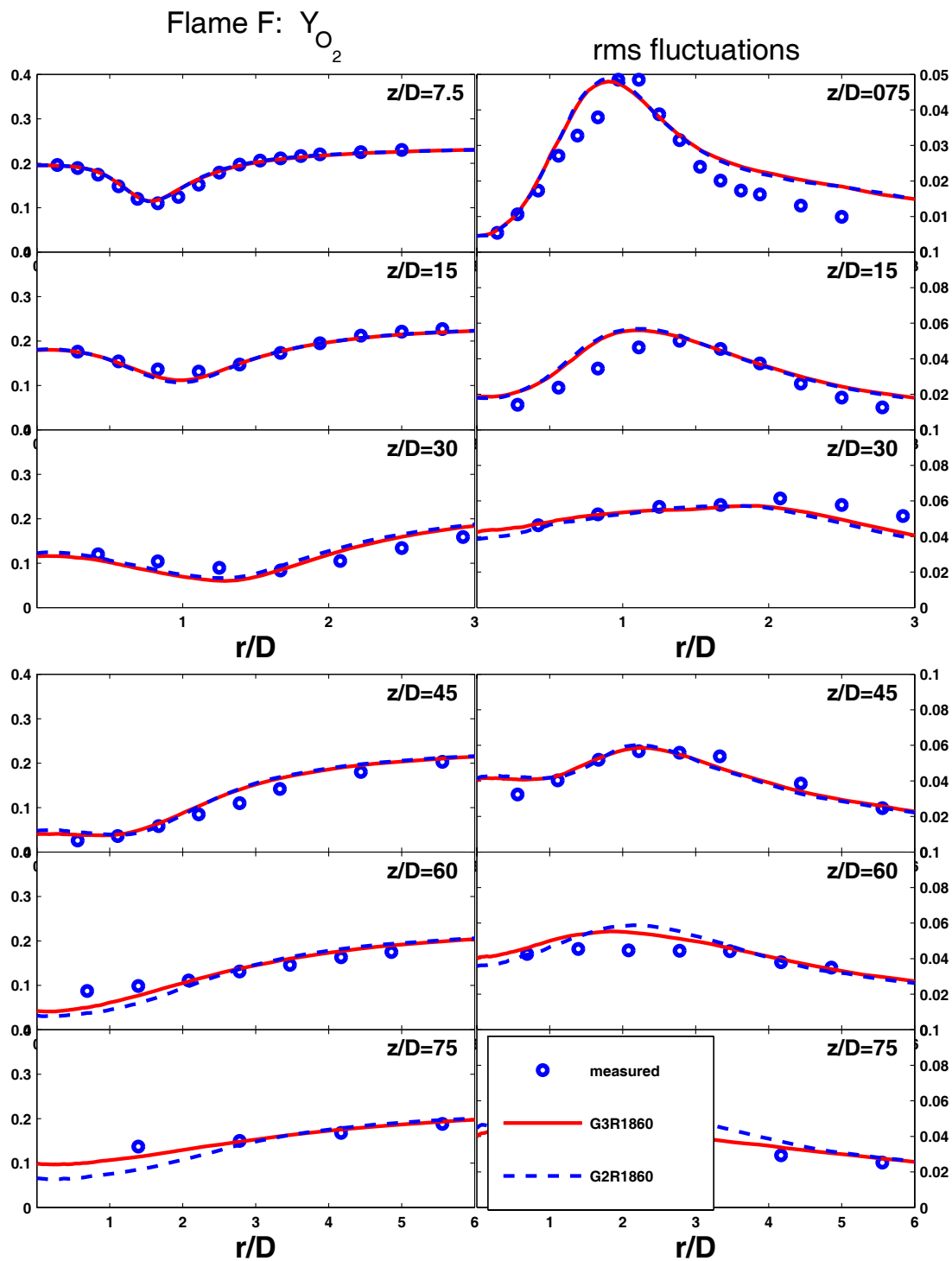
Part C: Unconditional means and rms's

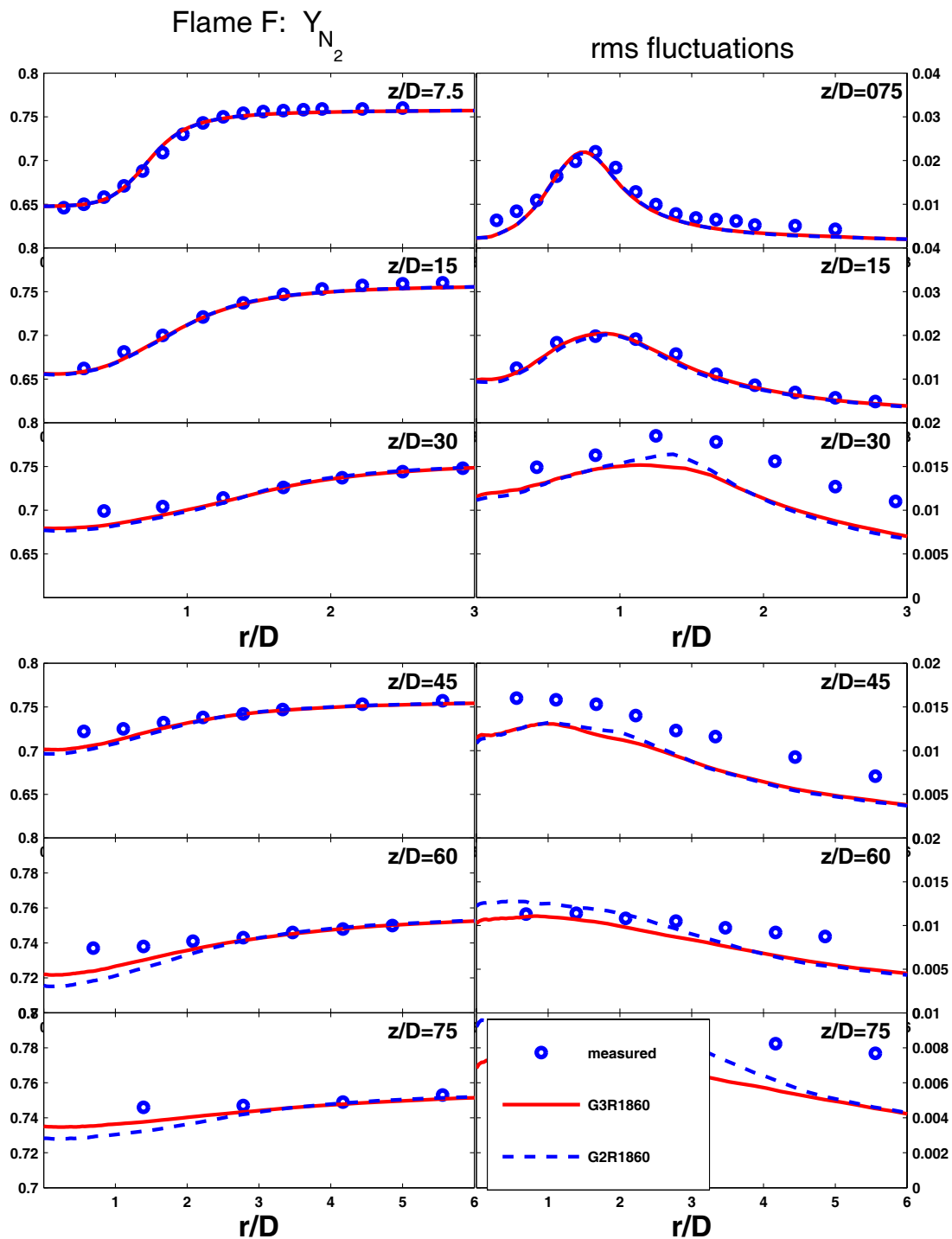
C-1 Calculations using GRI3.0 and GRI2.11 with base case configuration

