3SEC Strategy
for Evaluation of Combustion Processes

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Sequential **E**nlargement **C**ombination of
Separated **E**ffects **C**ontributions for
Side-by-side **E**xp/num **C**hecking

Strategy for **E**valuation of **C**ombustion **P**rocesses

Possible acronyms could be:

4SEC Processes or

3SEC Strategy for Evaluation of Combustion Processes.

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- Reactive mixing related to stratified medium with external source ignition
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Introduction 1

- Combustion is one of the most important process in the nature and in the man generated habitat which needs a very high level of interdisciplinary to be analyzed. **Chemistry, fluid-dynamic, electromagnetism are the main fundamental disciplines**, which involve all the matter state: solid, liquid, gas and plasma. The most crucial steps in the historical evolution of these disciplines are combustion processes.

Introduction 2

- The **Lavoisier** experiment on hydrogen oxidation is considered the critical moment in which chemistry itself has been founded
- The work of **Semenov** on the radical branching propagation has been developed in the contest of the study of combustion process.
- The work for the study of elementary reaction involved in the most important step of oxidation in combustion process.
- In fluid dynamic the works of **Rankine, Hugoniot, Chapman, Duffey, Jouguet, Karlovitz, von Karman** etc. are examples of the relevance of combustion in the science history.
- The electromagnetic has received fundamental contribution in the field of radiative heat transfer and of spectroscopy

Introduction 3

- In many academic curricula combustion is considered at the same level of discipline. This does not refer to the technological relevance of the combustion, but directly to its conceptual content, even though according to different schools, in which it is taught, it is in the orbit of one of the aforementioned disciplines. In other word combustion is a sort of multidisciplinary field and not **an interdisciplinary field, as it should be considered**

Introduction 4

- The corpus of knowledge on combustion and its relevance in strategic technological and economic fields make this subject at the dawn of the new millennium an active field of research and the scientific area where the interconnections between chemistry, fluid-dynamic, electromagnetism have to be studied more deeply. This is a challenge, which one has to be **aware to face in its comprehensive aspects**, otherwise approaches, which are mere drifts from casual starting points, are wildly proliferated without the needed check on the accuracy

Difficulties for evaluation of Combustion Processes. The need of a strategy

- **Direct Numerical Simulation** of reacting flows is a starting **guideline** for models based on continuum hypothesis. In this case the vector of the density, of the momentum density, , of the single species density , and of the sensitive enthalpy density :
- has to be predicted for whatever boundary and initial condition The vectors consists of **n+5 components** since n are the chemical species

Difficulties for evaluation of Combustion Processes. The need of a strategy

$$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot \left(\rho \underline{v} \right) = 0$$

$$\frac{\partial \rho \underline{v}}{\partial t} + \underline{\nabla} \cdot \left(\rho \underline{v}\underline{v} \right) + \nabla \cdot J_{v} = -\underline{\nabla} p$$

$$\frac{\partial \rho Y_i}{\partial t} + \underline{\nabla} \cdot \left(\rho \underline{v} Y_i \right) + \nabla \cdot J_{Y_i} = \dot{\rho}_i$$

$$\frac{\partial \rho h^s}{\partial t} + \underline{\nabla} \cdot \left(\rho \underline{v} h^s \right) + \nabla \cdot J_{h^s} = -\sum \dot{\rho}_i h_s^o$$

Difficulties for evaluation of Combustion Processes. The need of a strategy

- The first set of quantities which need specific submodels are the constitutive equations, referred as "**diffusion models**"
- The second set of quantities which need specific submodels are temporal variations of species densities associated to their chemical destruction or creation.. for two/three/four parameters, named kinetic constants. The whole set of equations and kinetic constants are usually referred as "**chemical kinetics models**".

Difficulties for evaluation of Combustion Processes. The need of a strategy

- The presence of interface discontinuities forces the Direct Numerical Simulation to include the description of the kinetic of such surfaces and momentum, heat and mass transfer associated to them. They can be considered time-dependent internal boundary conditions, which are defined through hypotheses and equations.
- "**atomization/fragmentation-submodels**"
- "**entrainment submodels**"
- "**state transition submodels**"

Difficulties for evaluation of Combustion Processes. The need of a strategy

- Turbulent approach consists in **averaging** the quantities either over the **time** (Reynolds, Fabvre average) or over the **space** (volume average) or on ensemble of "occurrences" of the variables with **filters** (e.g. Large Eddy Averaging) or without filters (e.g. probability density functions approaches).

Difficulties for evaluation of Combustion Processes. The need of a strategy

- In synthesis a great number of " approaches-submodels" have to be introduced in order to describe **multiscale** (turbulent), **multicomponent**, **multiphase**, **multidimensional** reacting flows. A not exhaustive list of these approaches-submodels is the following

  - i) Turbulent (LES, RANS, k-E,.......)
  - ii) Mixing (curl, IEM, EMST,LEM,CMC........)
  - iii) Chemical kinetics (detailed, reduced,two steps,.......)
  - iv) ChemistryCoupling (Flamelet, SurfaceDensity, EBU......)
  - v) Atomization (TAB, Ranz-Taylor,Weber, Rayleigh)
  - vi) State transition (D2, film boiling,.........)

Difficulties for evaluation of Combustion Processes. The need of a strategy

- If one assumes that at least five types of submodels can be used for the first **three categories of submodels** one can calculate that **125 combinations** are possible. This number can reach the incredible value of **15625** if other three categories of submodels are added always with five possible choices for each of them.

Difficulties for evaluation of Combustion Processes. The need of a strategy

- Multi-dimensionality can be reduced by focusing on **projections** or **sections** of the solutions of the aforementioned equations, which describe satisfactorily the most important part of the whole solution dominion. They may be defined either in the time coordinate as **Poincaré sections**, or in space dominion as **interfaces and isosufaces** in homogeneous phase or in both time and space as trajectories, intermaterial surfaces and progressive surfaces

Difficulties for evaluation of Combustion Processes. The need of a strategy

- In synthesis the problem is complicated and complex:
  - It is **complicated** because it is composed of many interrelated parts and has to be dealt with the contemporaneous use of many relationship. This in turn entails that the construction of the model can be subjected to uncontrollable errors.
  - The problem is also **complex** because the interaction of the different effects in the direct numerical approach or of the different submodels is highly not linear according to the equation nature.

Difficulties for evaluation of Combustion Processes. The need of a strategy

- It is clear that complicated and complex problems need recognized strategies to be faced.

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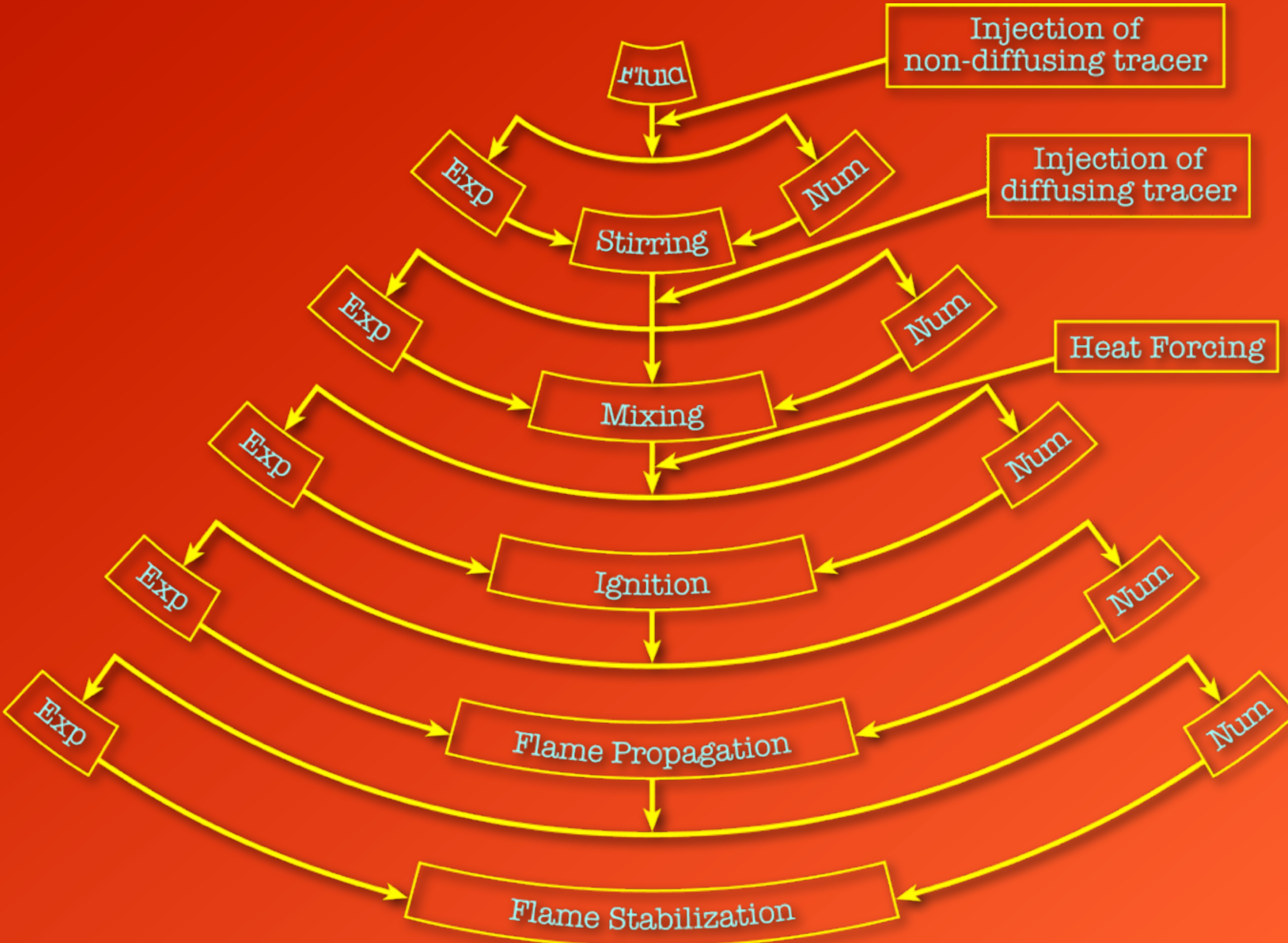
- The first reason for this is that without strategy the problem is faced with the specification of a **long list of submodels**, which are motivated only for some parts of them.
- The second reason is that the submodels can be chosen with the criterion that they are interlinked in a particular way. **This link has to be found for each single strategy** and it can guide at least the choices related to the model core. This is needed not only for formal self-consistency of the model, but also because complicated problems need simplifications also in the communication and in the expert use of the single pieces.

It is clear that complicated and complex problems need recognized strategies to be faced.

- This means that **validation** has to be performed in an intelligent way with selection of **representative samples** of cases and with very deeply evaluation of the submodels based on well sounded submodels and on well identified interaction with model core.
- Therefore **isolation** of single effects to neglect contemporaneously the effect both in physical and numerical model **may be not feasible** for strongly interlinked subprocesses. Very few papers have been devoted to this subject whereas this is the central assumption of nearly every model.

It is clear that complicated and complex problems need recognized strategies to be faced.

- It can be tought as divided in six parts, which corresponds to a "Separated Effect Contribution" (**SEC**).
- It allows "Sequential Enlargement Combination" (**SEC**) of the "separated effects"
- and the " Side-by-side Experimental/Numerical Checking" (**SEC**) of the appropriate characterization of the field obtained by the introduction of new "separated effect".


