Numerical Simulation of Accelerating Premixed Flames in Closed Tubes

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Acknowledgement:

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Overview

Objective:

- Development and test of a simplified model for gas and dust explosions
- Emphasis on safety assessment
- Possibility to perform parameter studies

Numerical Model:

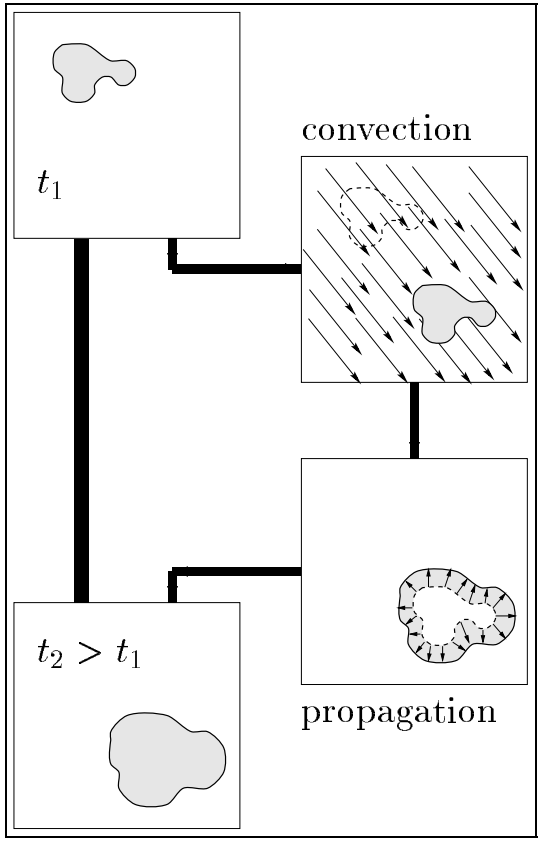
- one dimensional calculation
- Front tracking techniques + Godunov type method
- Kinematic description of turbulent flame propagation
- Different physical effects as *'independent'* submodels

Experimental Conditions from Literature:

- Closed tubes
- Length diameter ratio $L/D \approx 20$
- Hasson, Avinor, Burcat: C_2H_4 and O_2
- Phylaktou, Andrews: CH_4 and air

Front Tracking Method

Problem:

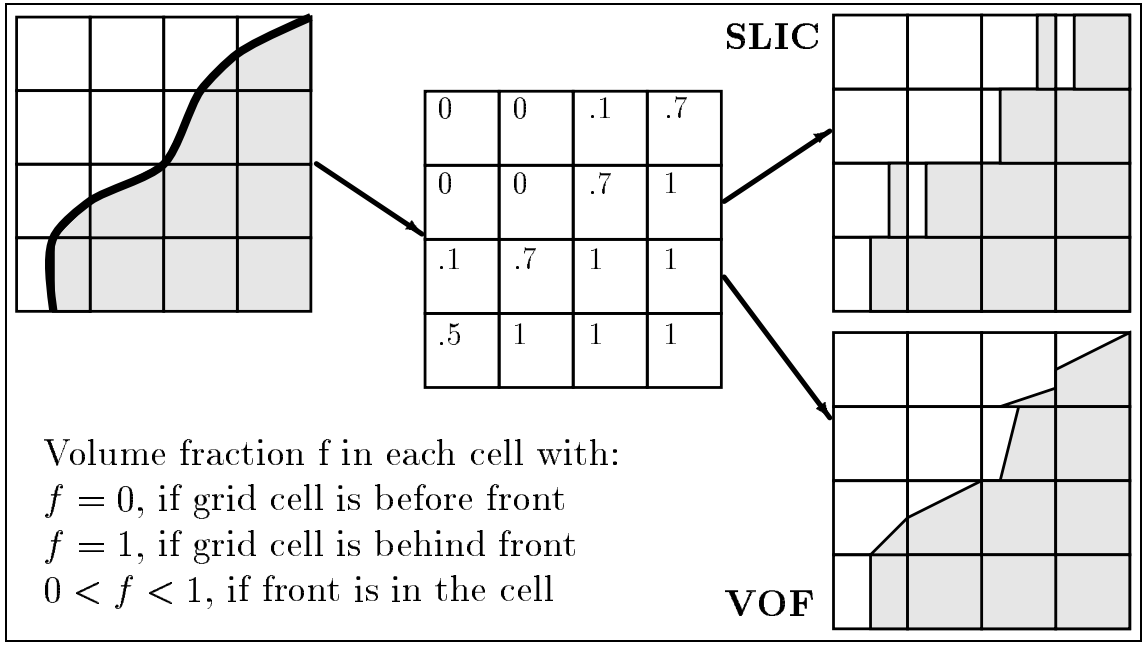


Transport equation for an interface $F(X,t) = 0$ (see Markstein):

$$\frac{\partial F}{\partial t} + V_u \nabla F - S_u |\nabla F| = 0$$

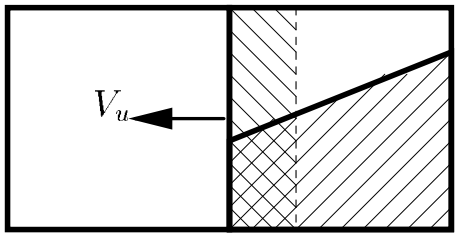
with flow velocity V_u
and propagation velocity S_u

Reconstruction:



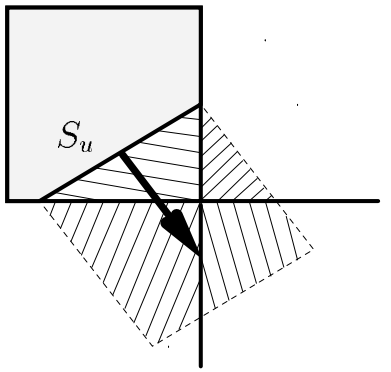
Volume fraction f in each cell with:
$f = 0$, if grid cell is before front
$f = 1$, if grid cell is behind front
$0 < f < 1$, if front is in the cell

Convection:



- staggered grid
- velocity at cell faces
- convectiv flux depends on interface position

Propagation:



Propagation
- normal to interface
- outward

Calculation of Flow Field

Euler equations in 1-D

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}(\rho u) = 0 \qquad \text{(mass)}$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) + \frac{\partial p}{\partial x} = 0 \qquad \text{(momentum)}$$

$$\frac{\partial e_t}{\partial t} + \frac{\partial}{\partial x}[(e_t + p)u] = \dot{H} \qquad \text{(energy)}$$

with

$e_t = e + \frac{1}{2}\rho u^2$

$\dot{H}$ summarizes additional effects on energy equation:

- heat losses to the tube walls

  $\alpha * (T - T_0)$

  with

  $\alpha = \alpha_u * (1 - f) + \alpha_b * f$
- ignition sources

Coupling of Front Tracking and Euler equations:

Introduction of transport equation for a progress variable ξ

$$\frac{\partial}{\partial t}\xi + \frac{\partial}{\partial x}(\xi u) = s$$

with

$s = \frac{f^n - f^{n-1}}{\Delta t}$

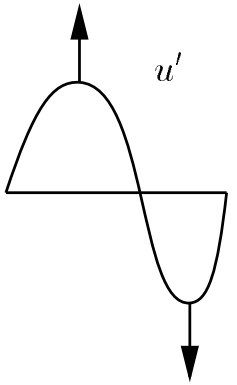
Heat of reaction

- For reactants and products constant compositions are assumed.
- These compositions are **once** calculated for each mixture with Gordon/McBride equilibrium code.
- Composition in each cell is mixture of reactants and products.
- Internal energy of gas is calculated from the given composition.