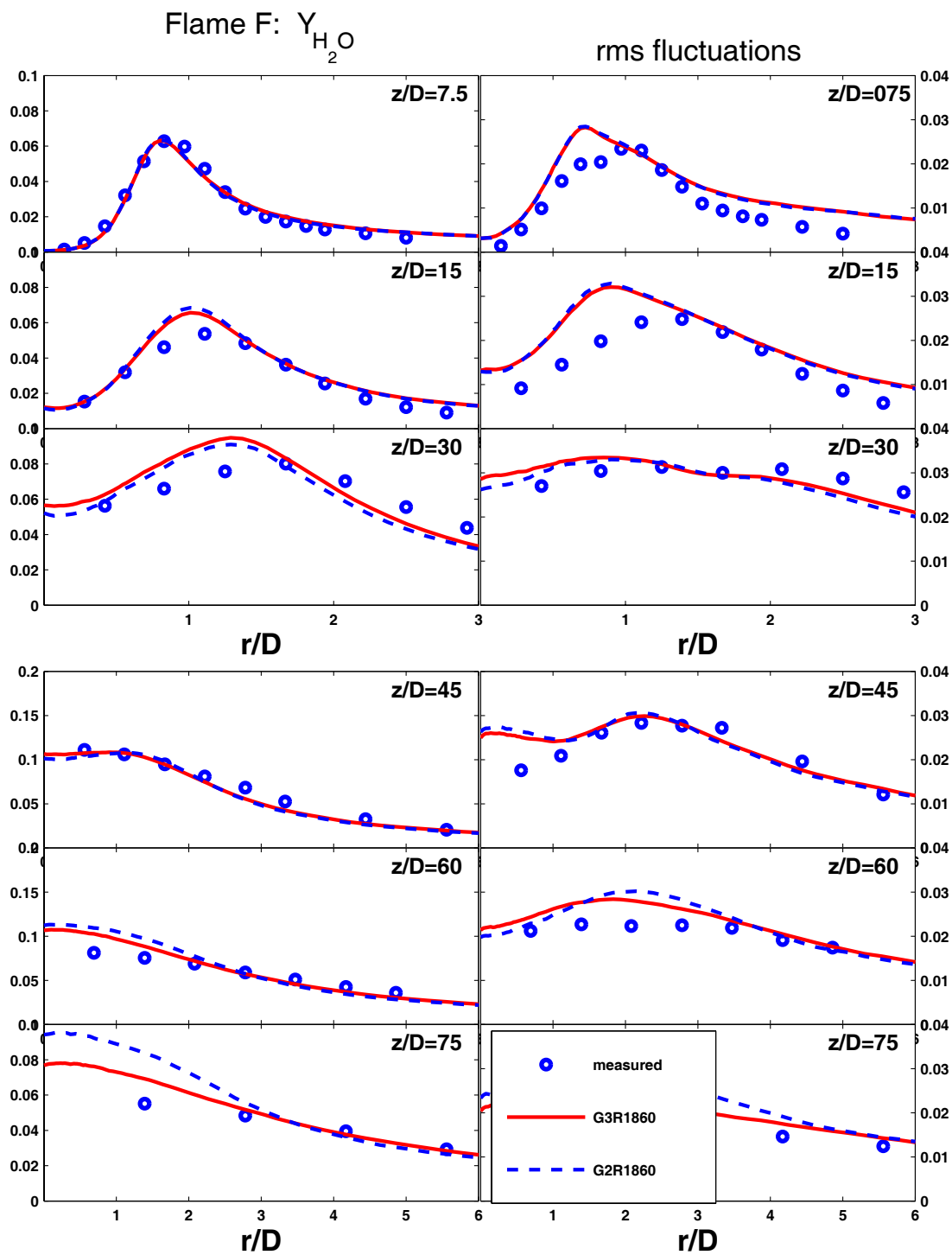
(1) Flame F

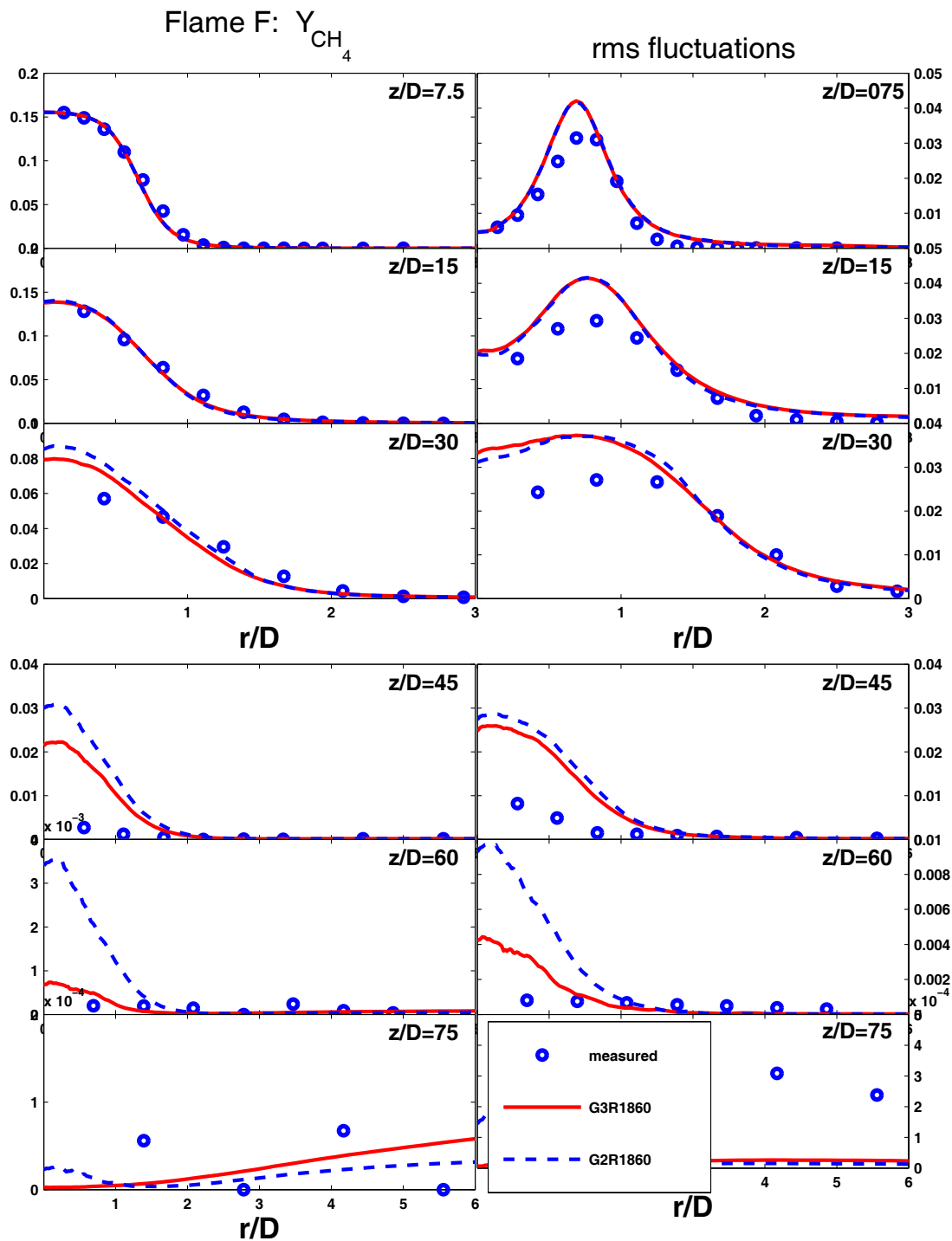