Fluid
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Exp
Num
Stirring
Injection of diffusing tracer
Exp
Num
Mixing
Heat Forcing
Exp
Num
Ignition
Exp
Num
Flame Propagation
Exp
Num
Flame Stabilization

Isothermal single component fluid-dynamic.

- The first step of the 3SEC strategy is the characterization of the **isothermal fluid-dynamics**.
- The **Lagrangian** characterization is needed, because the entanglement between the fuel and the oxidant have to be ensure and evaluated on quantitative basis.
- The fluid- dynamic characterization should be performed both in Eulerian and Lagrangian way on a **broad spectrum of scales**.

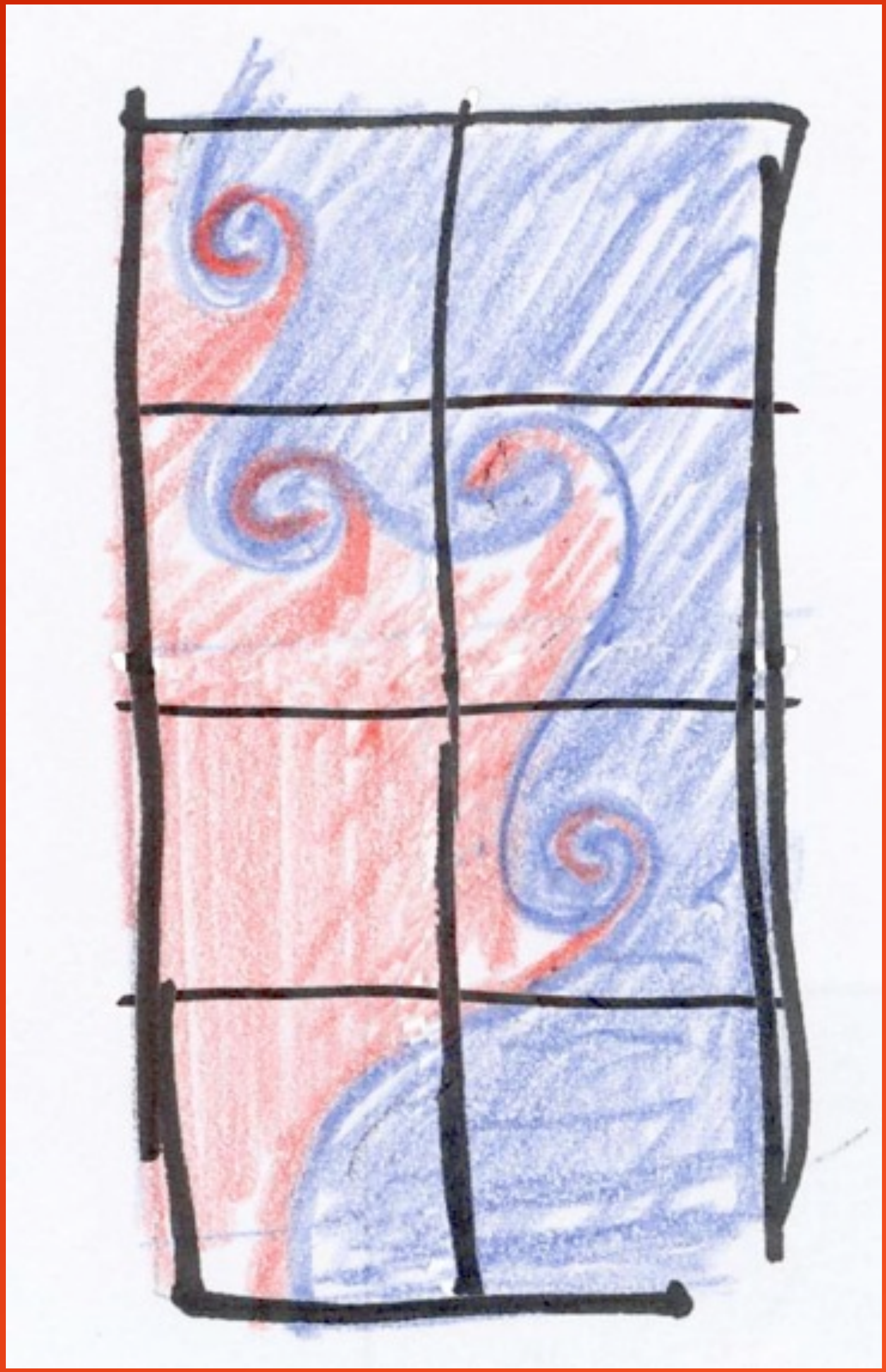
Stirring

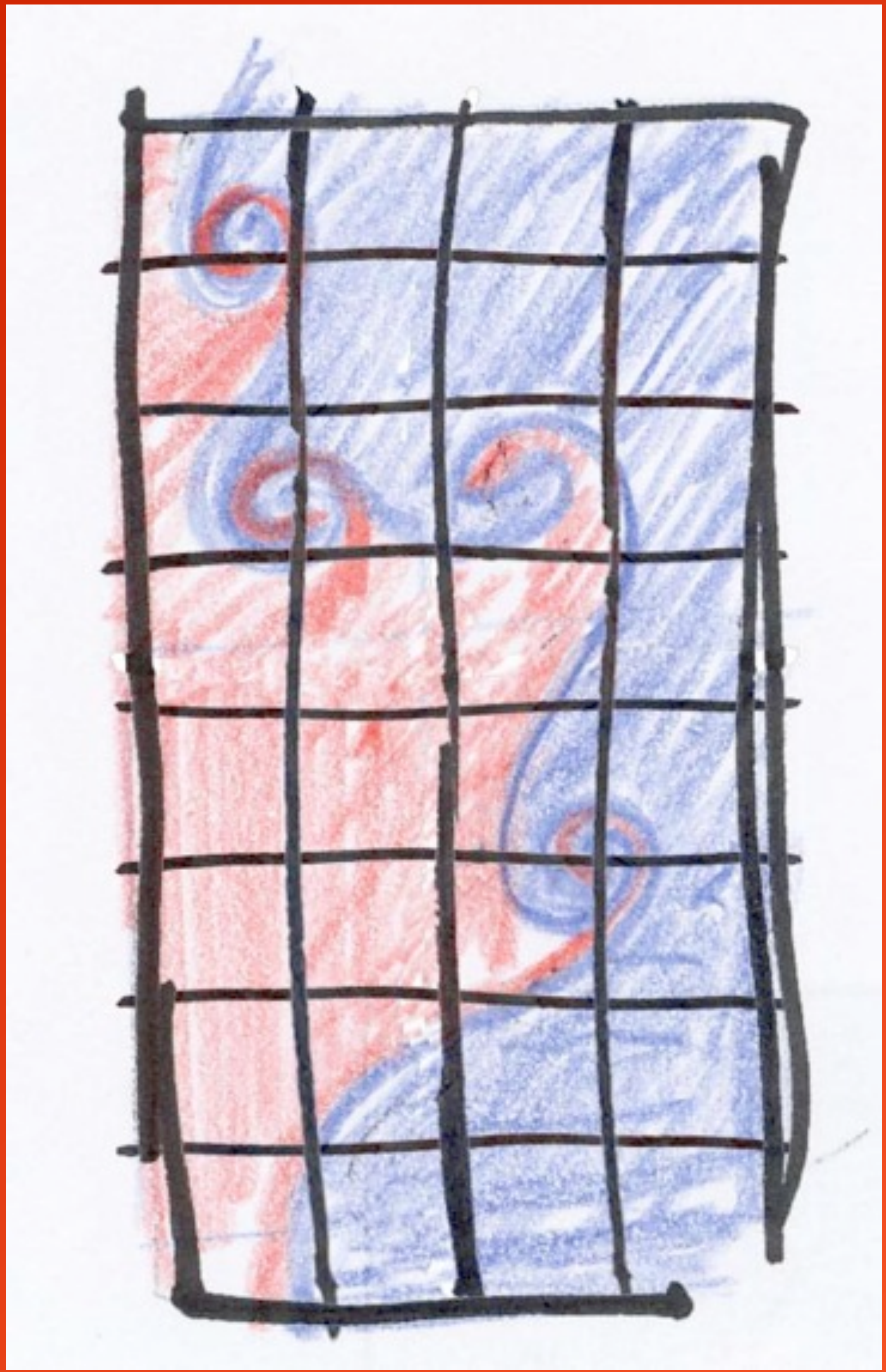
- When a non diffusive tracer is introduced into part of the flow it determines an **interface**. This is the surface of the flow where the concentration of the tracer is discontinuous, that is where it passes from zero to a finite value on an infinitely thin surface.