Turbulent burning velocity

$$\frac{s_b}{s_l} = 1 + k_1(\frac{u'}{s_l})^n \quad (1 - exp(-k_2 s_l t))$$

Increase of laminar flame area due to turbulence



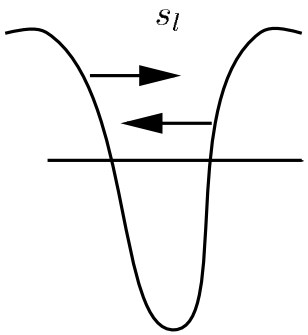
Decrease of laminar flame area due to front propagation

usual form of equation

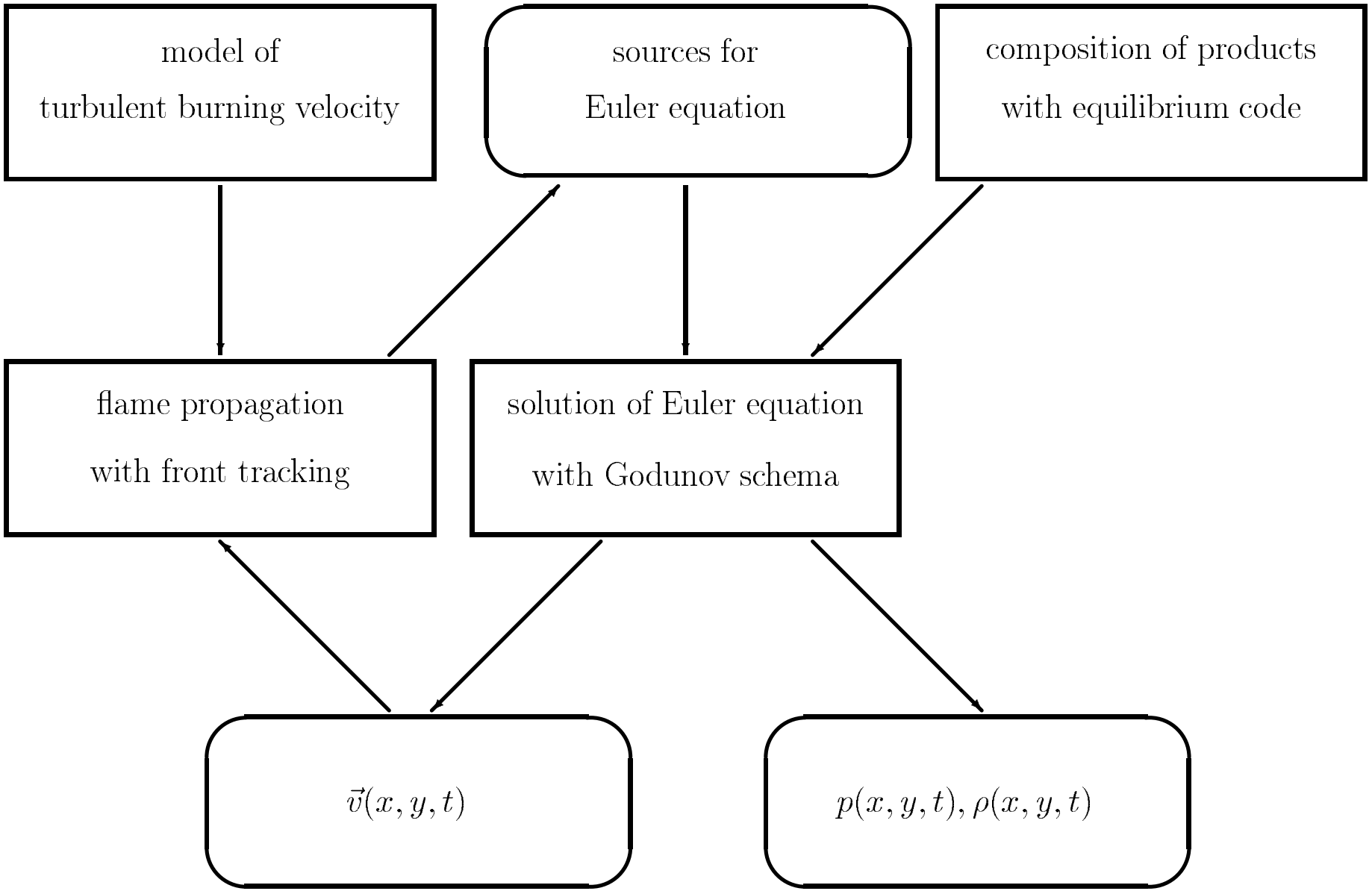
additional term to account for the transition from laminar to turbulent flame during the ignition phase

u' is assumed proportional to mean flow velocity $\bar{u}$:

$$u' = 0.2\bar{u}$$



Numerical Model

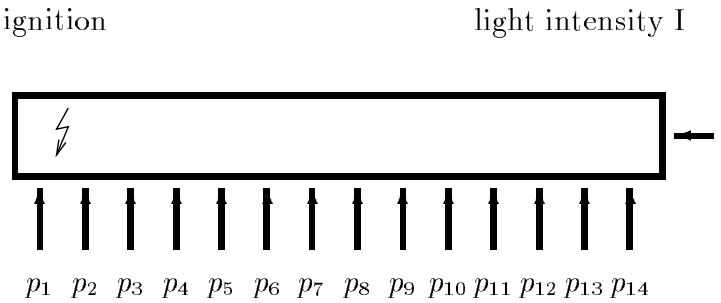


Test calculations and comparison with experiments

Experiments from
A. Hasson, M. Avinor, A. Burcat:
Combustion and Flame 49: 13-26 (1983)

fuel oxidizer	C_2H_4 with O_2
equivalence ratio	0.47 to 2.31
laminar burning velocity	4.0 to 5.5 m/s
length of tube	1300 mm
tube diameter	56 mm
L/D ratio	23
initial pressure	0.11 - 0.88 bar
heat transfer coefficients	adiabatic
initial ignition energy	0.5 J, 3 J and 10 J
grid size	100 cells
maximum time step	0.001 s
coefficient k_1 for s_b	5.0
coefficient k_2 for s_b	300 - 13000 1/m

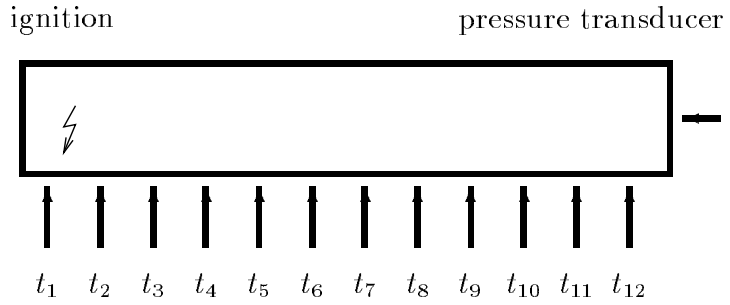
Schematic Setup:



Experiments from
H. Phylaktou, G.E. Andrews,
Combust. Sci. Tech, 1991, Vol.77, pp.27-39

fuel oxidizer	CH_4 with air
equivalence ratio	0.6 to 1.55 (6% to 14%)
laminar burning velocity	0.15 to 0.44 m/s
length of tube	1992 mm or 2981 mm
tube diameter	162 mm
L/D ratio	12.3 or 18.4
initial pressure	1 bar
heat transfer coefficients	$\alpha_u = 100 W/m^2K$
	$\alpha_b = 300 W/m^2K$
initial ignition energy	16 J
grid size	20 or 50 cells
maximum time step	0.001 s
coefficient k_1 for s_b	2.7
coefficient k_2 for s_b	550 1/m

Schematic Setup:

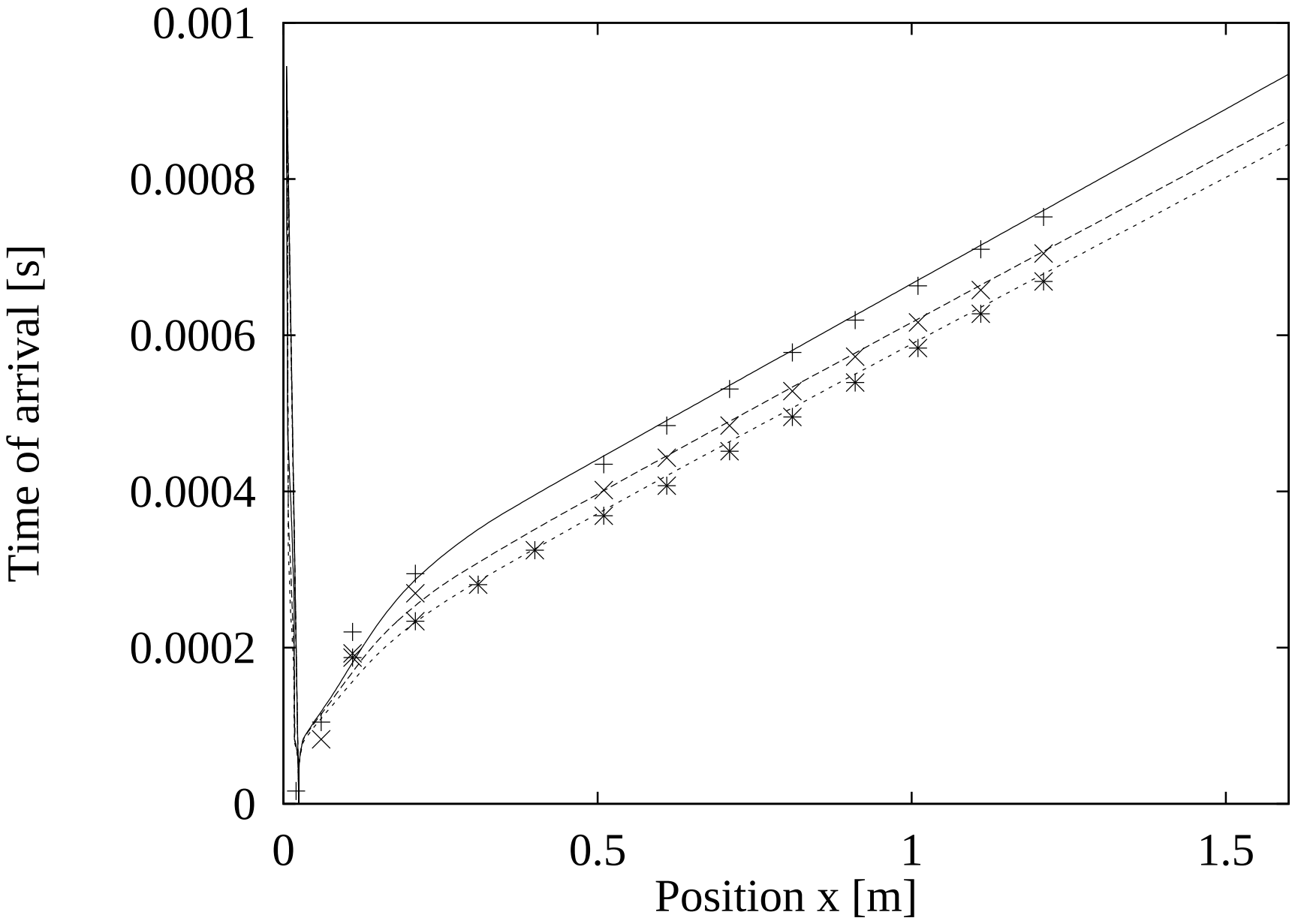


Conclusions

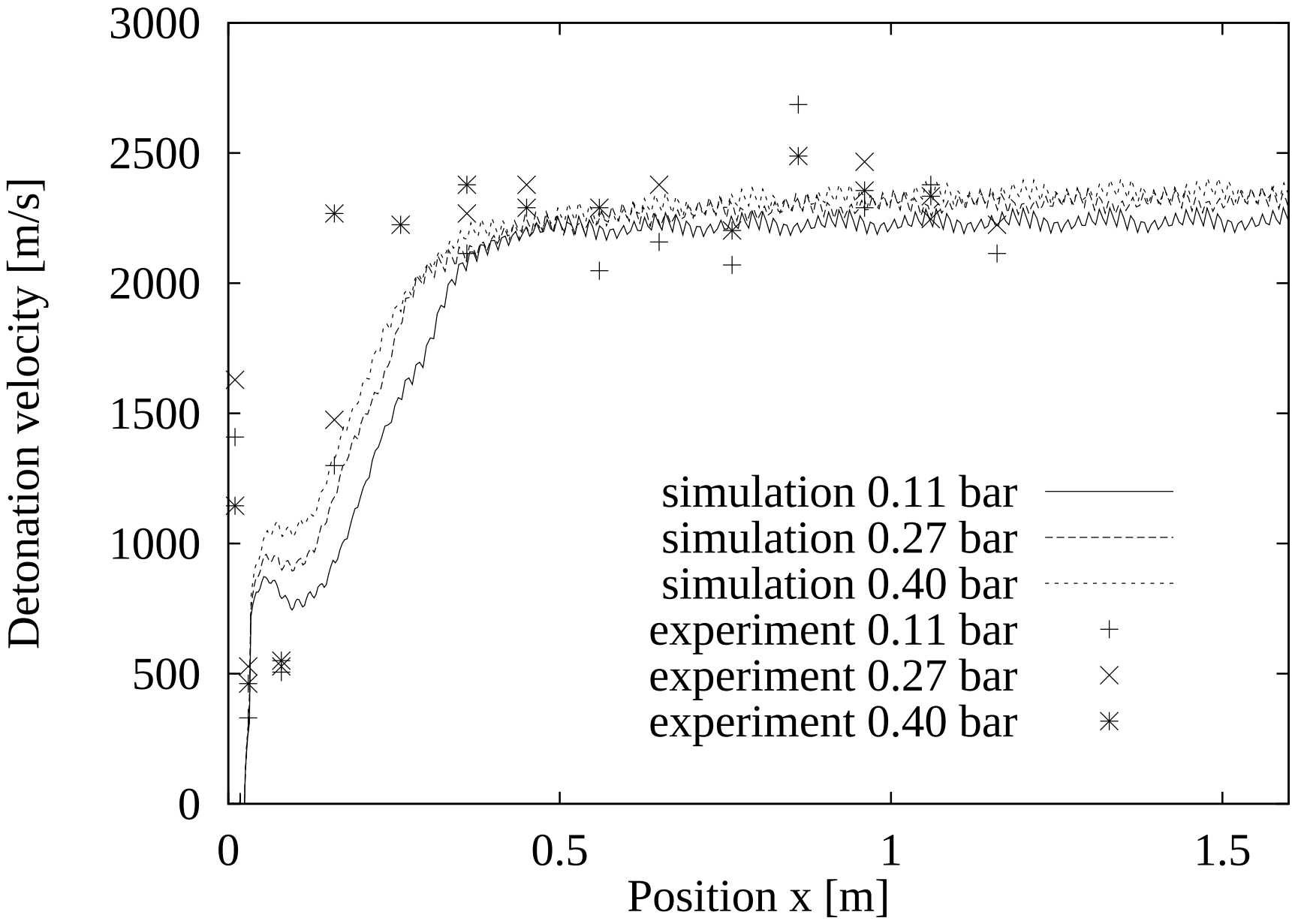
- A numerical model for turbulent flame propagation in tubes was developed which combines front tracking methods with a Godunov type solver of the Euler equations.
- The turbulent burning velocity is modeled as a function of laminar burning velocity, turbulence intensity and time.
- Advantages of this model are:
  - Turbulent flame propagation is described by a kinematic model.
  - System of differential equations is not stiff.
  - Only moderate computational effort.
  - Parameter studies are possible.

- Test calculations were performed for a wide range of experimental conditions from turbulent flames to detonations.
- For all calculations satisfactory agreement with experimental data was achieved.