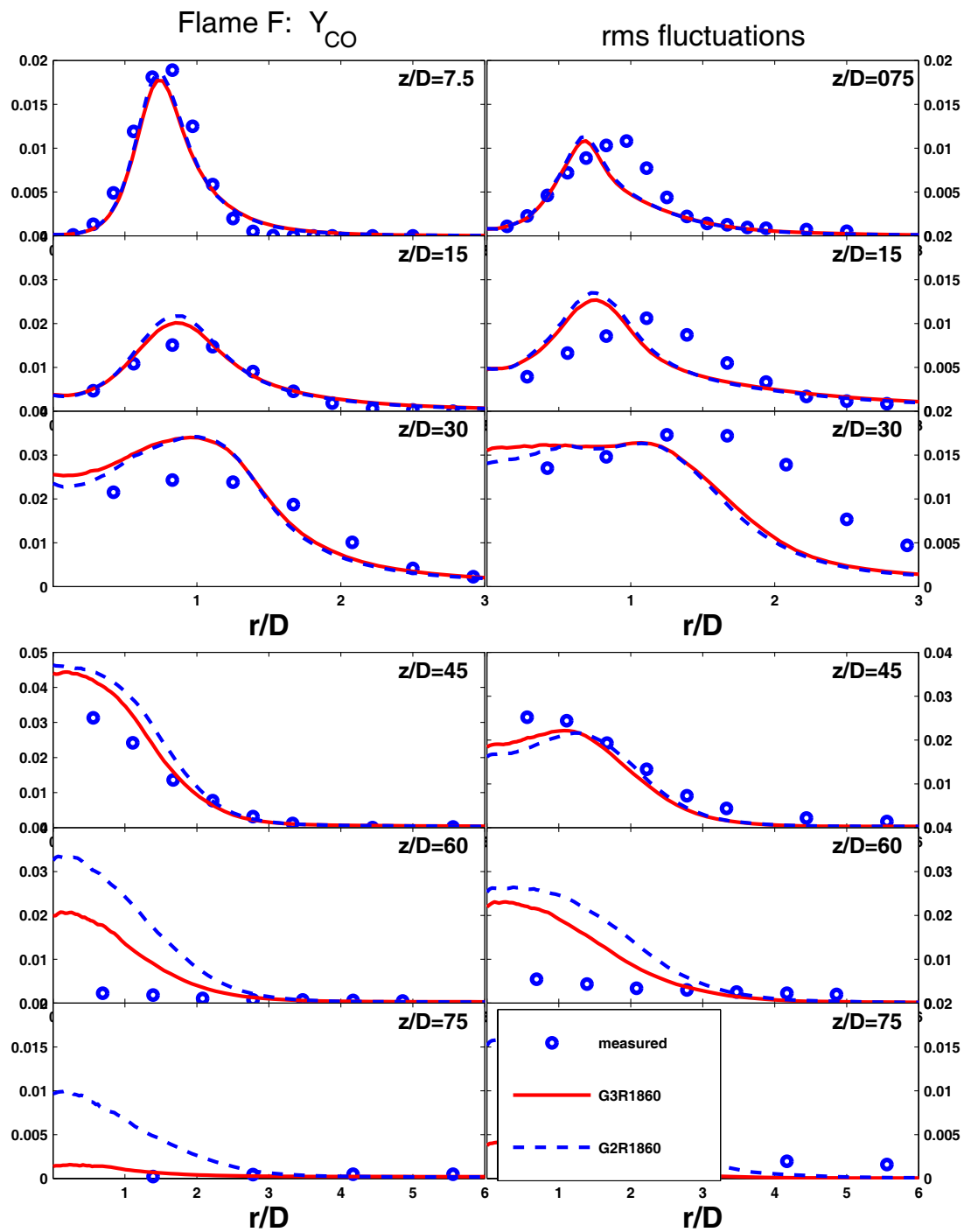


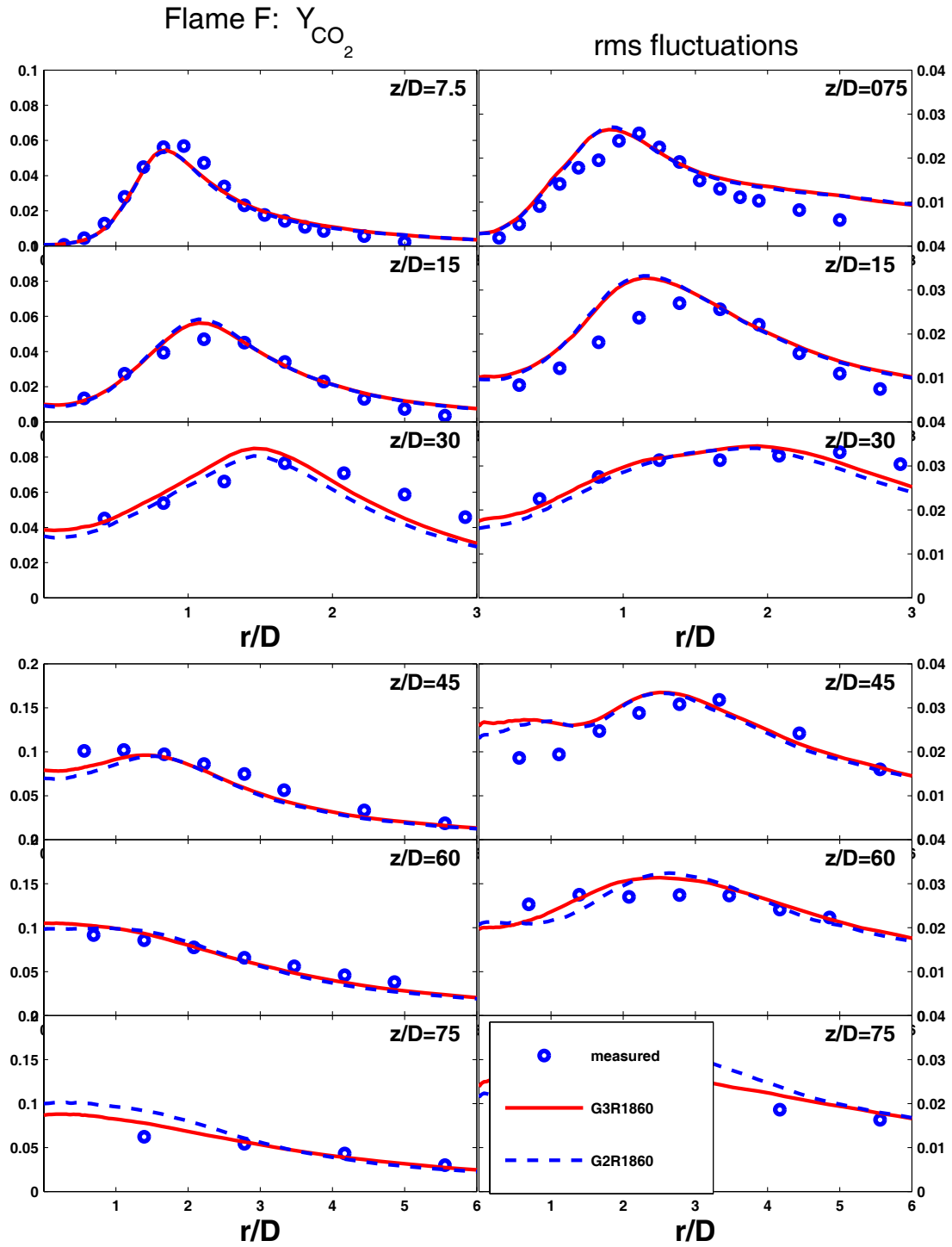