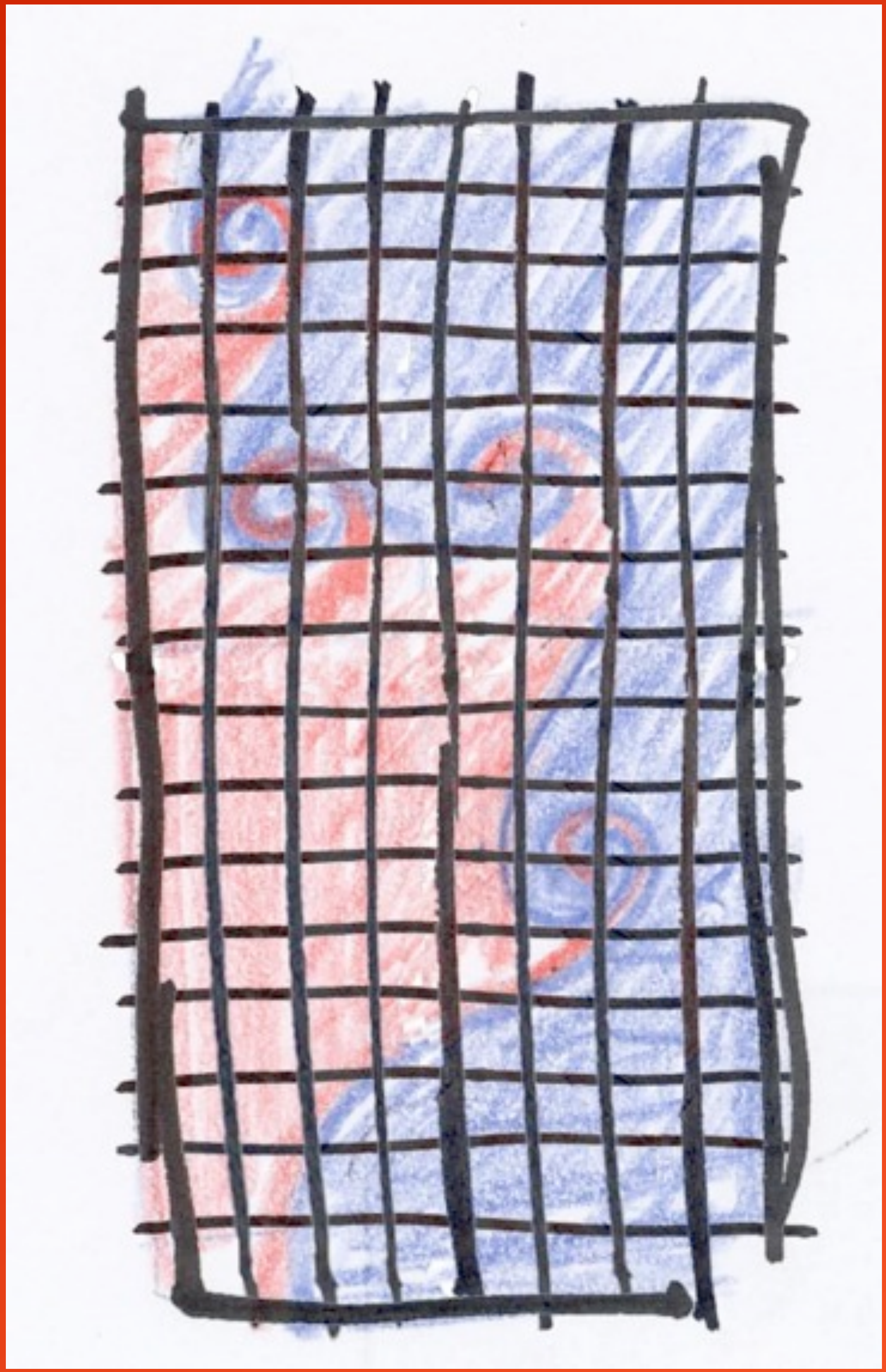
- 6 interfacce

stirring

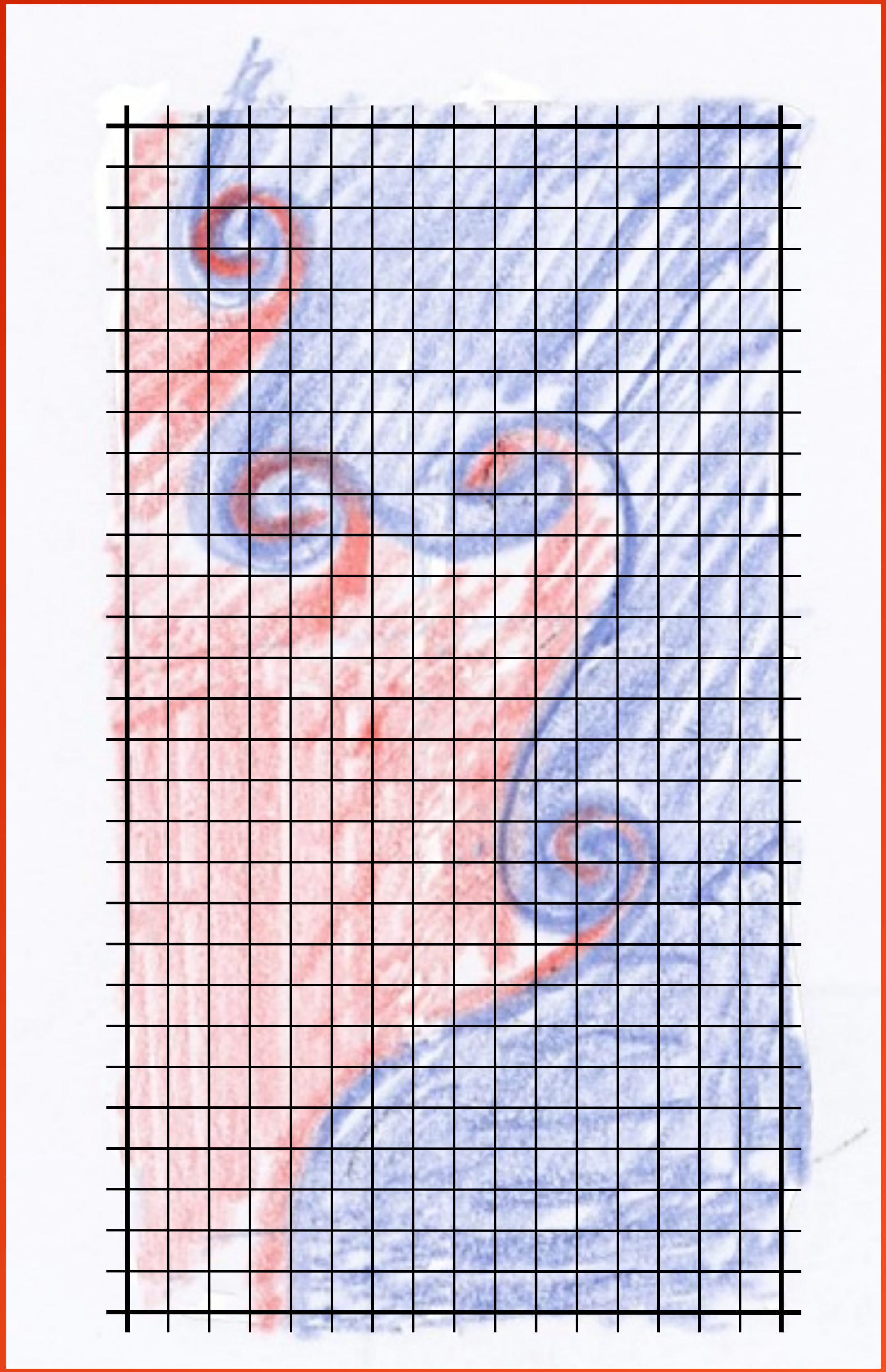
- Intrinsic properties
  - Interface is continuous
  - Interfaces are not intersecting
  - Interface is oriented
- Extrinsic properties
  - Multiscalarity (fractal)
  - Dimensional equivalence
  - Morphology
  - Single or multiple box crossing