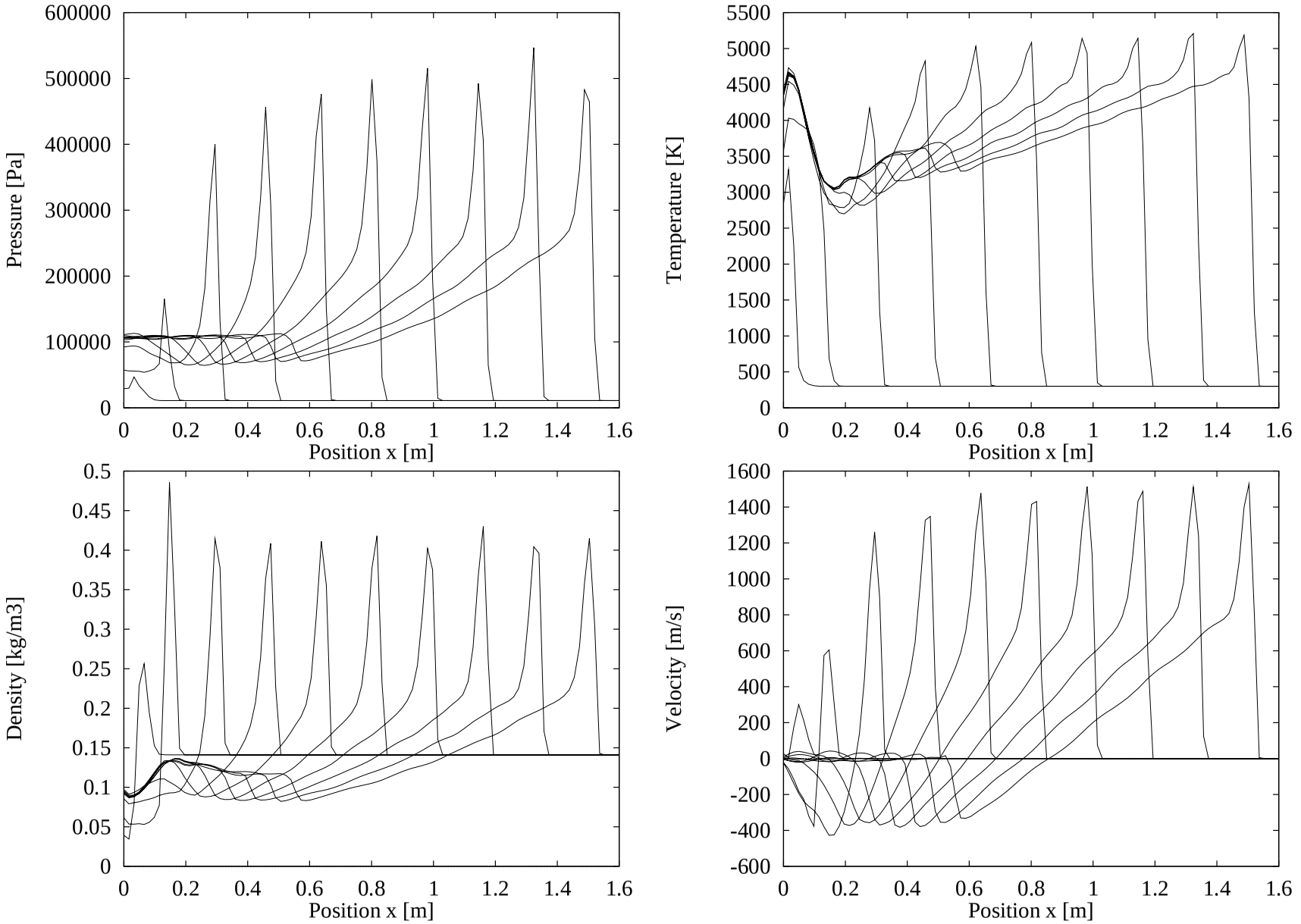
- Further calculations are needed to determine a general expression for the model parameters.
- Extension of the model to 2-D calculations is straight forward and development of the computer program is on its way.



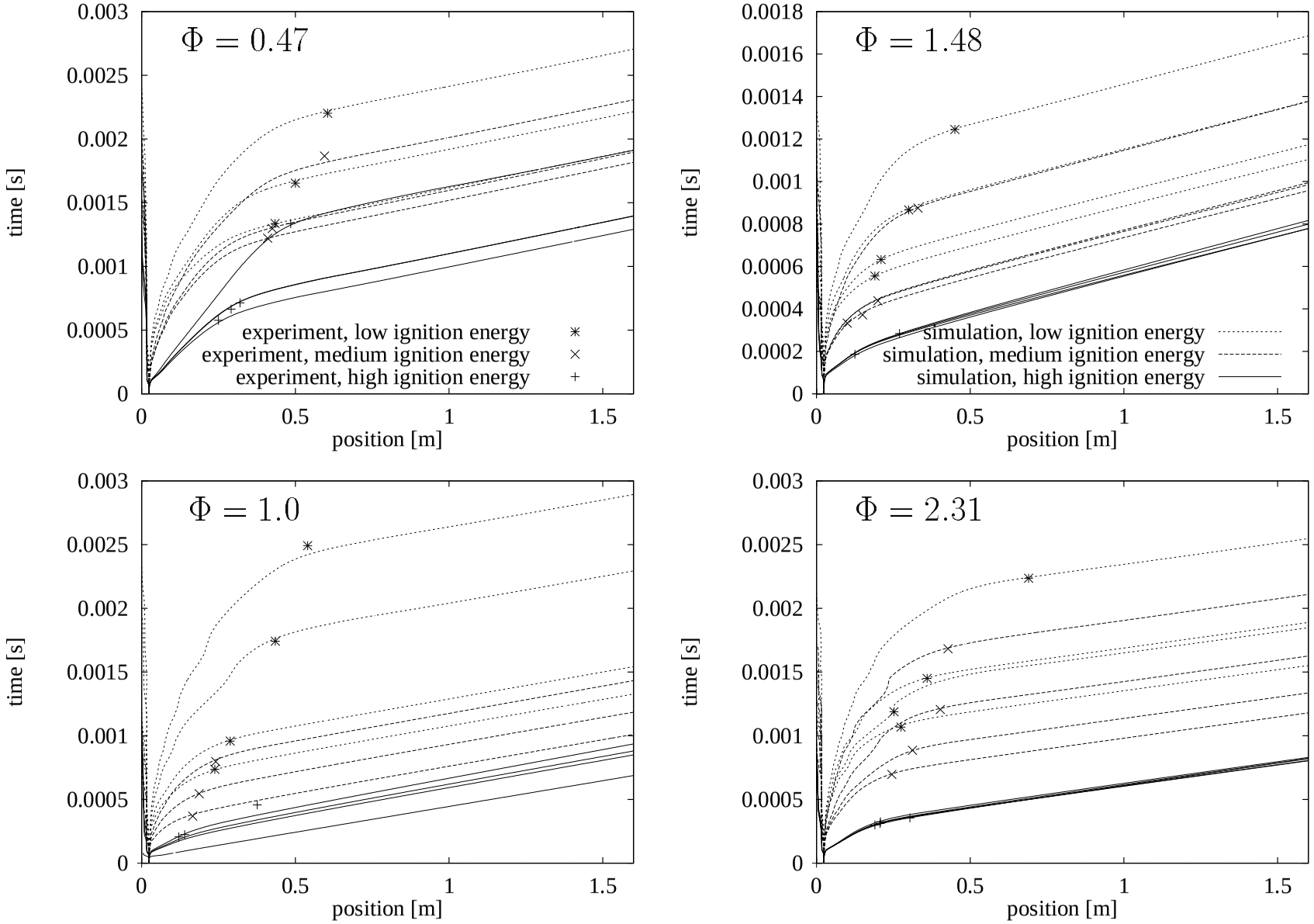
$C_2H_4 + O_2$, $\Phi = 1.0$: x-t-diagram of flame propagation



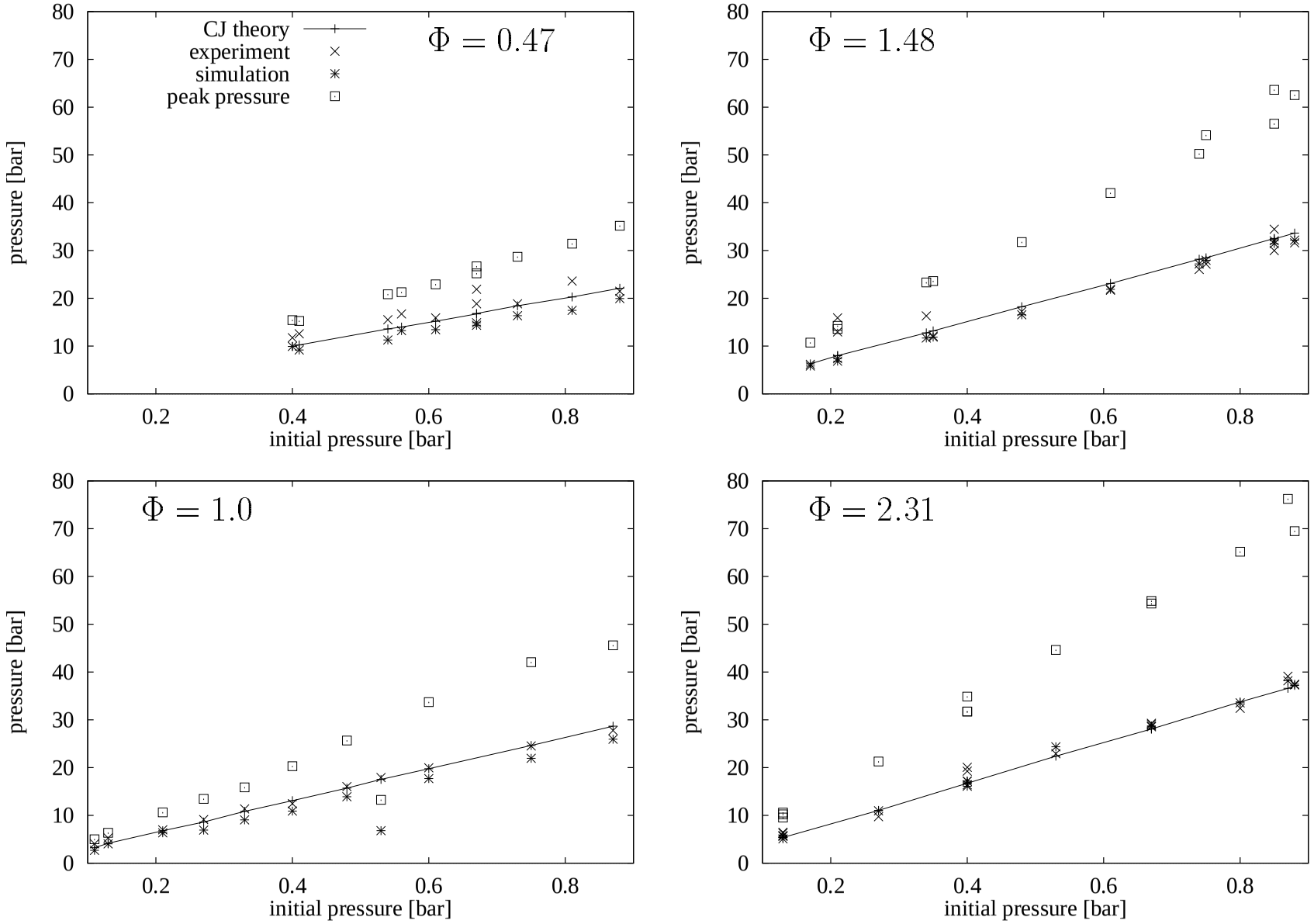
$C_2H_4 + O_2$, $\Phi = 1.0$: front velocity along tube