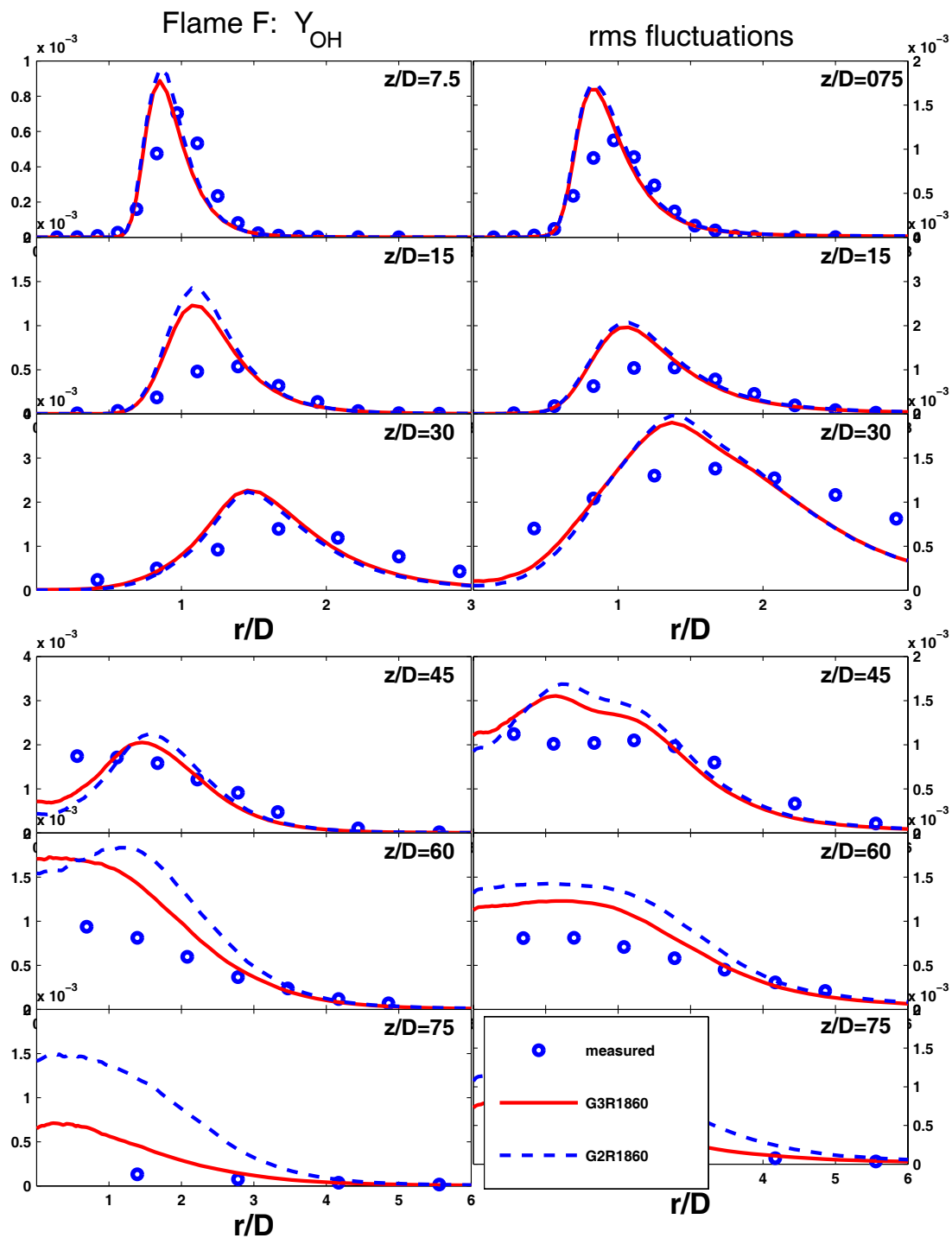


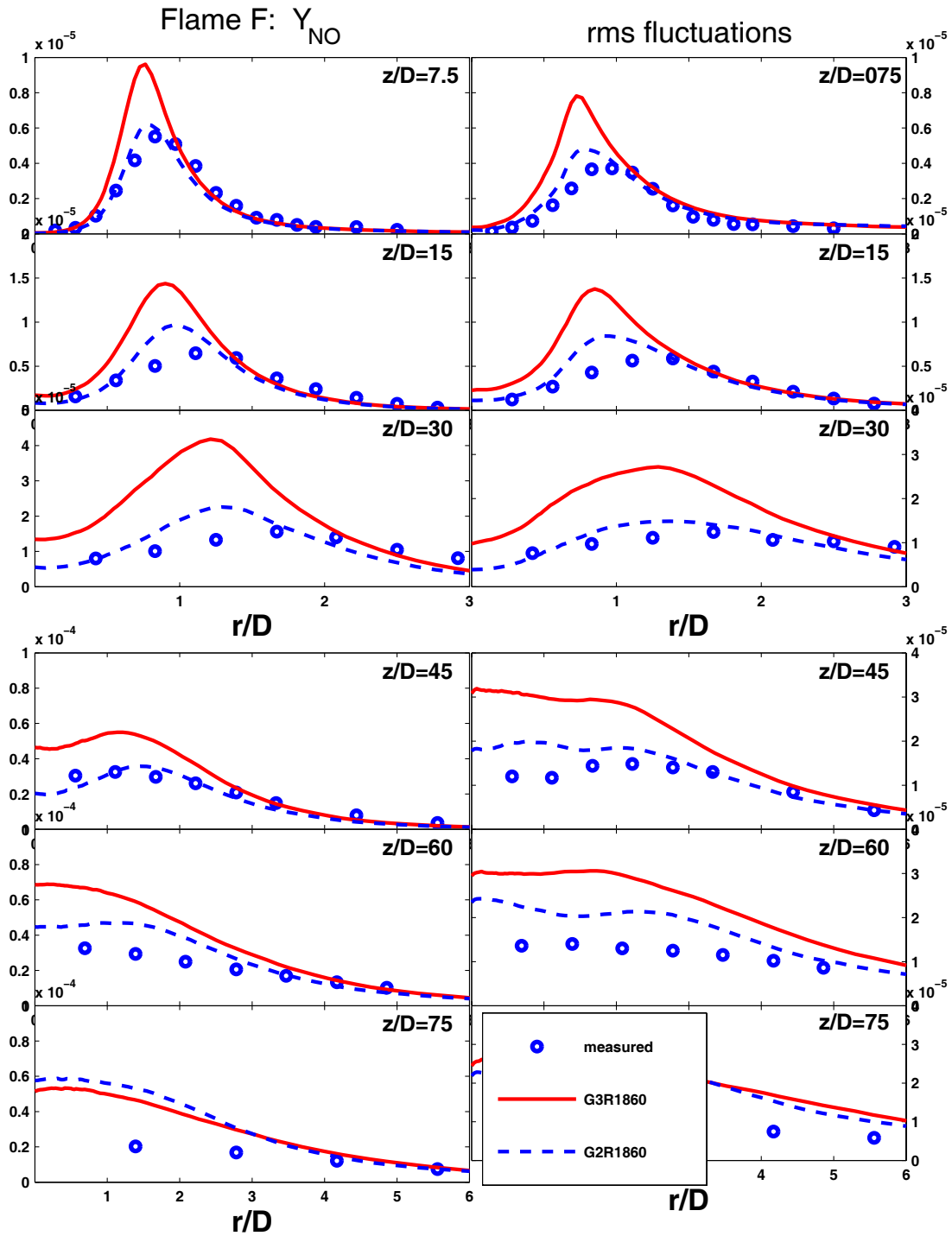




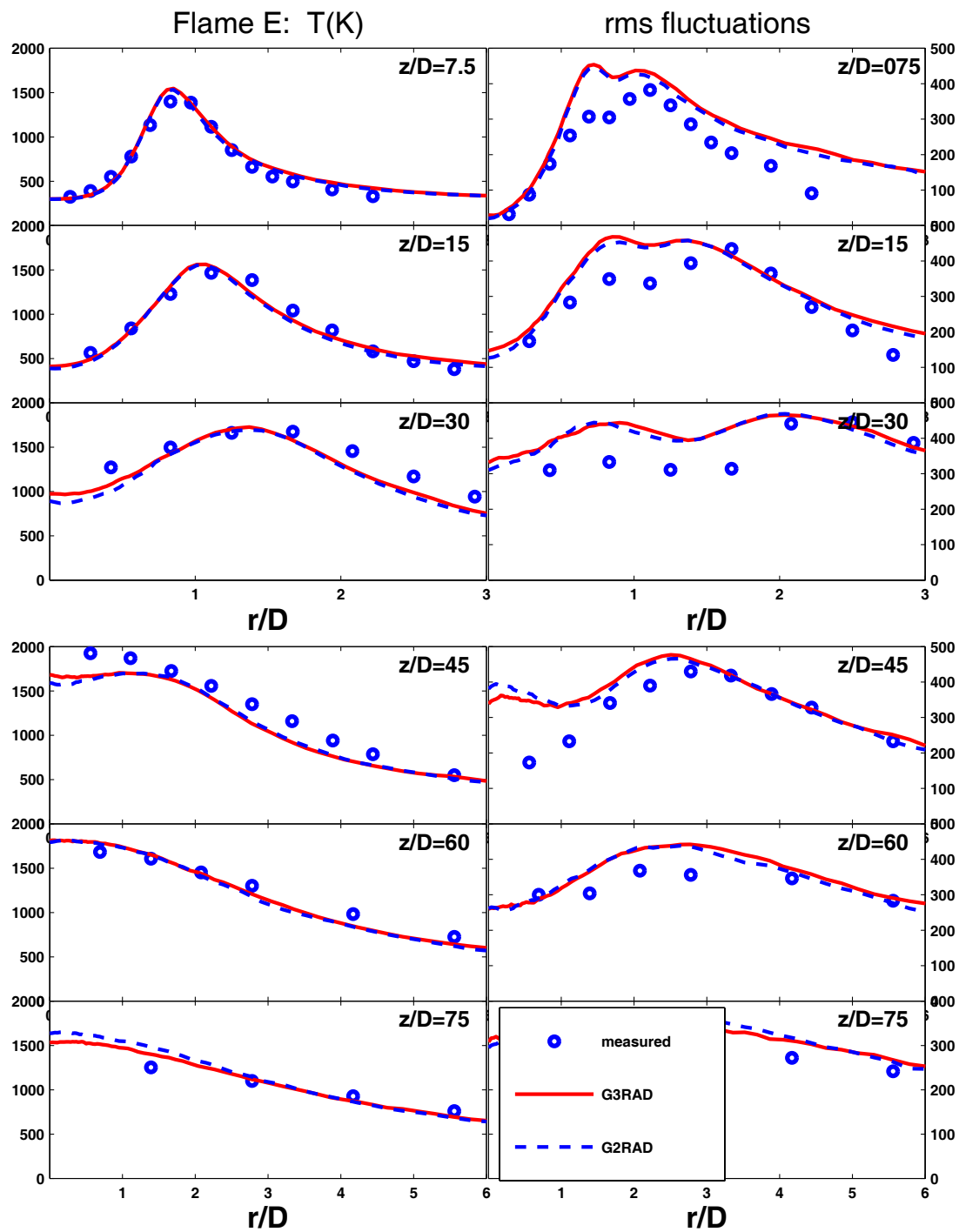