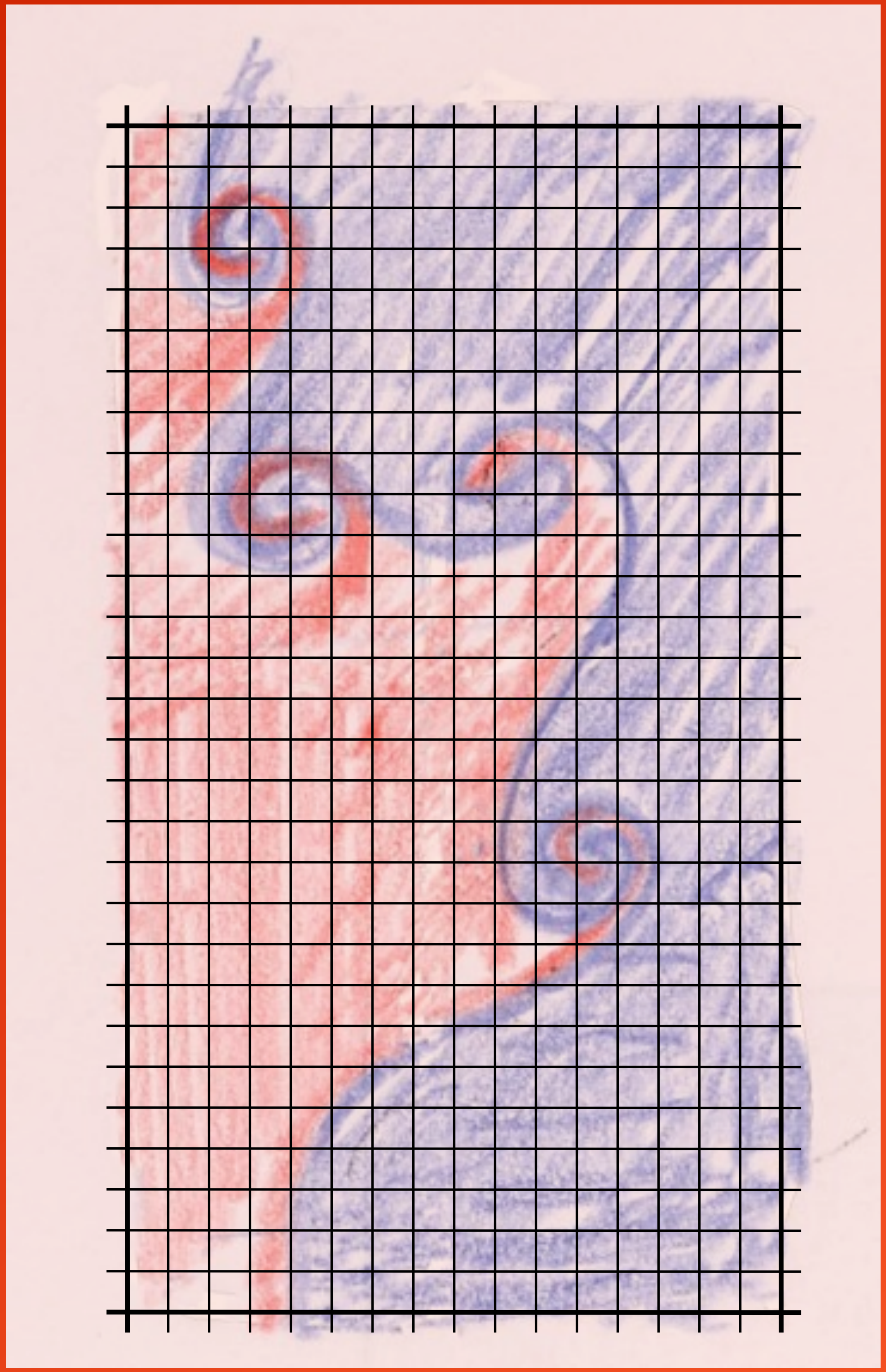




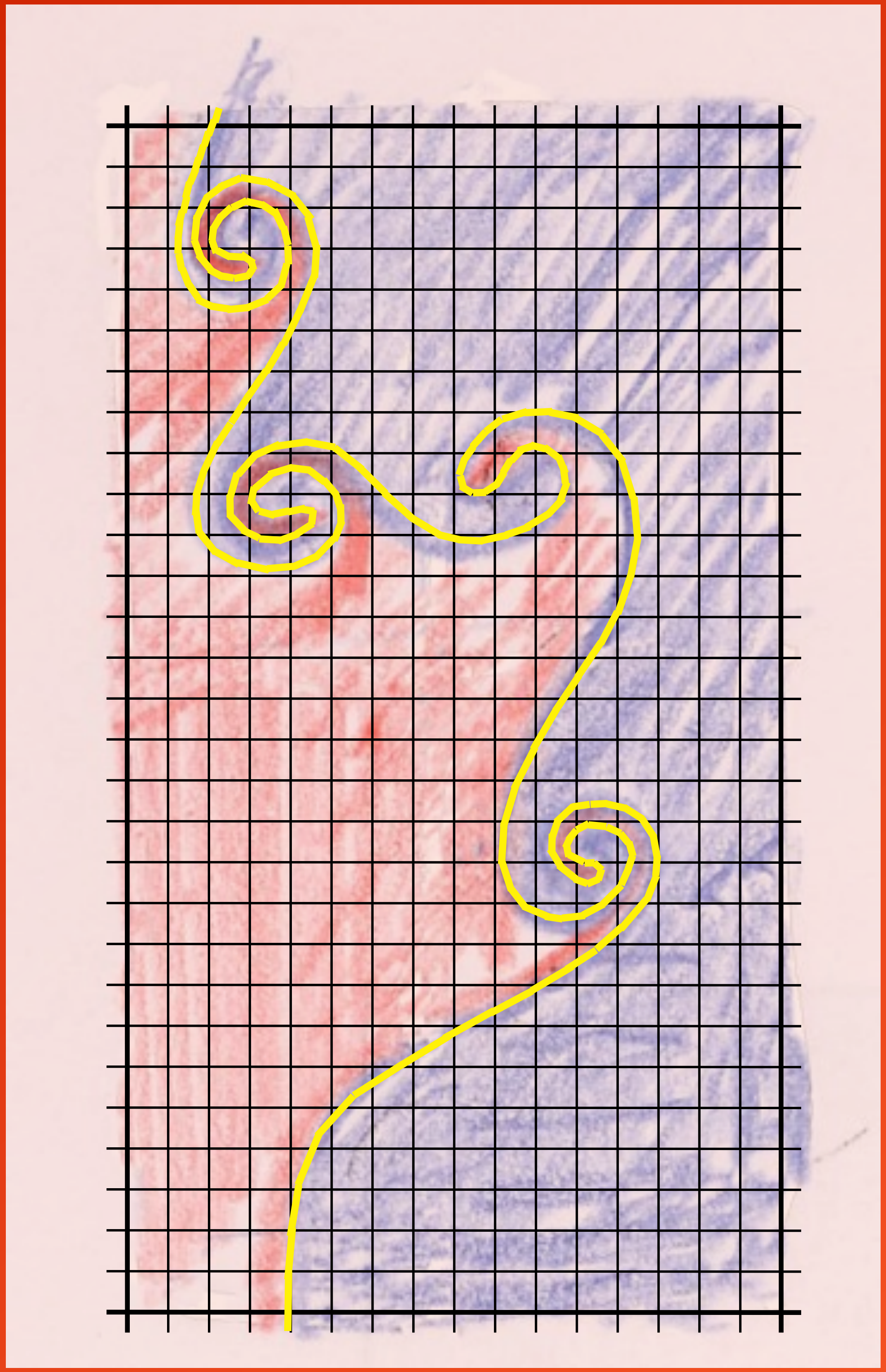
Interface is continuous



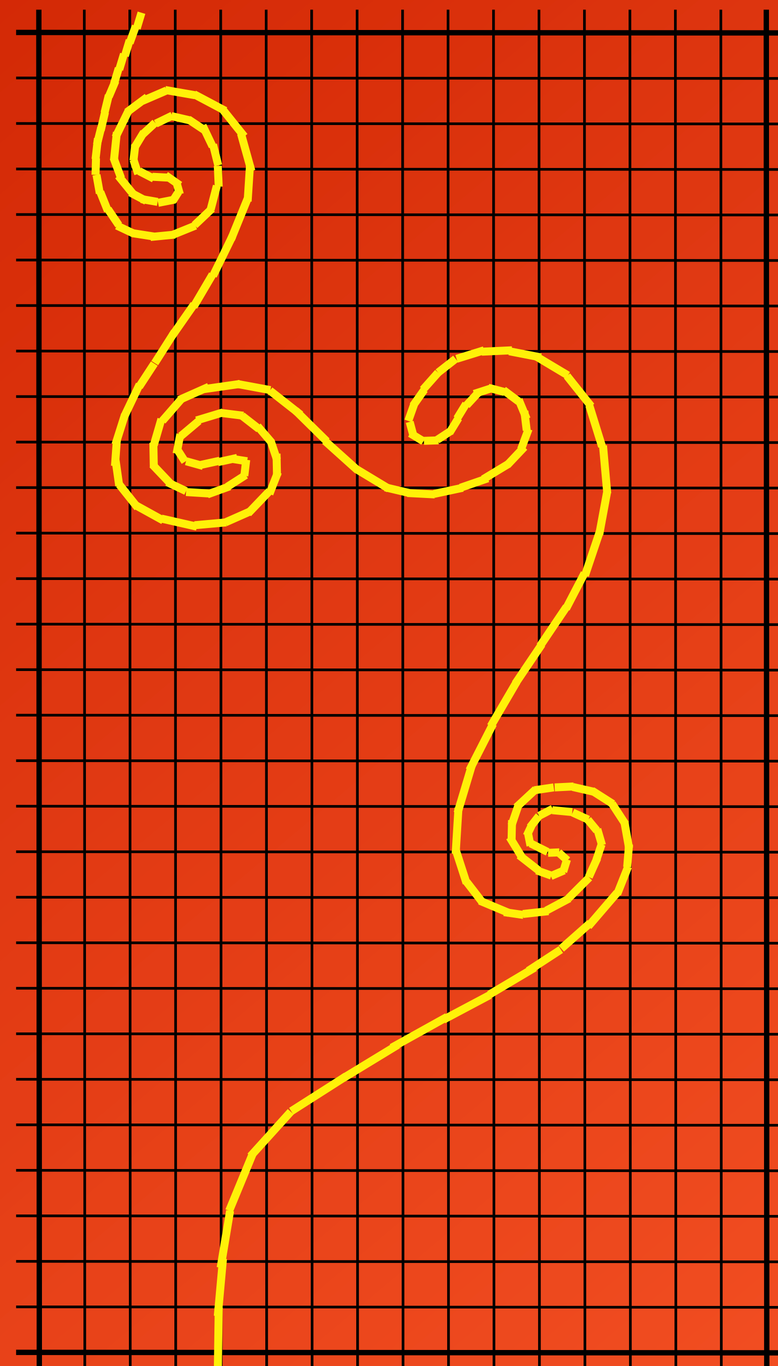
Interface is continuous



Interface is continuous



Single or multiple box crossing



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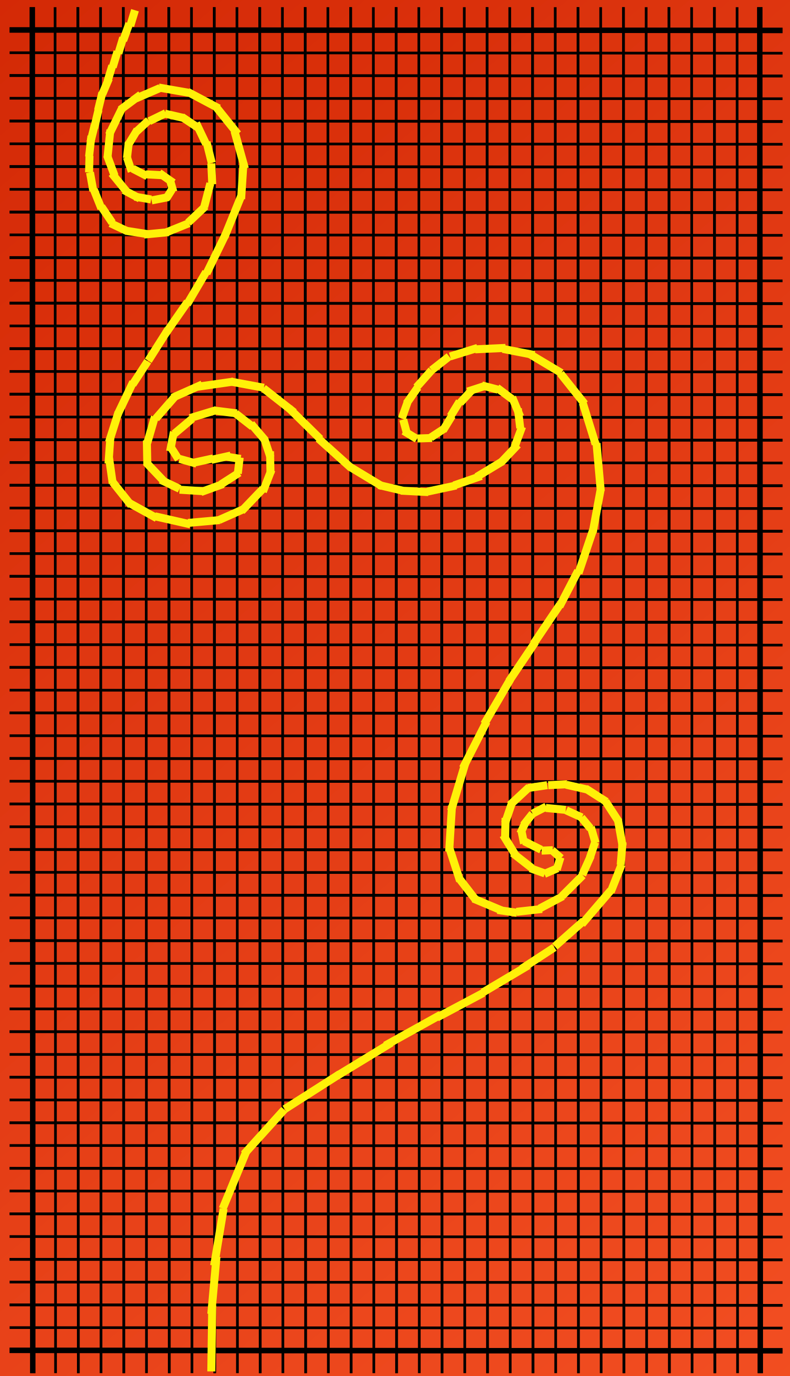