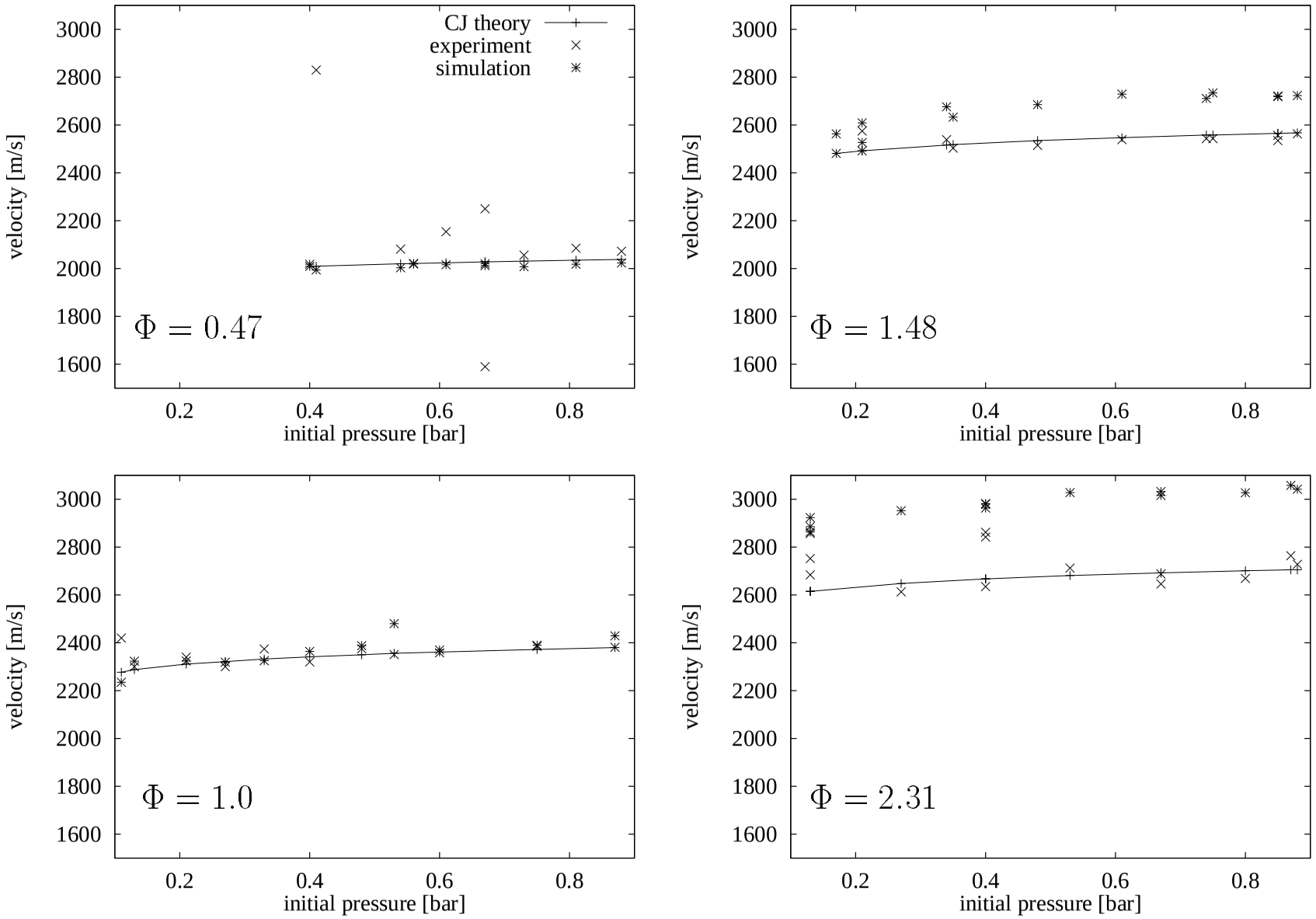
$C_2H_4 + O_2$, $\Phi = 1.0$: profiles along tube at various times



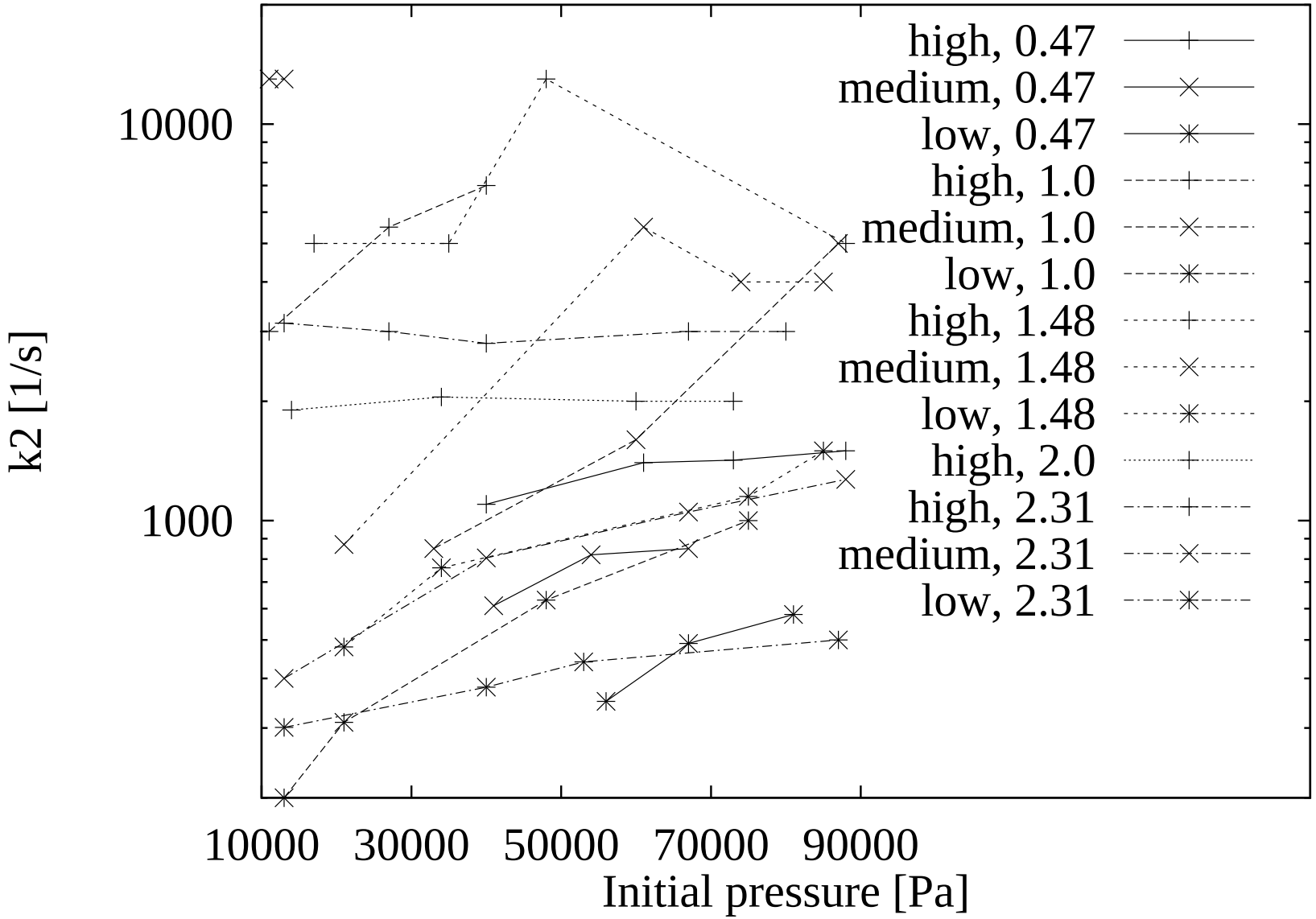
$C_2H_4 + O_2$: x-t-diagrams for all available experimental data