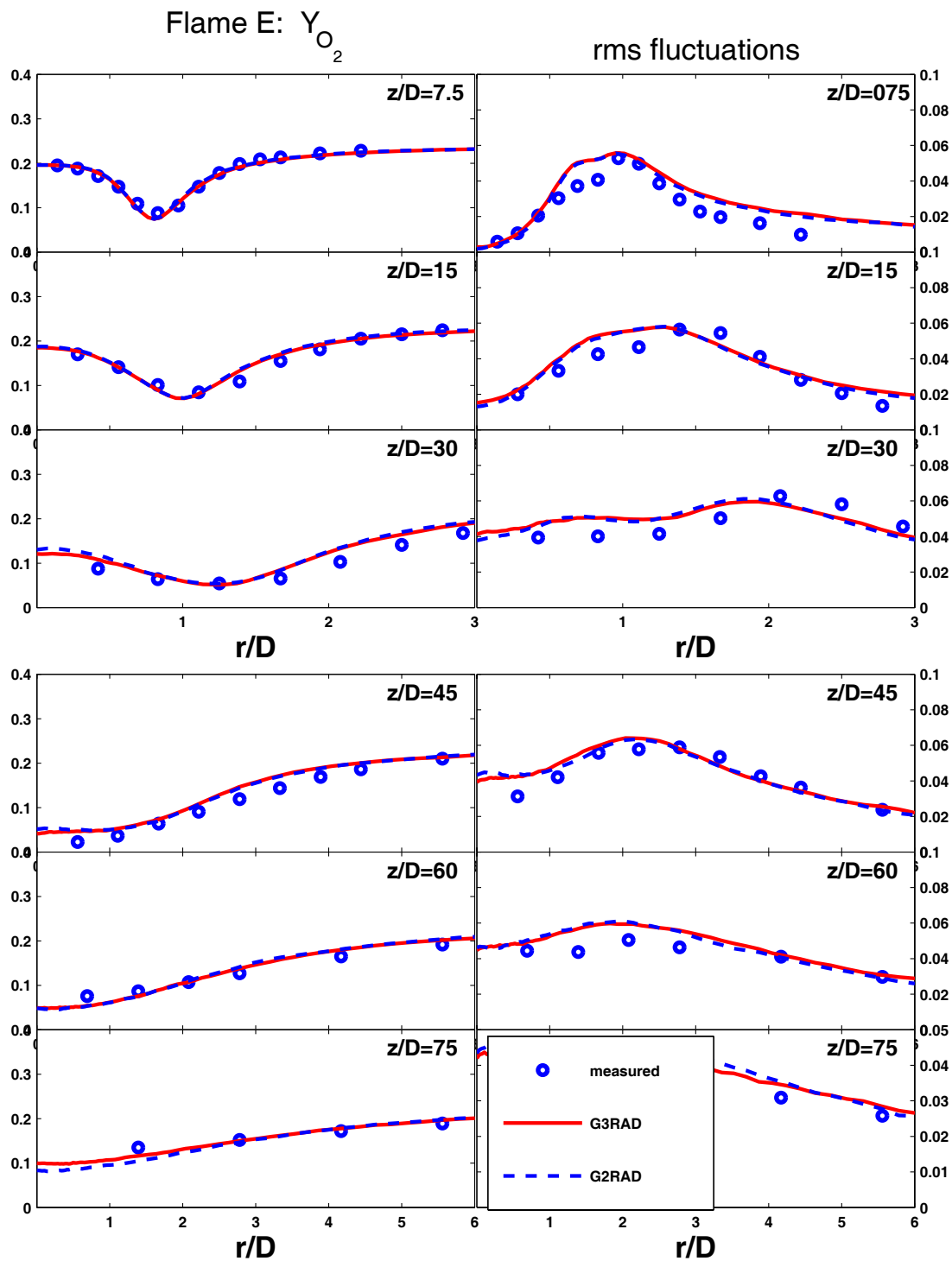


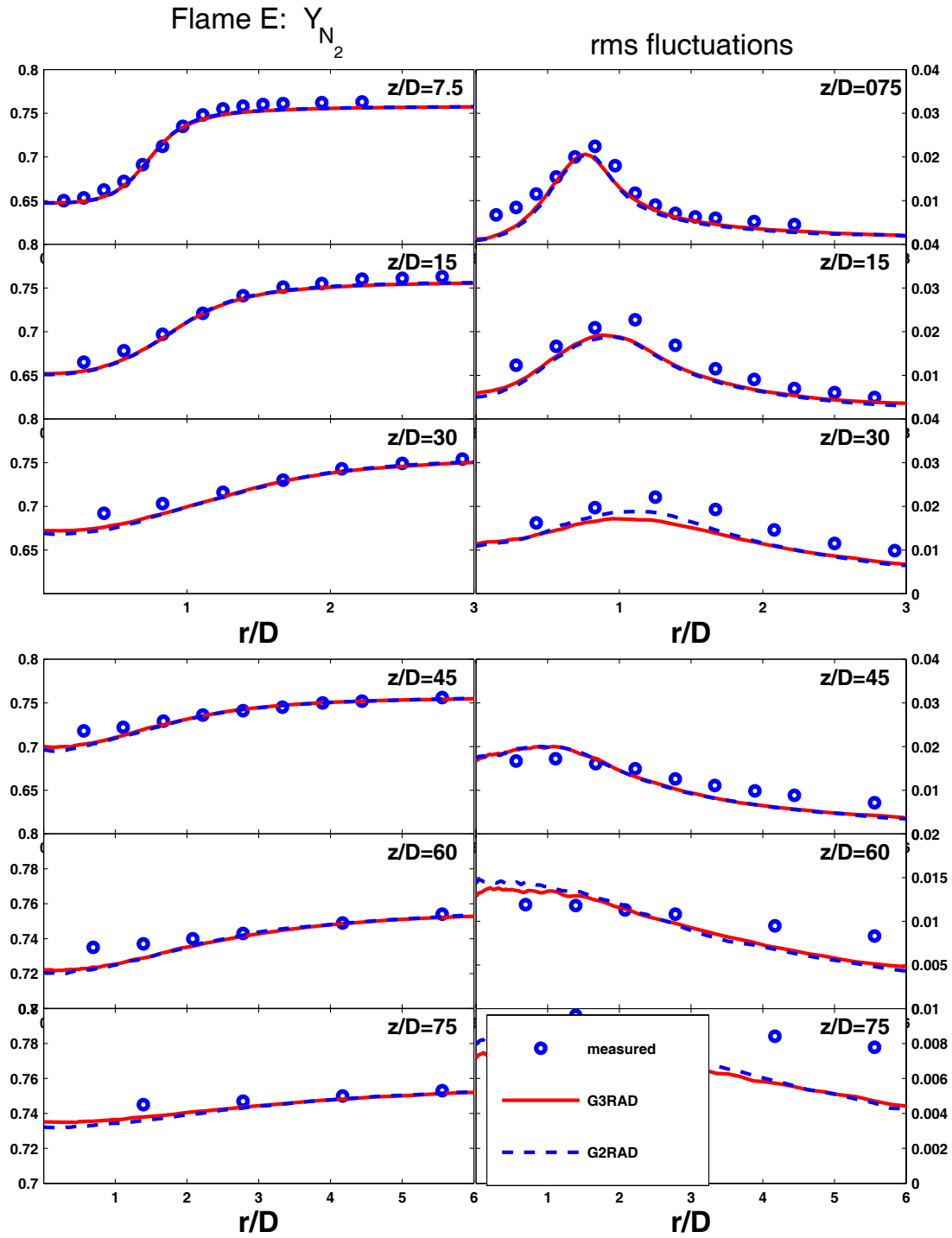