Convex, concave, stratified, convoluted

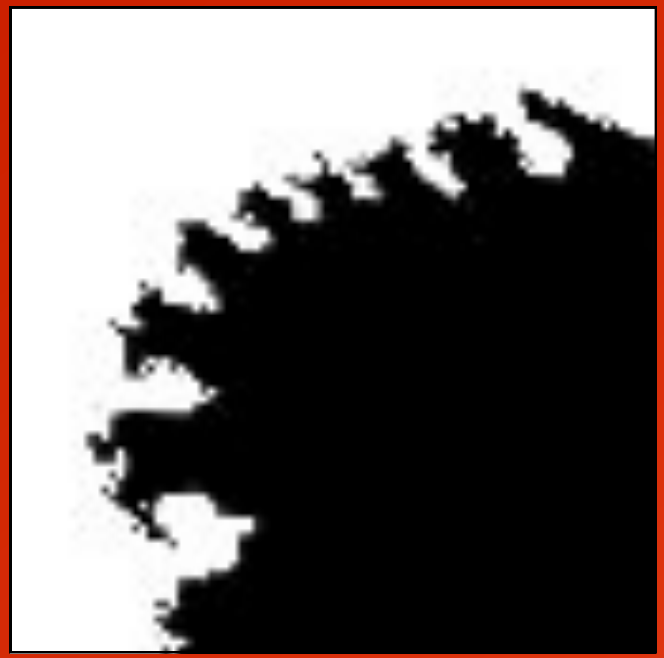
a

Convex, concave, stratified, convoluted

a

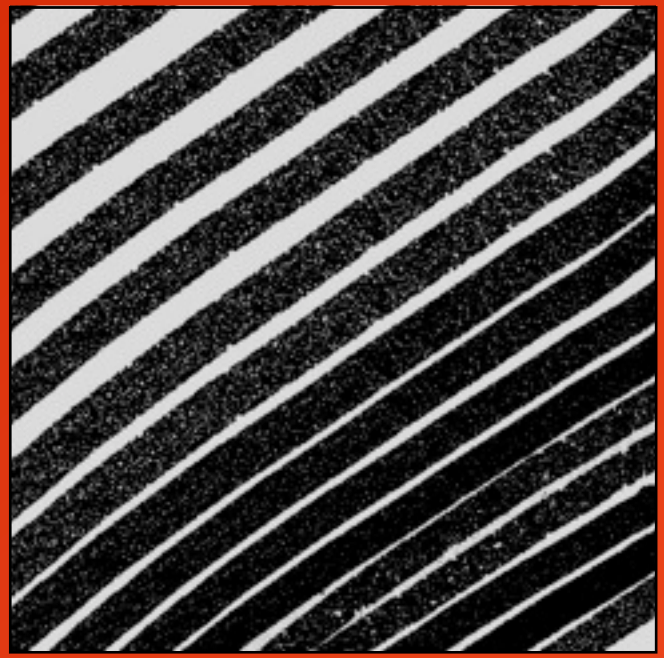
b

Convex, concave, stratified, convoluted



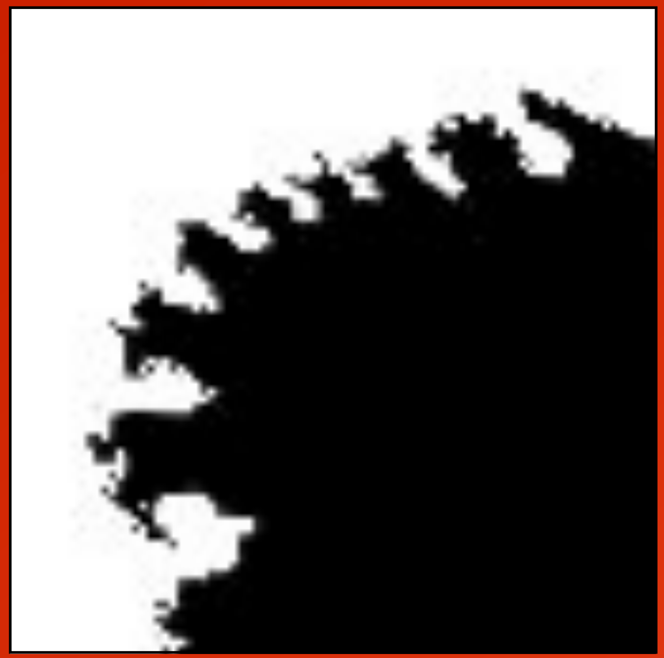
a

b



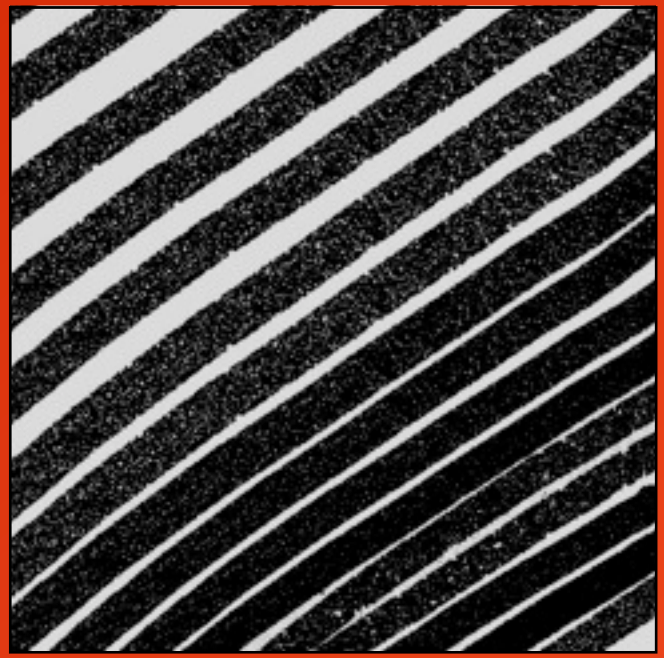
c

Convex, concave, stratified, convoluted



a

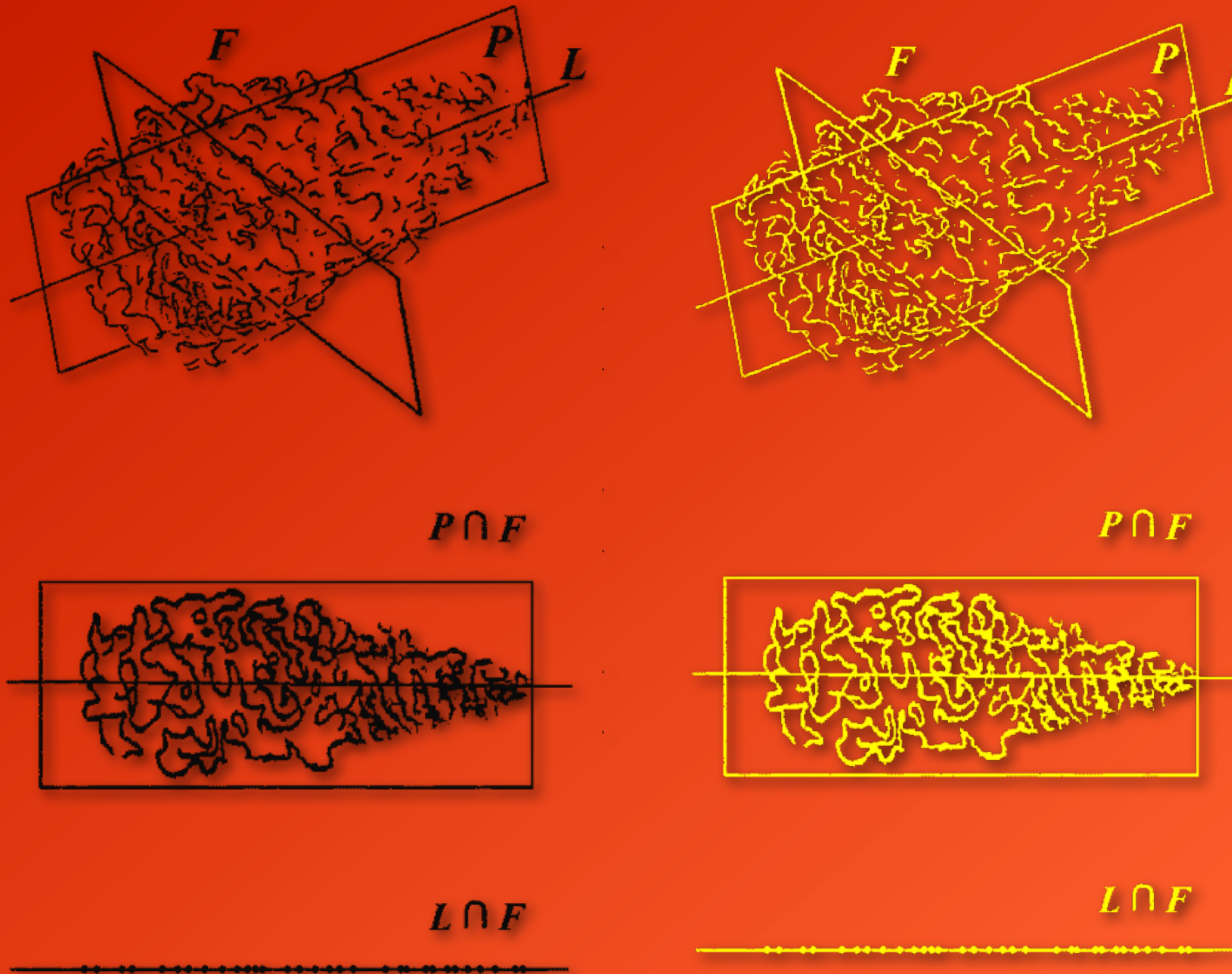
b

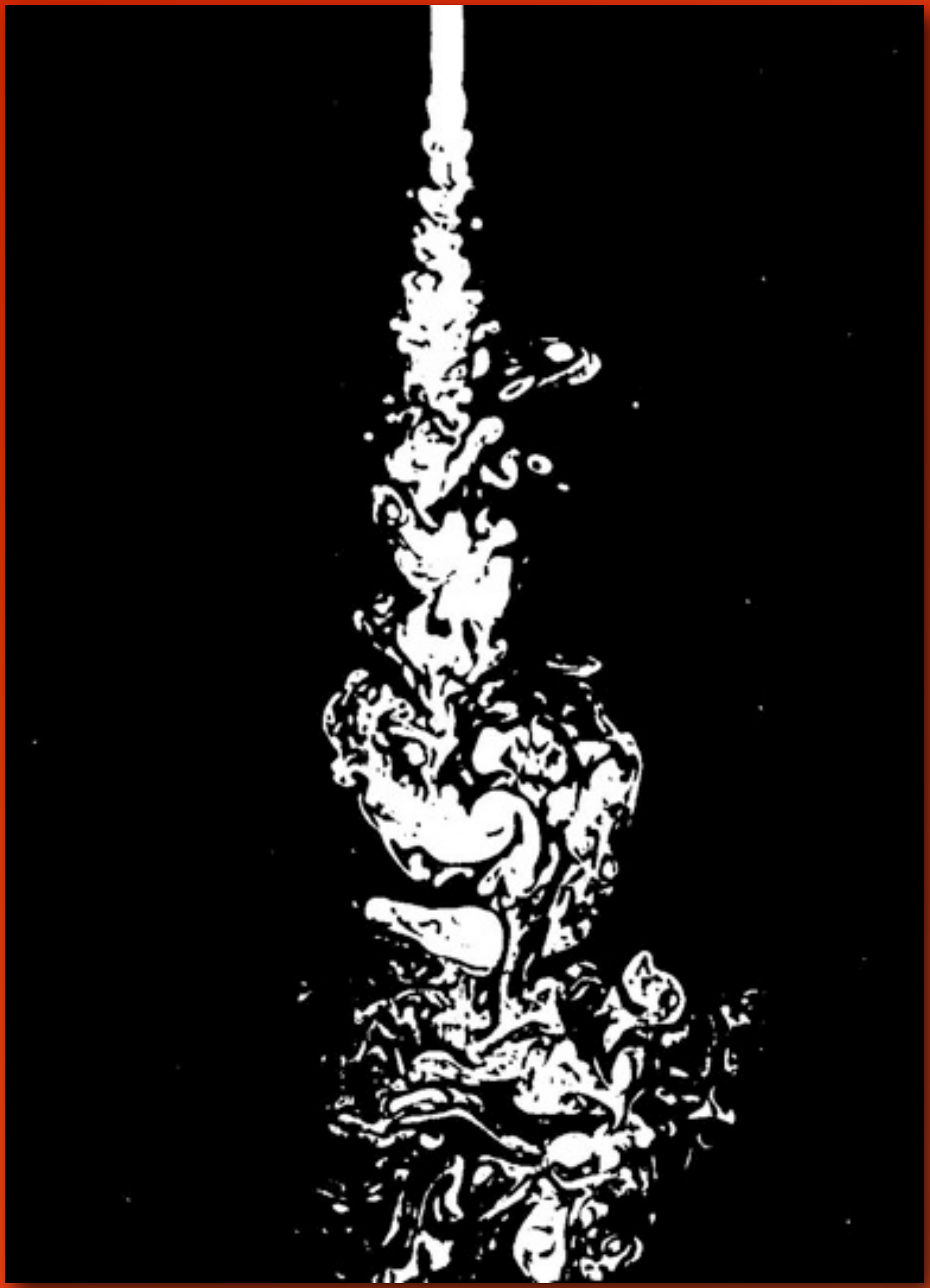


c

d

Planar and linear sectioning

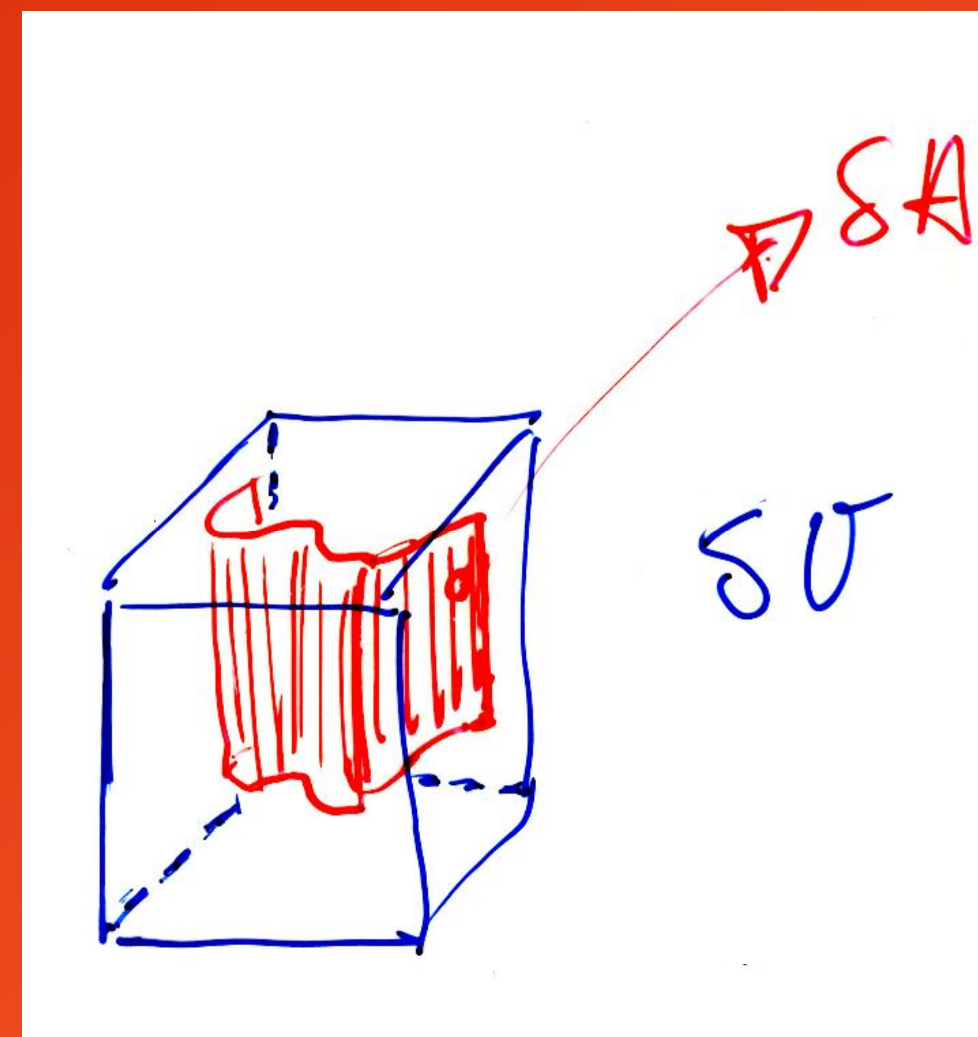


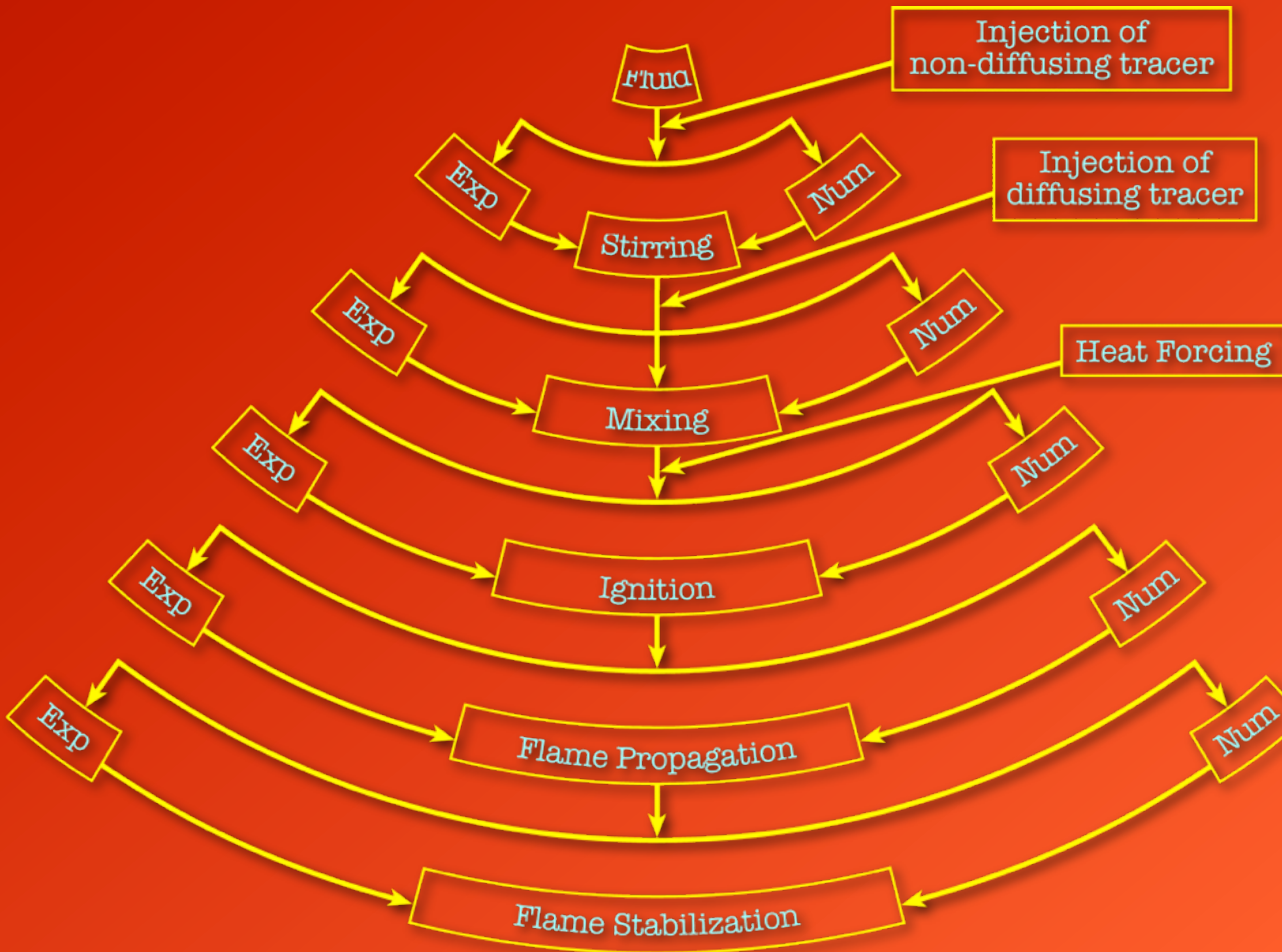


$$\Sigma = \langle \Sigma' \rangle = \left\langle \frac{\delta A}{\delta V} \right\rangle = \frac{\langle \delta A \rangle}{\delta V}$$