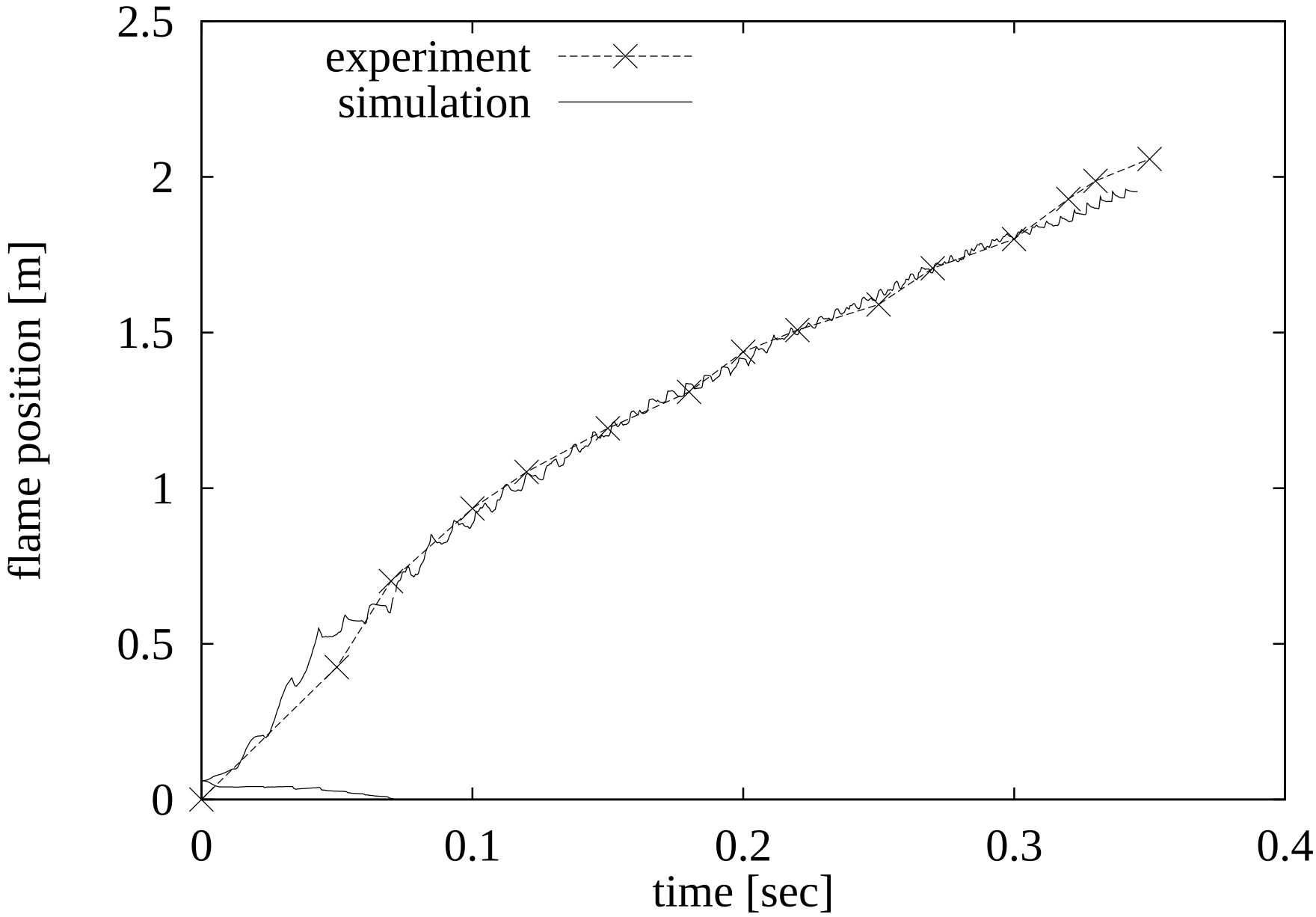
$C_2H_4 + O_2$: detonation pressure as function of initial pressure



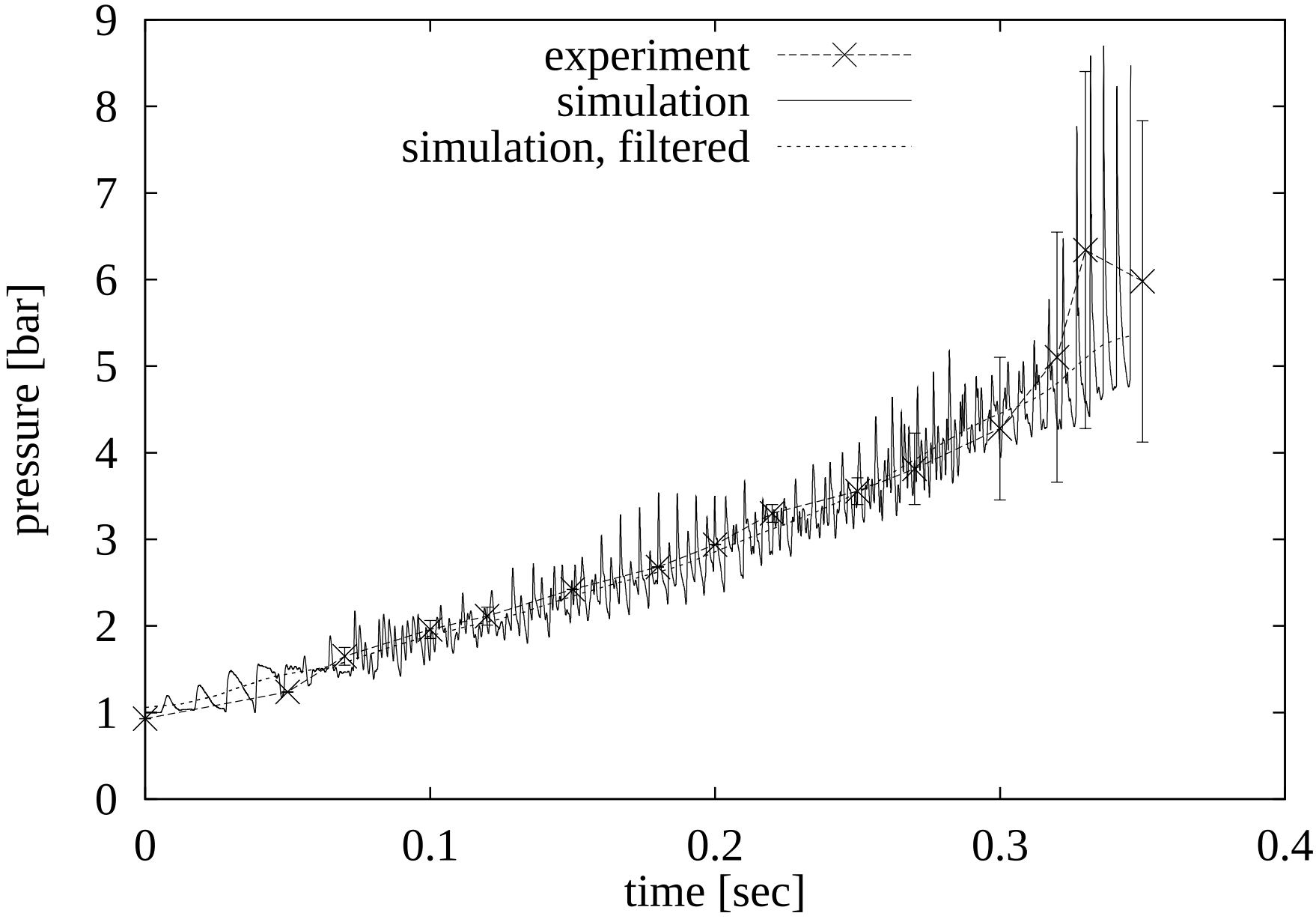
$C_2H_4 + O_2$: detonation velocity as function of initial pressure