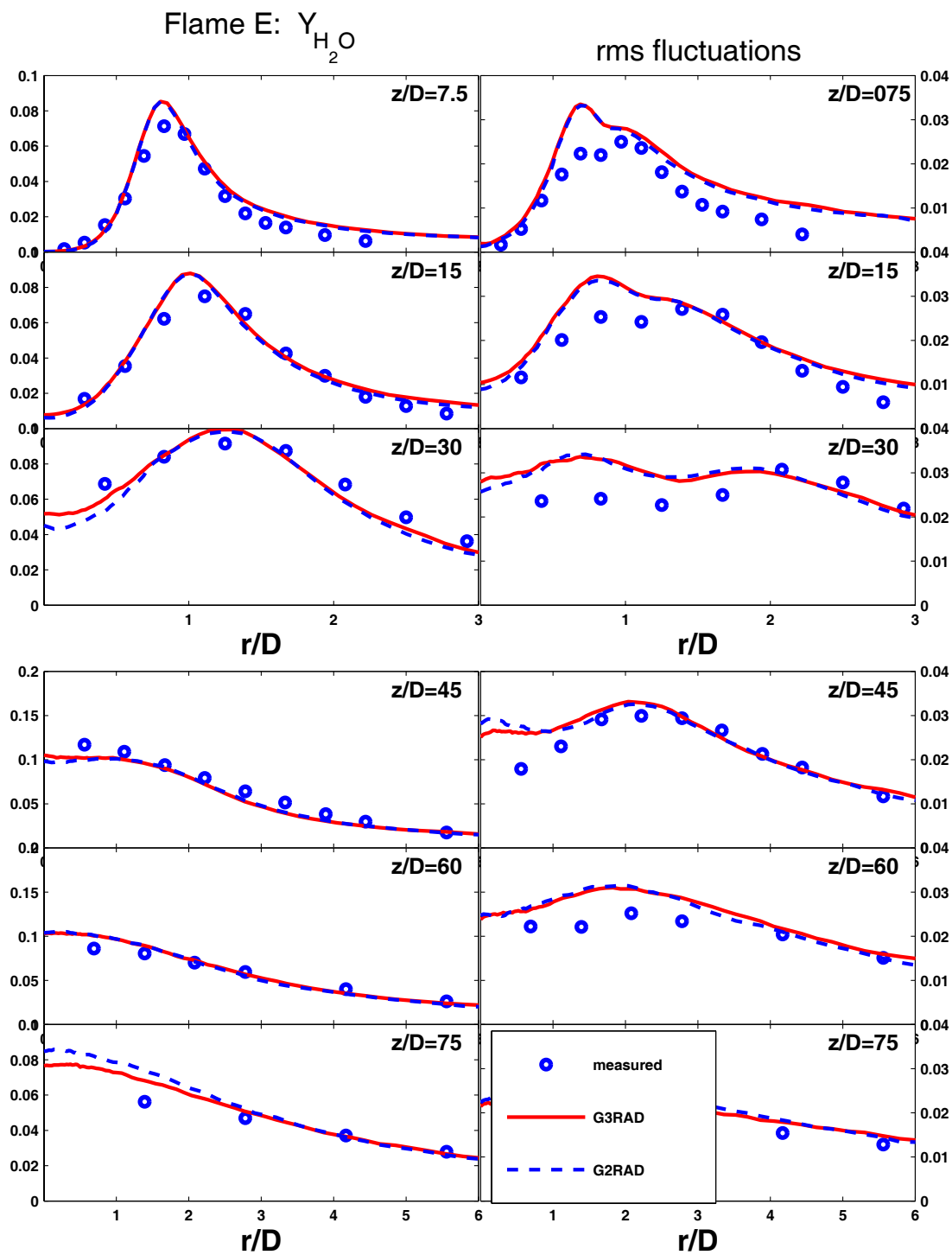


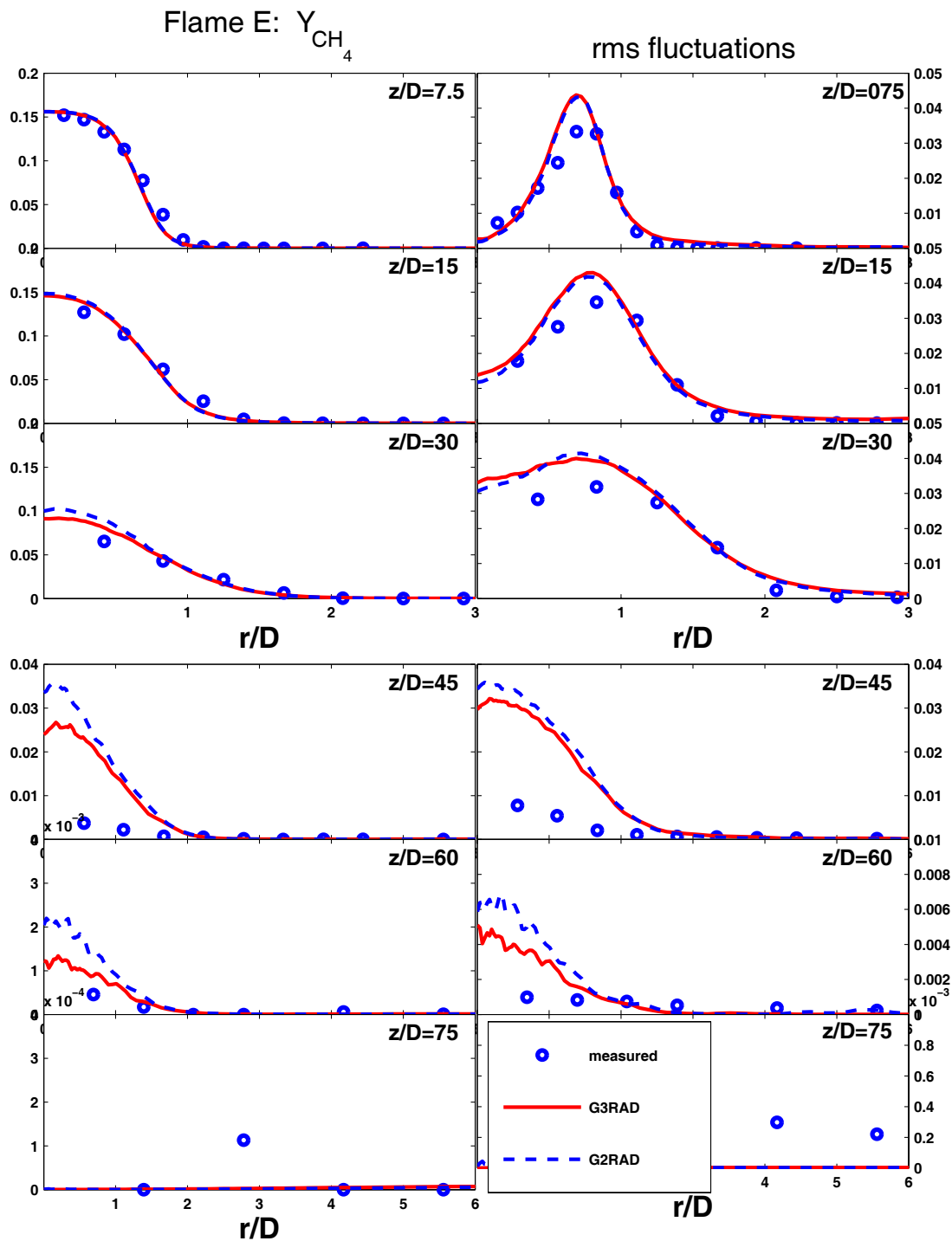
(2) Flame E