$$\langle Q \rangle_s = \frac{\langle Q\delta A \rangle}{\langle \delta A \rangle} = \frac{\langle Q\Sigma' \rangle}{\Sigma} = \frac{\langle Q\delta A \rangle}{\Sigma \delta V}$$

$$\frac{\partial \Sigma}{\partial t} = \underline{\nabla} \cdot \left(\left\langle \underline{v}^{tot} \right\rangle_s \Sigma \right) = \left\langle K^{tot} \right\rangle_s \Sigma$$

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Flame Propagation
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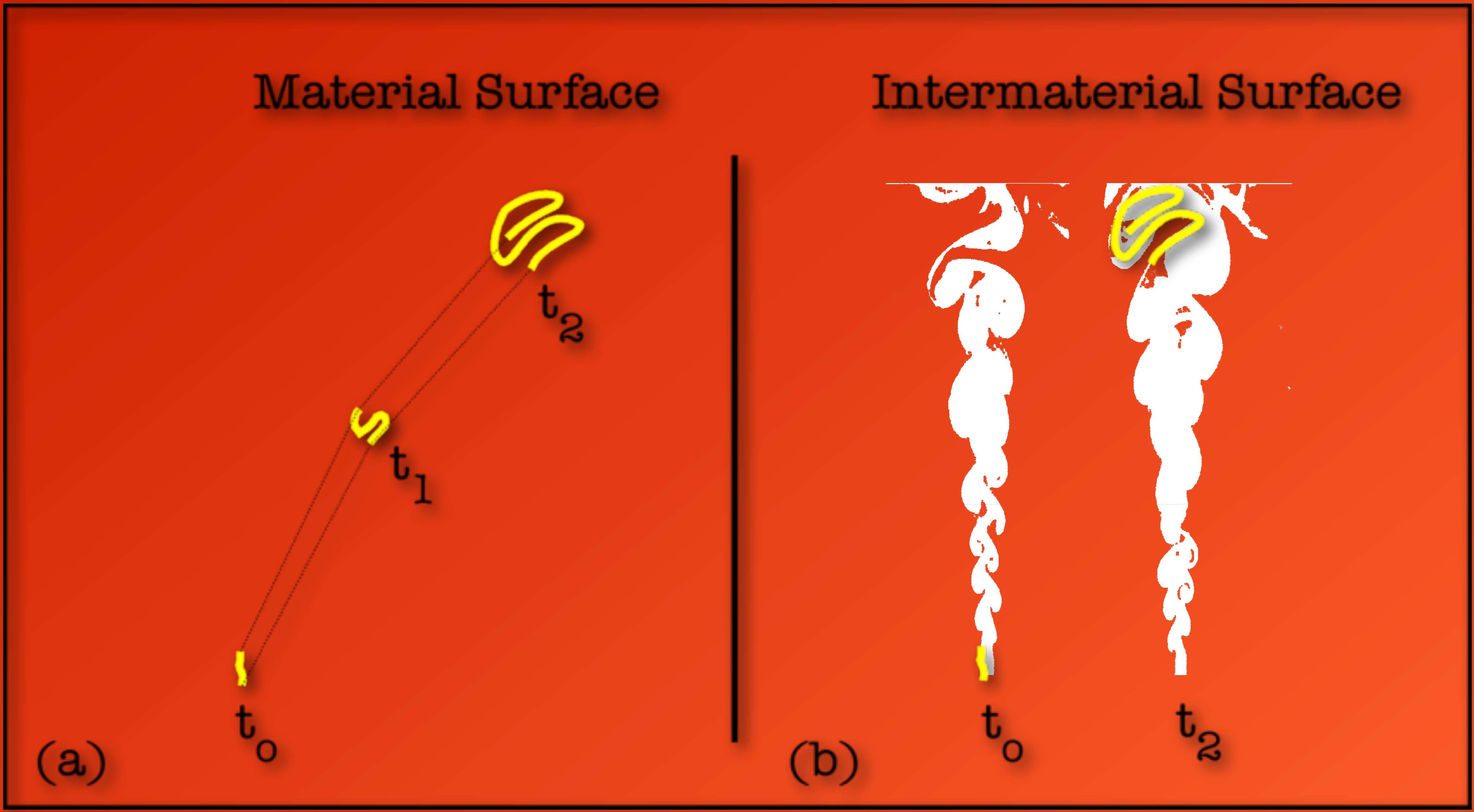
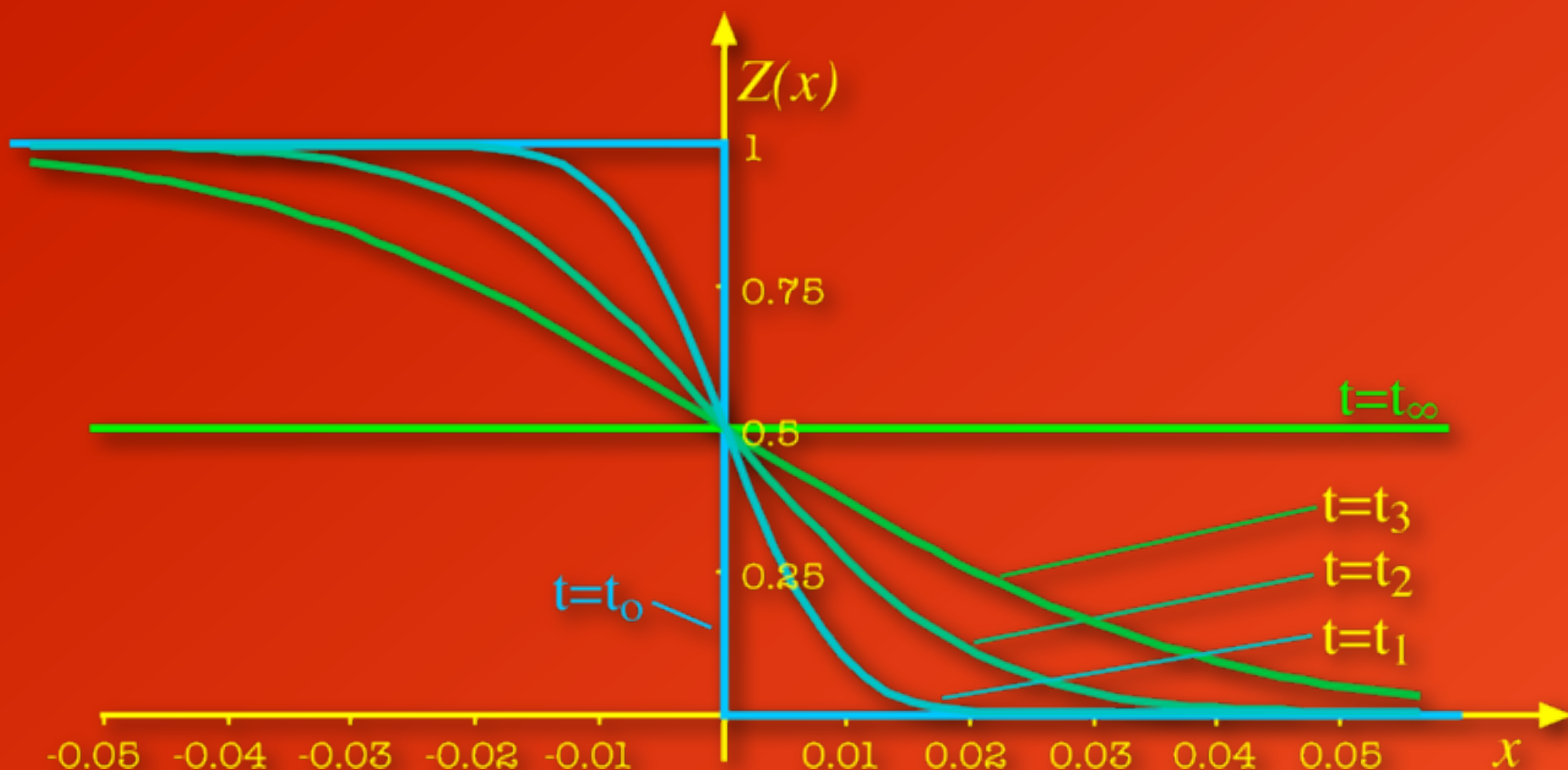
Flame Stabilization