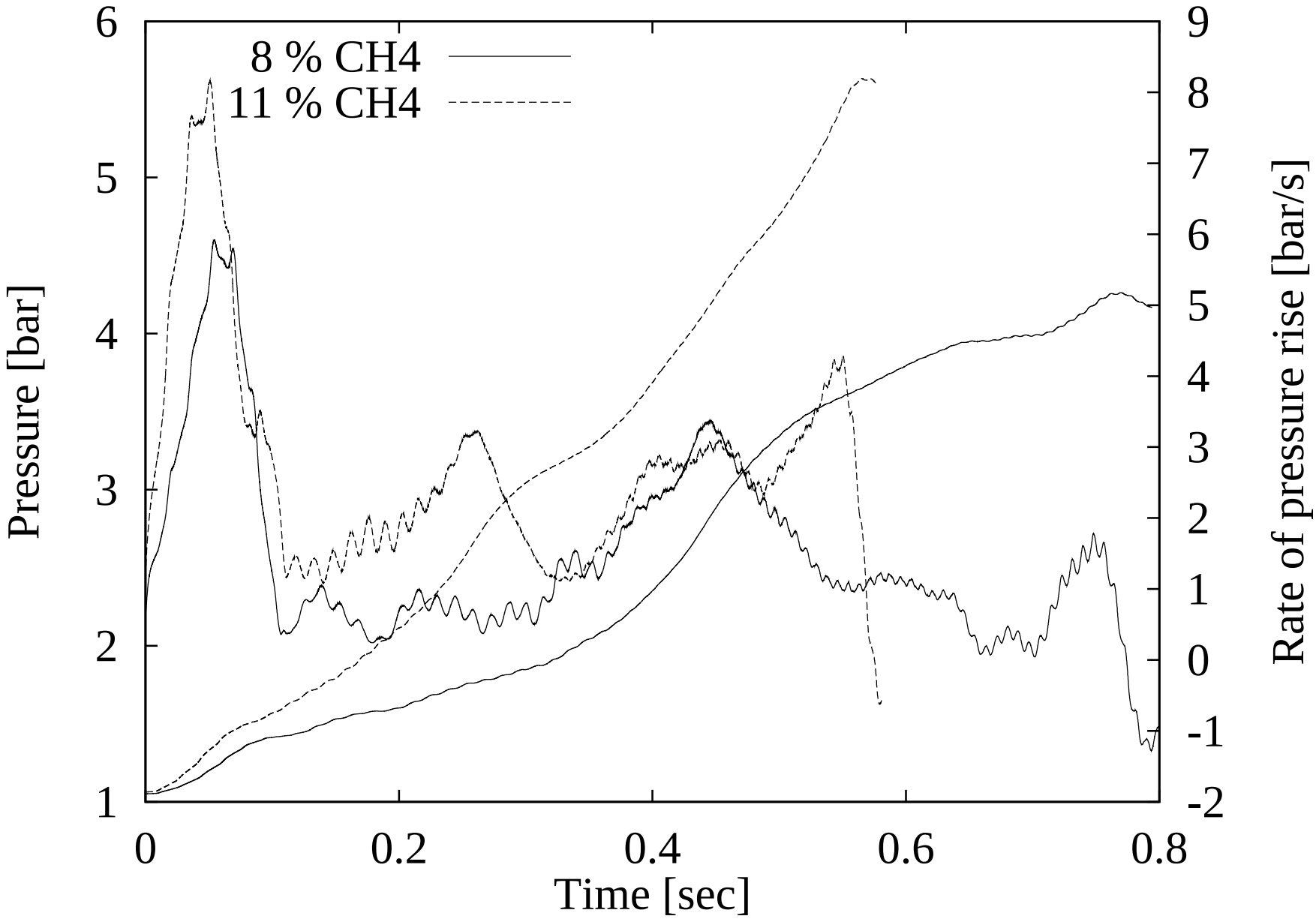
$C_2H_4 + O_2$: parameter k_2 as function of initial pressure



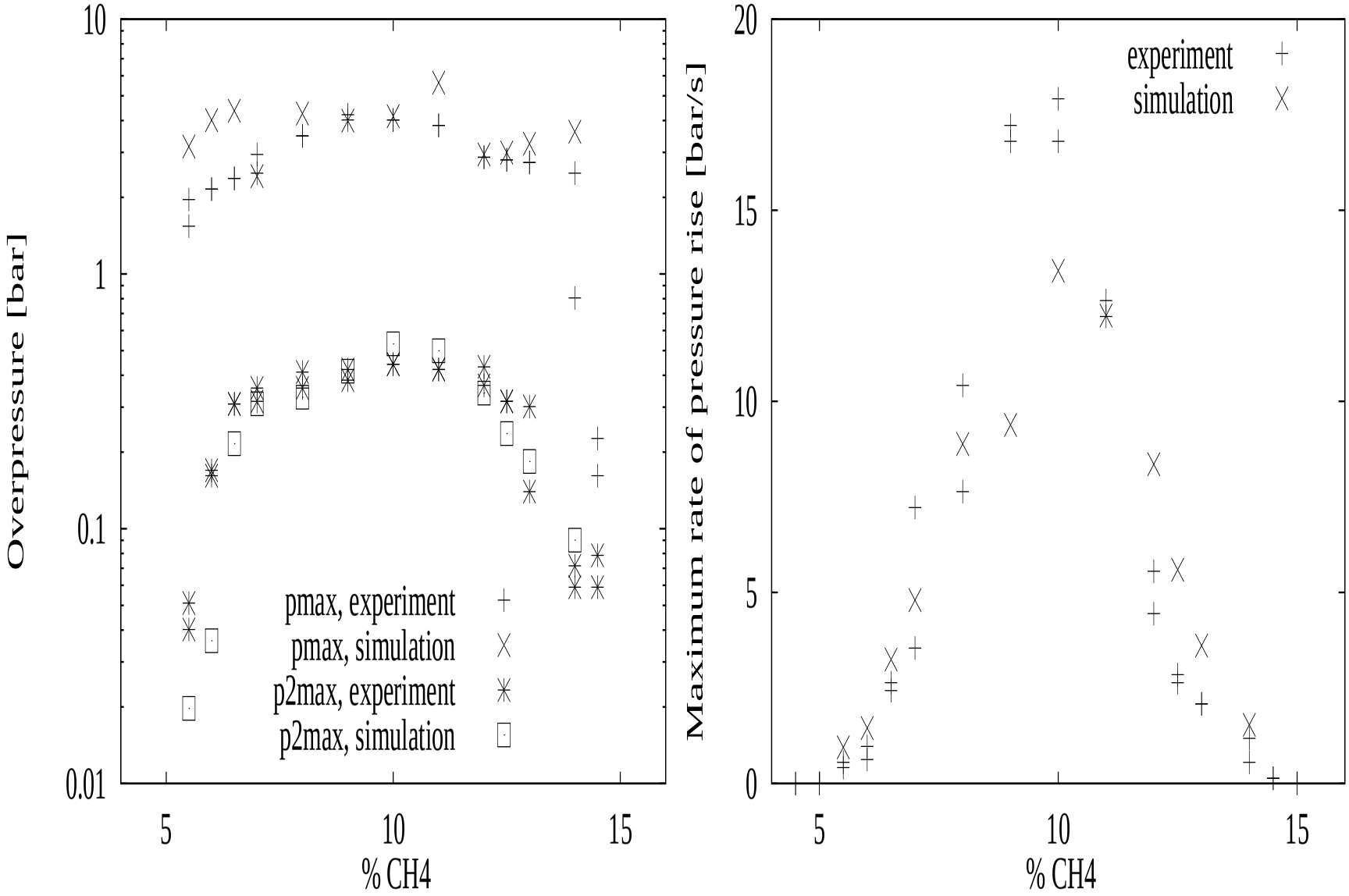
$10\ \%\ CH_4 + air$: x-t-diagram of flame propagation