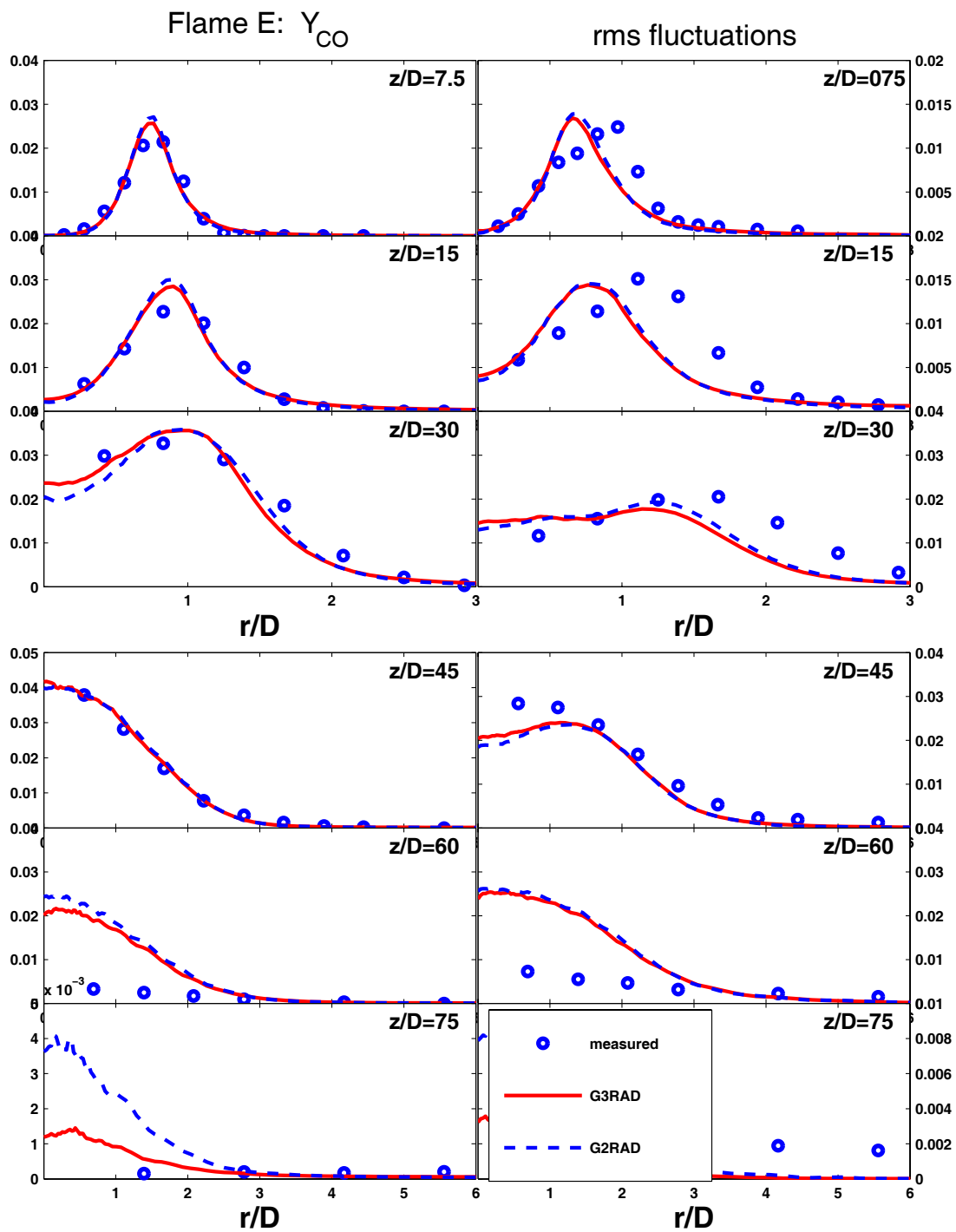


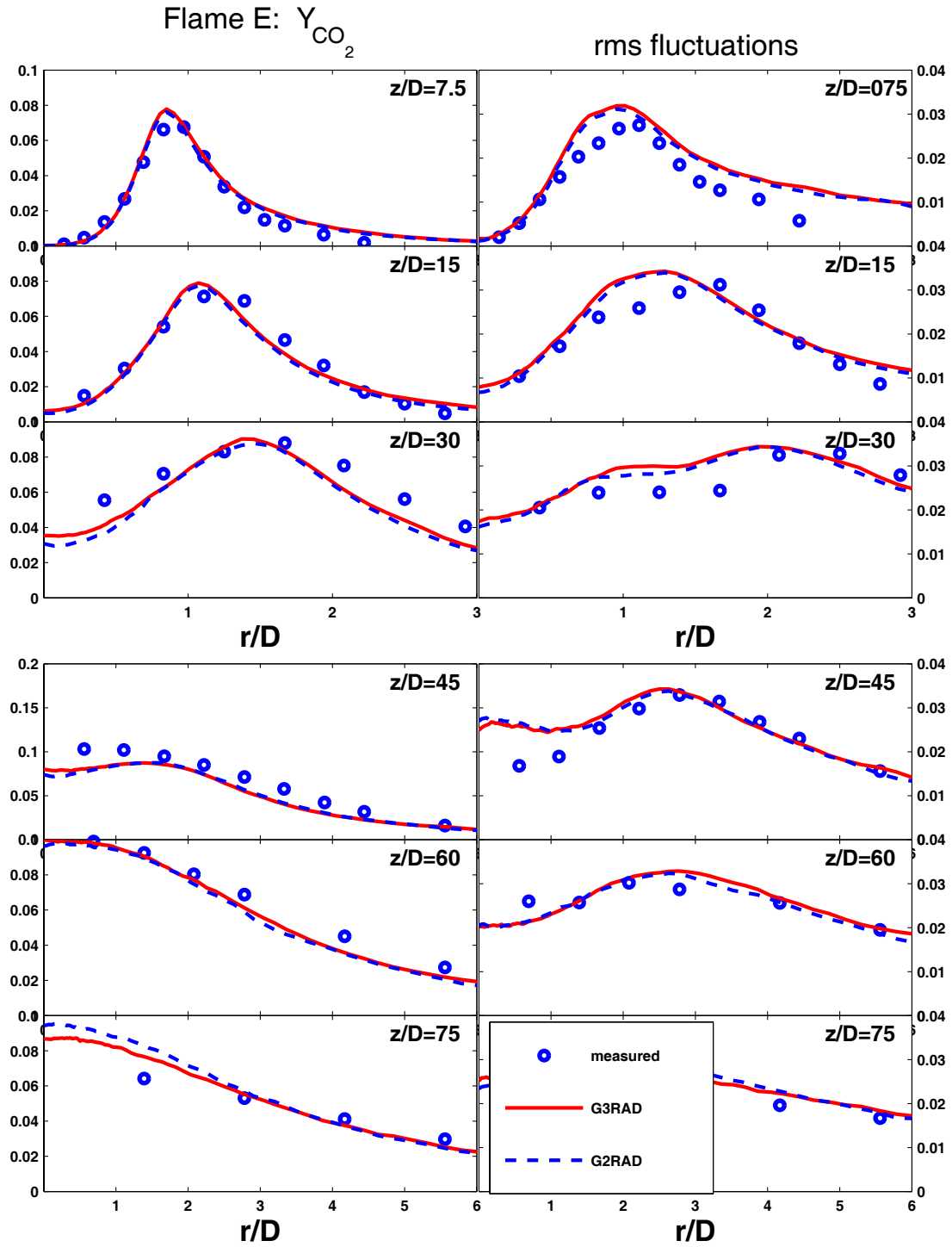