Schematic of material and intermaterial surface evolution



Isolated mixing layer

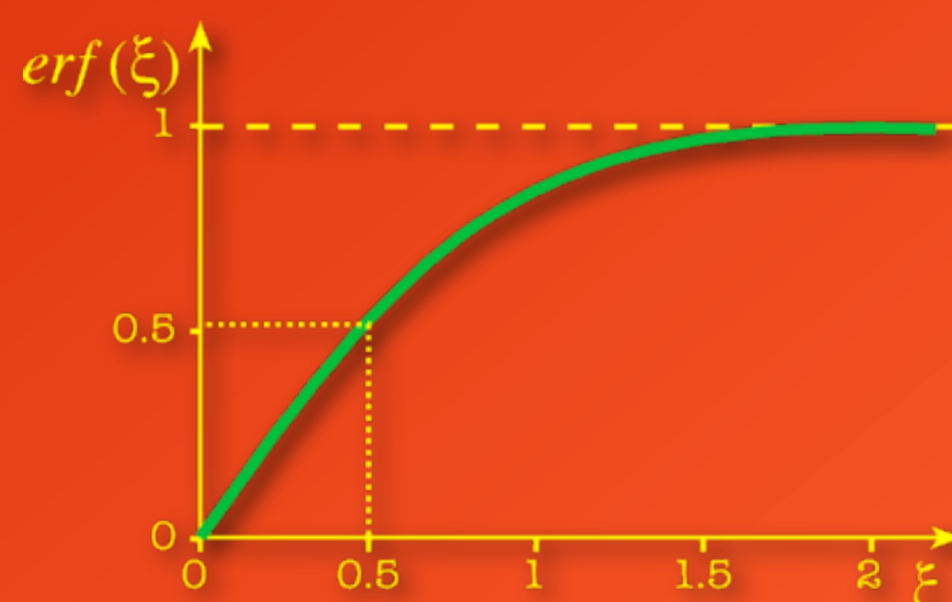


$$\frac{\partial Z}{\partial t} - D\underline{\nabla}^2 Z = 0$$

$$\frac{Z - Z_o}{Z_\infty - Z_o} = erf\left(\xi = \frac{x}{\delta_m}\right)$$

$$\delta_m = \delta_{0.9} = \sqrt{4Dt}$$

$$erf\left(\xi\right) = \frac{2}{\sqrt{\pi}}\int_0^\xi e^{-x^2}dx$$

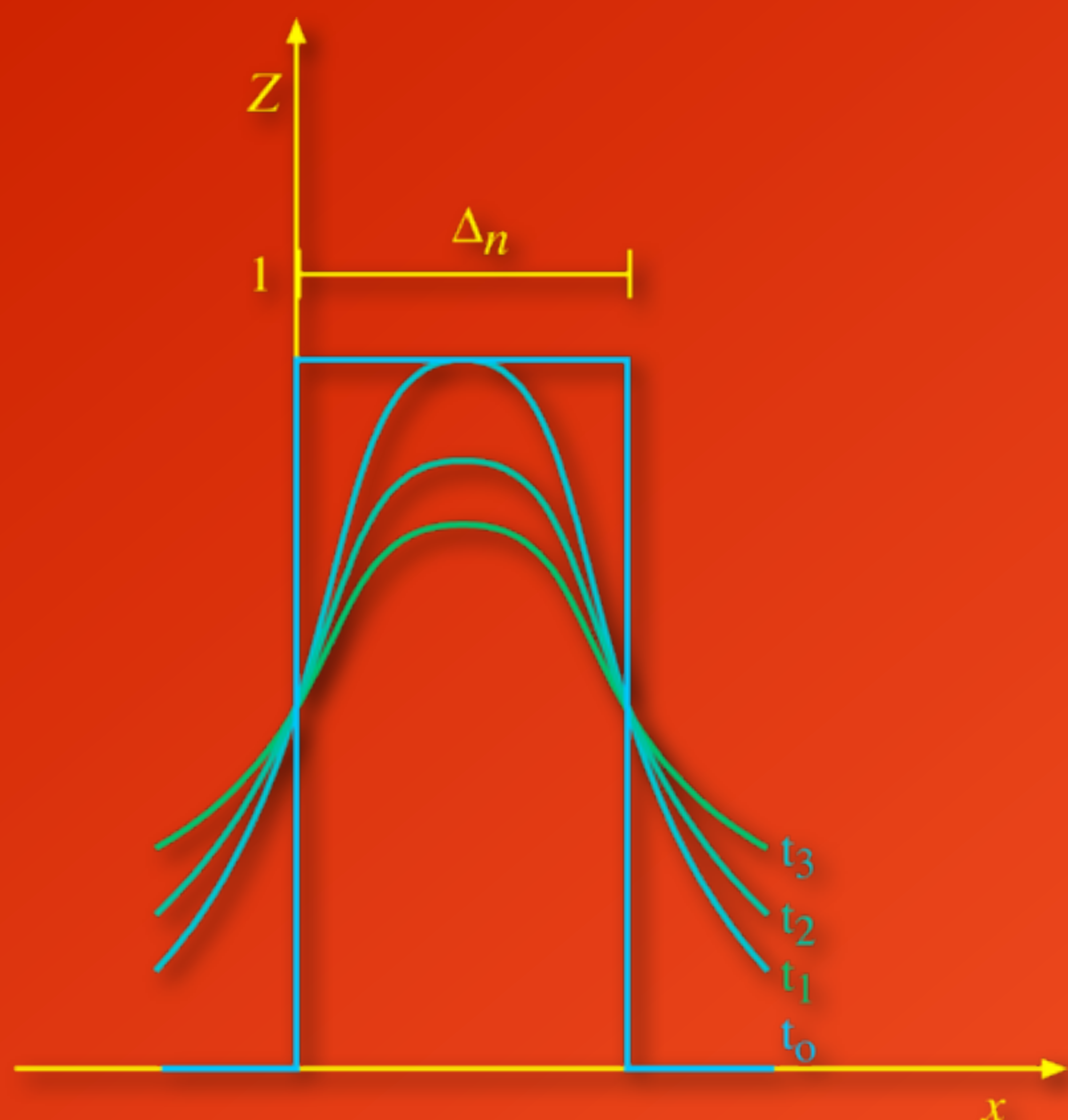


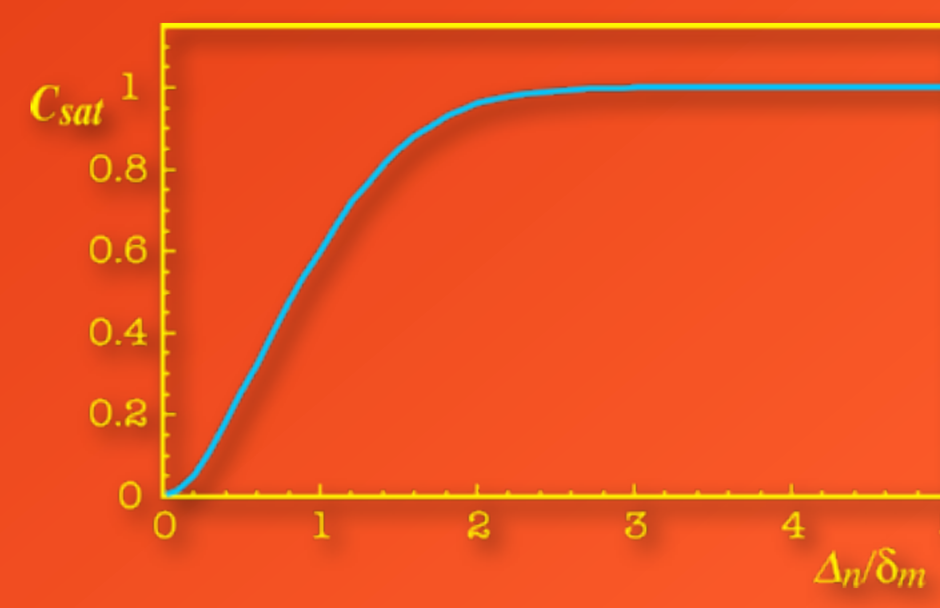
Example of 1D mixture fraction distribution in a double diffusive layer