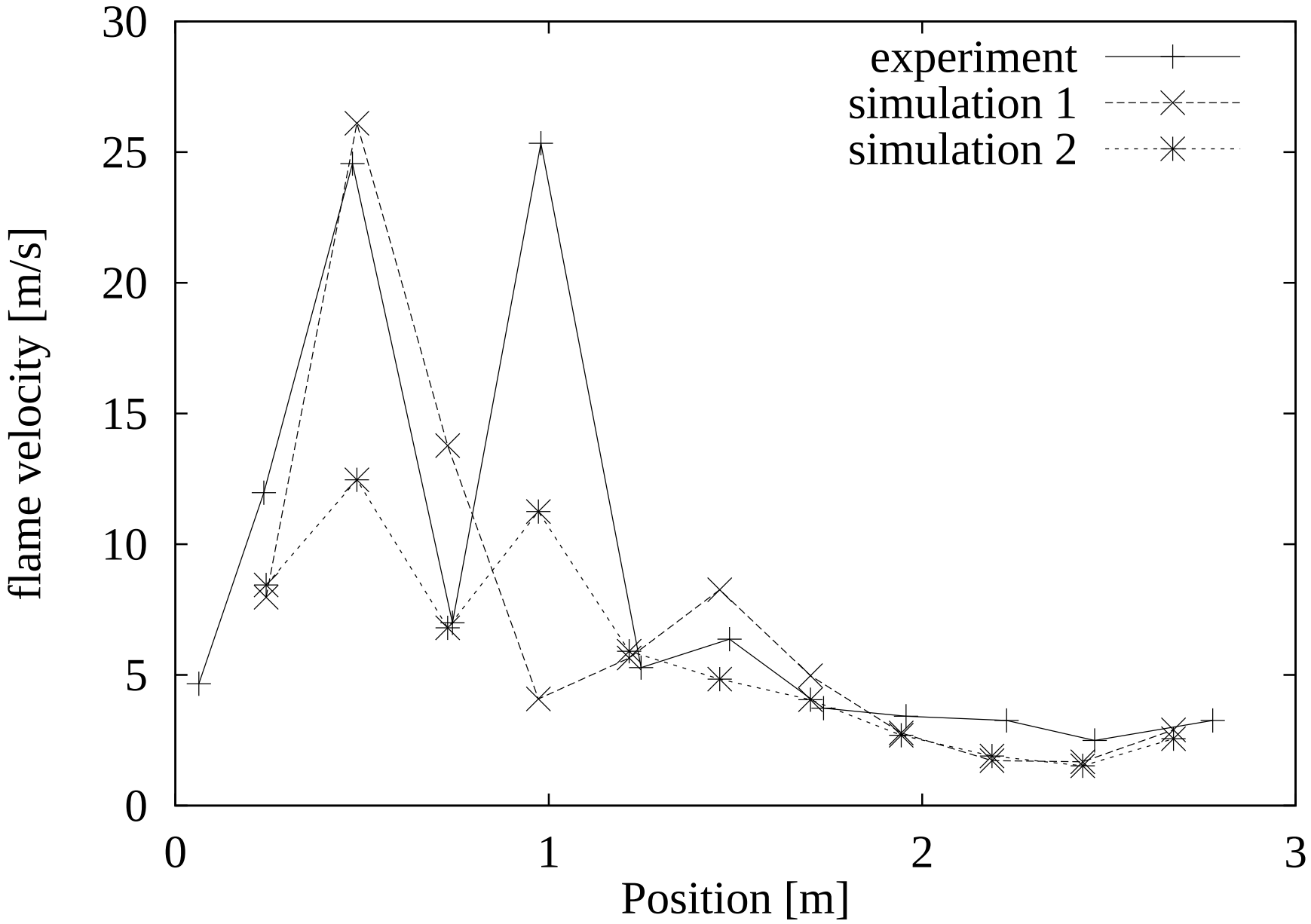
$10\ \%\ CH_4 + air$: pressure at end of tube



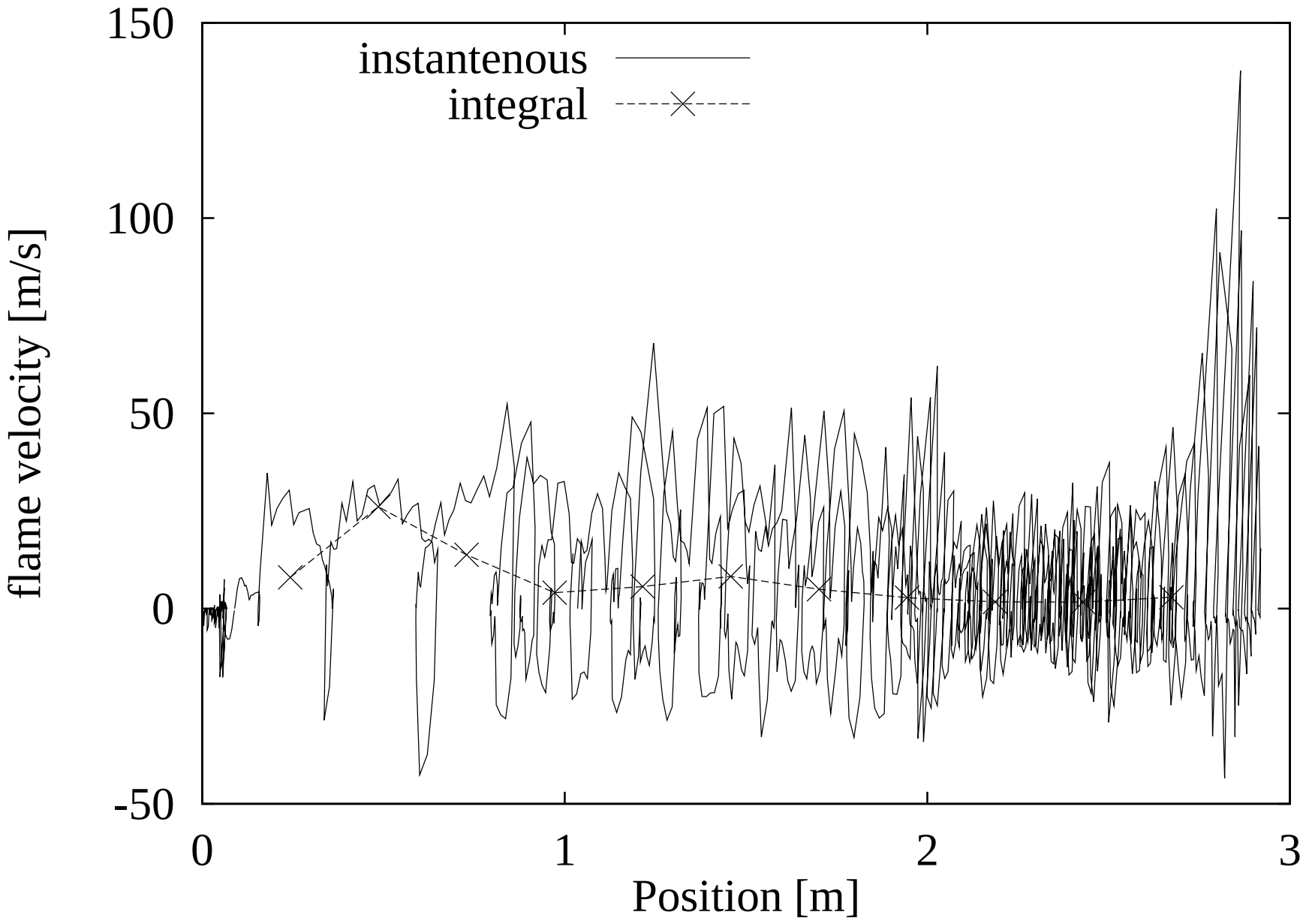
$CH_4 + air$: pressure and rate of pressure rise for 2 simulations



$CH_4 + air$: maximum pressure and maximum rate of pressure rise



$10\ \%\ CH_4 + air$: mean flame velocity along tube axis



$10\ \%\ CH_4 + air$: instantaneous and mean flame velocity