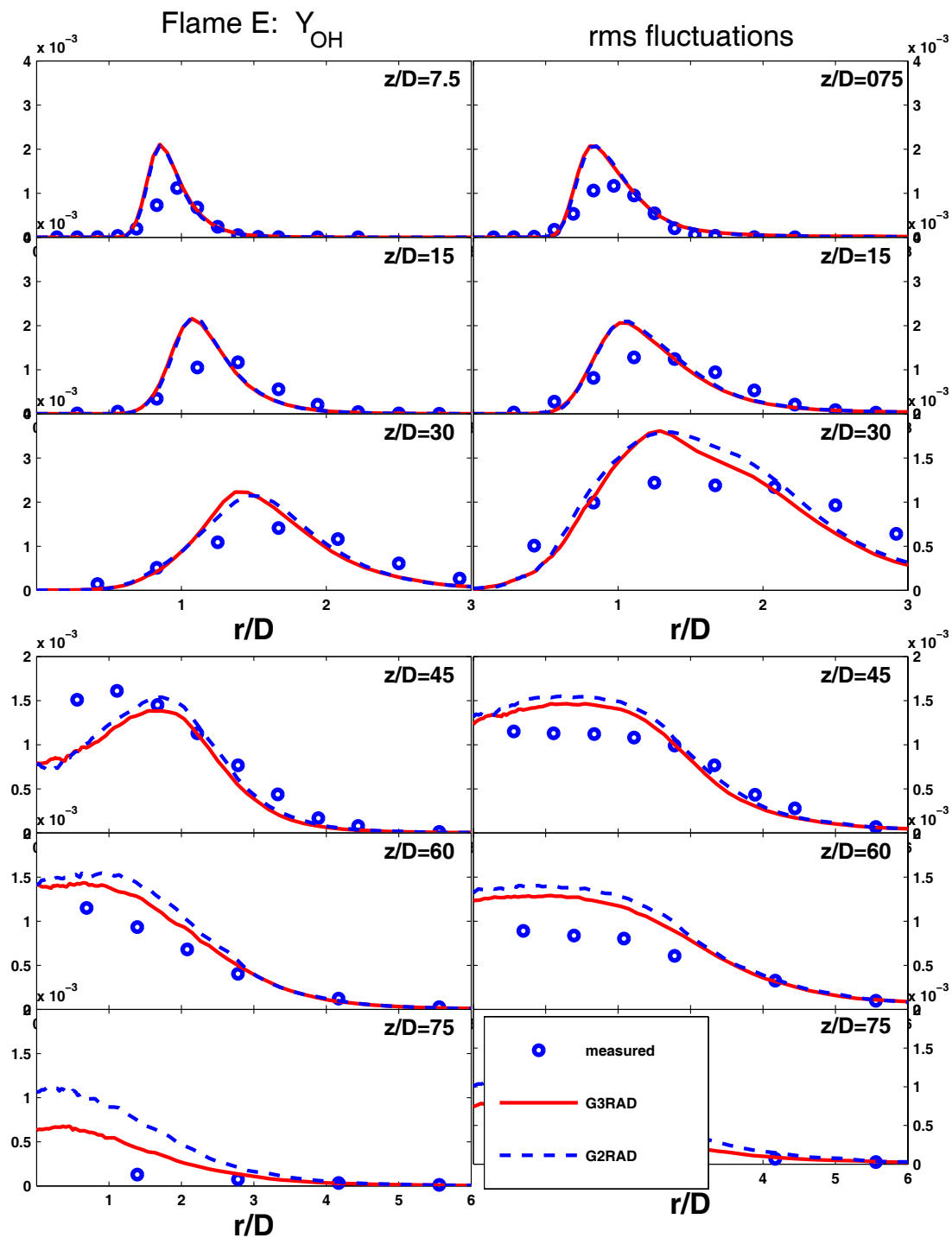


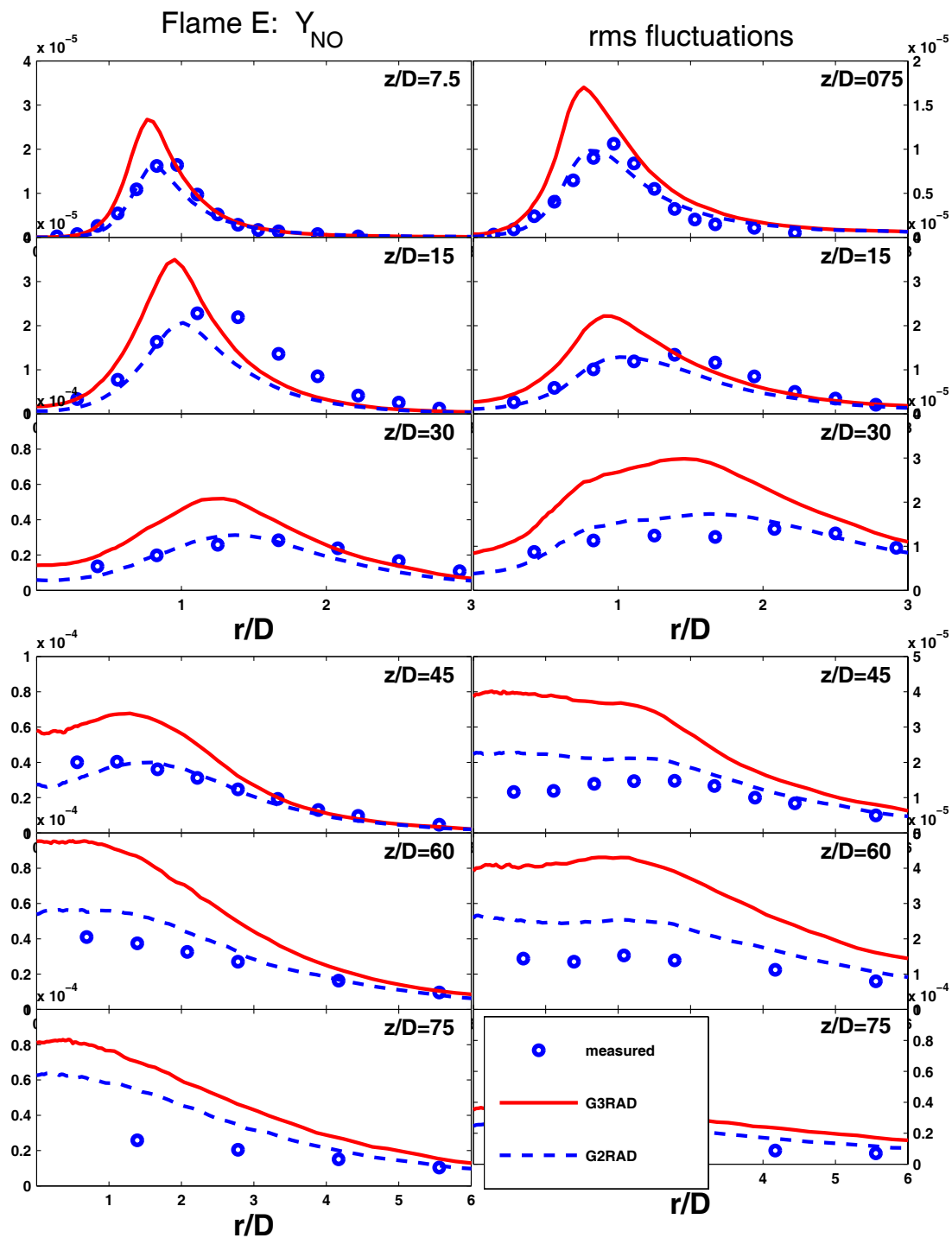












(3) Flame D