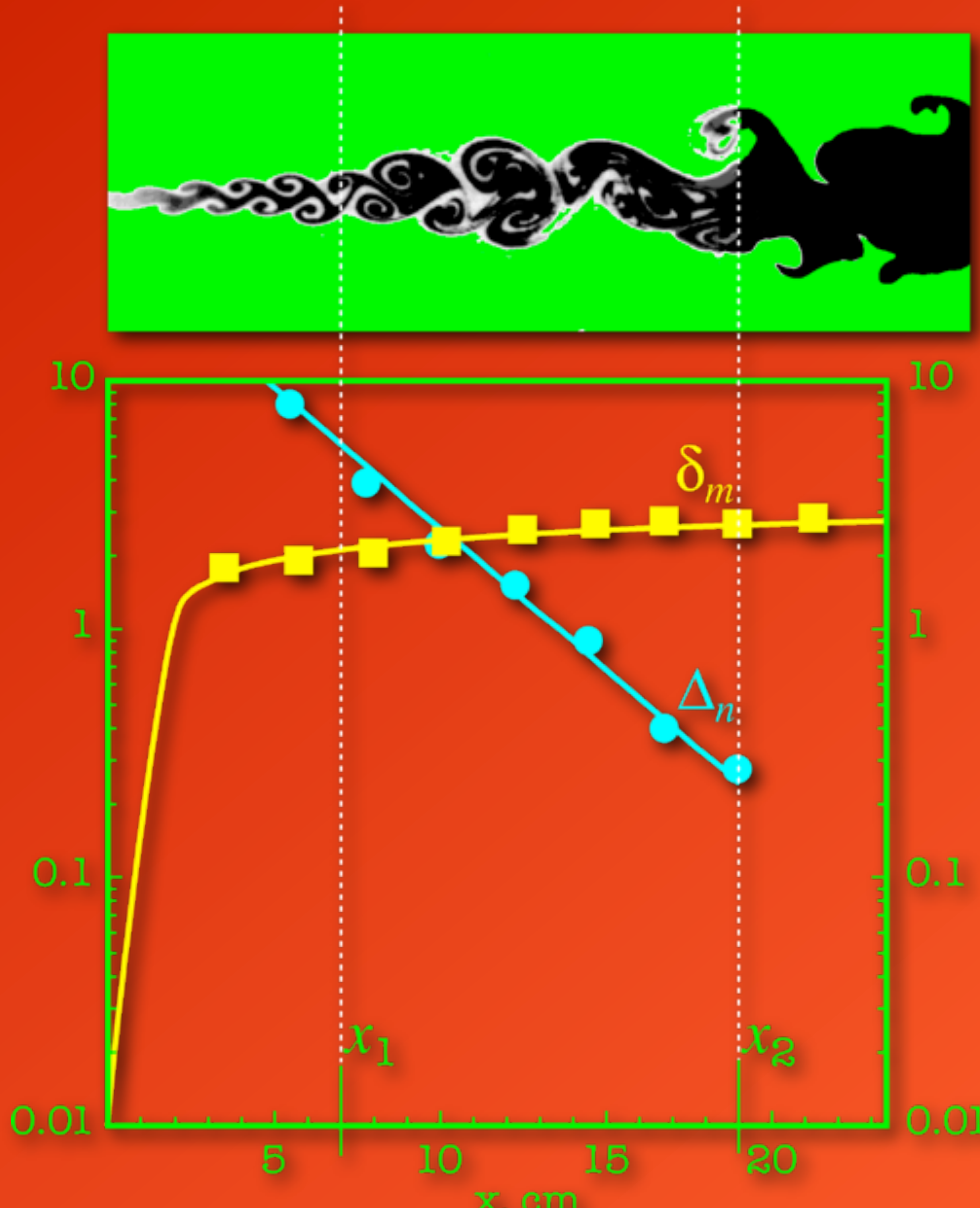
$$Z = \frac{1}{2}\left[erf\left(\frac{x}{\delta_m}\right) - erf\left(\frac{x-\Delta_n}{\delta_m}\right)\right]$$

$$\frac{\phi_{\Delta_n}}{\phi_{\Delta_\infty}} = C_{st} = 4 - e^{-\left(\frac{\Delta_n}{\delta_m}\right)^2}$$

$$\phi_{\Delta_\infty}(t, x_n) = \frac{\rho DSR}{\sqrt{\pi}\delta_m}$$

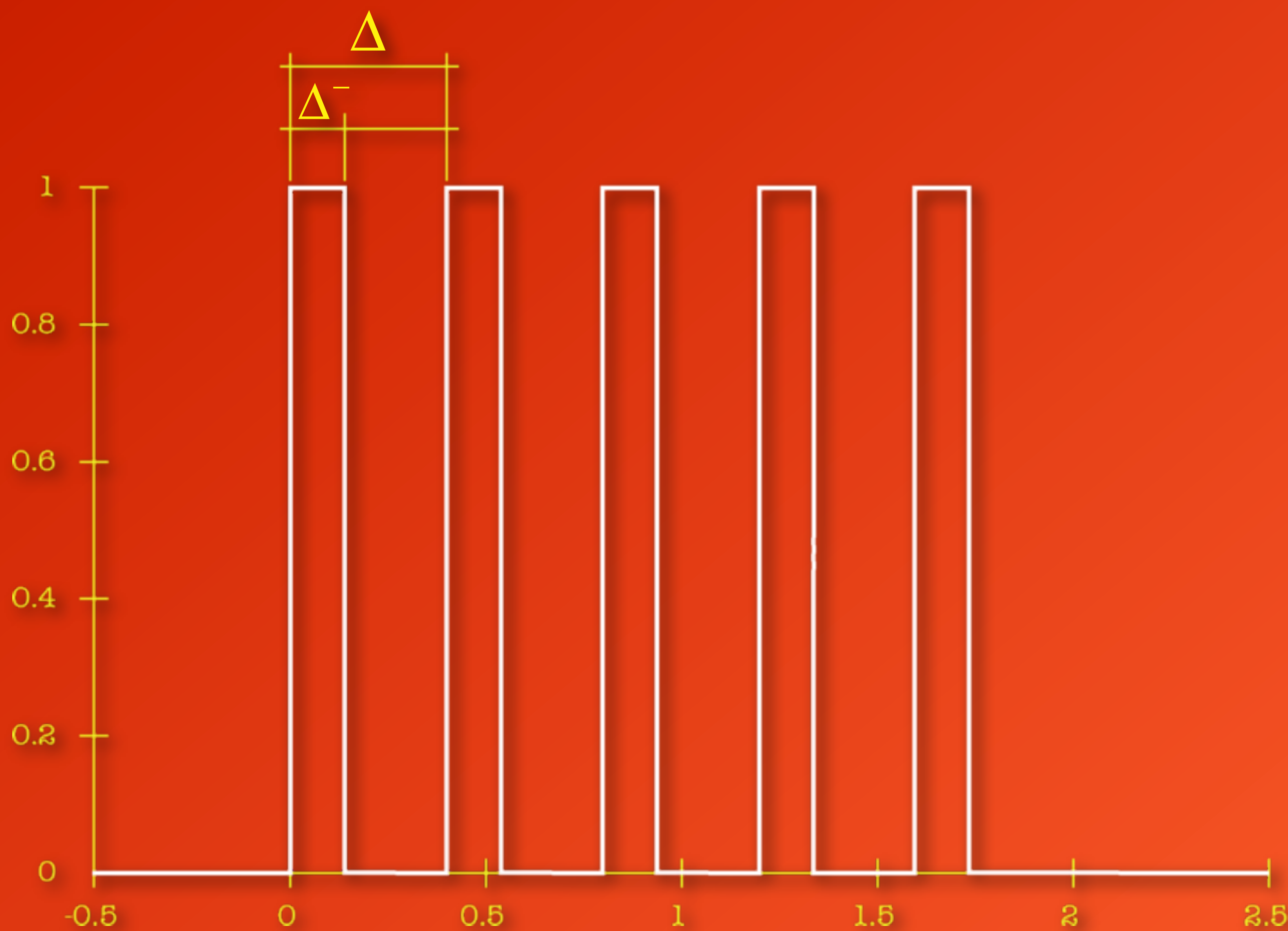






10
1
0.1
0.01
10
1
0.1
0.01
δ_m
Δ_n
x_1
x_2
5
10
15
20
x, cm

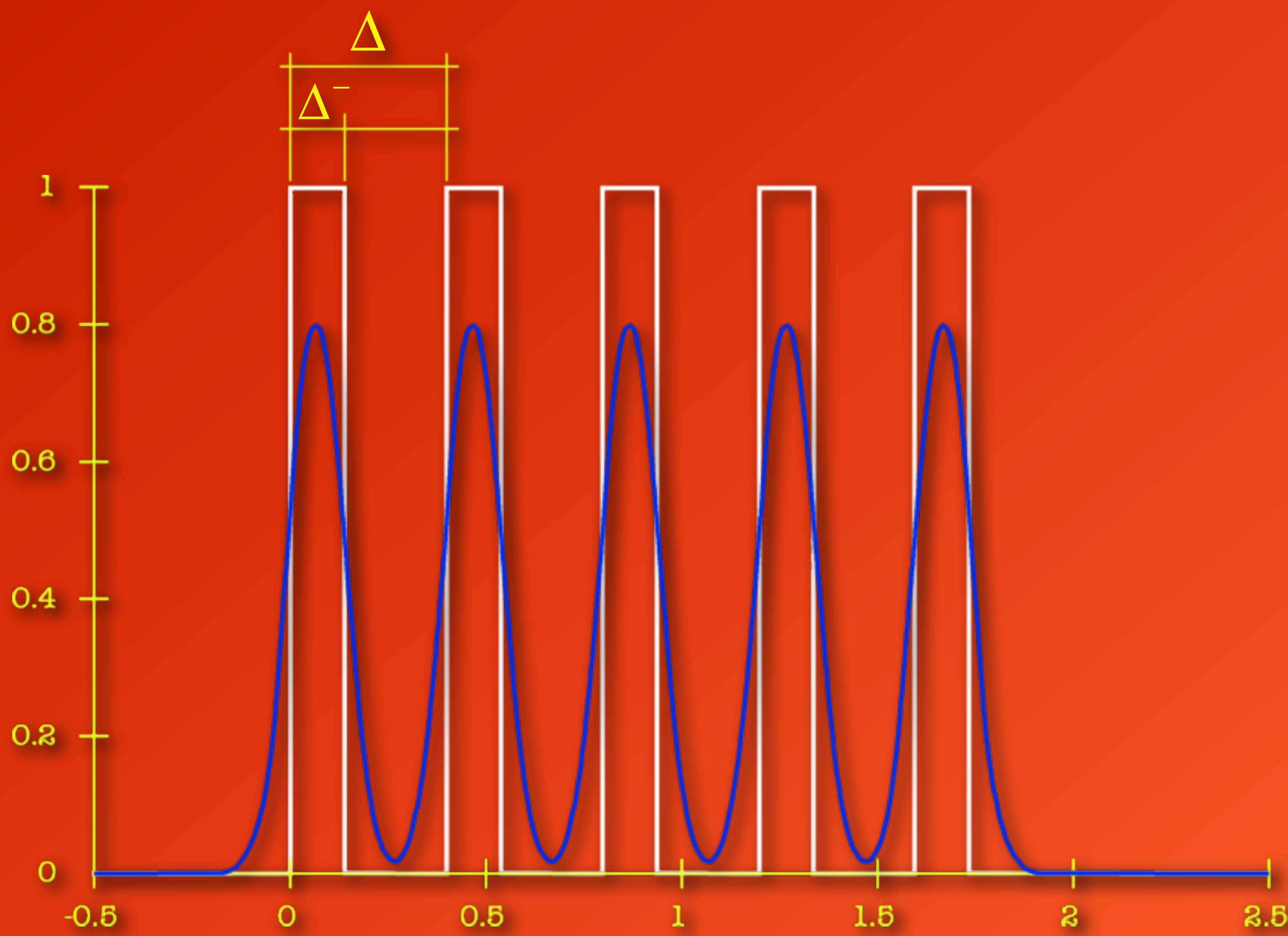
multiple layer



$$n = 4$$

$$Z = \sum_{i=0}^{n} \frac{1}{2}\left[erf\left(\frac{x - n\Delta - \Delta^-}{\delta} \right) - erf\left(\frac{x - n\Delta}{\delta} \right) \right]$$

multiple layer



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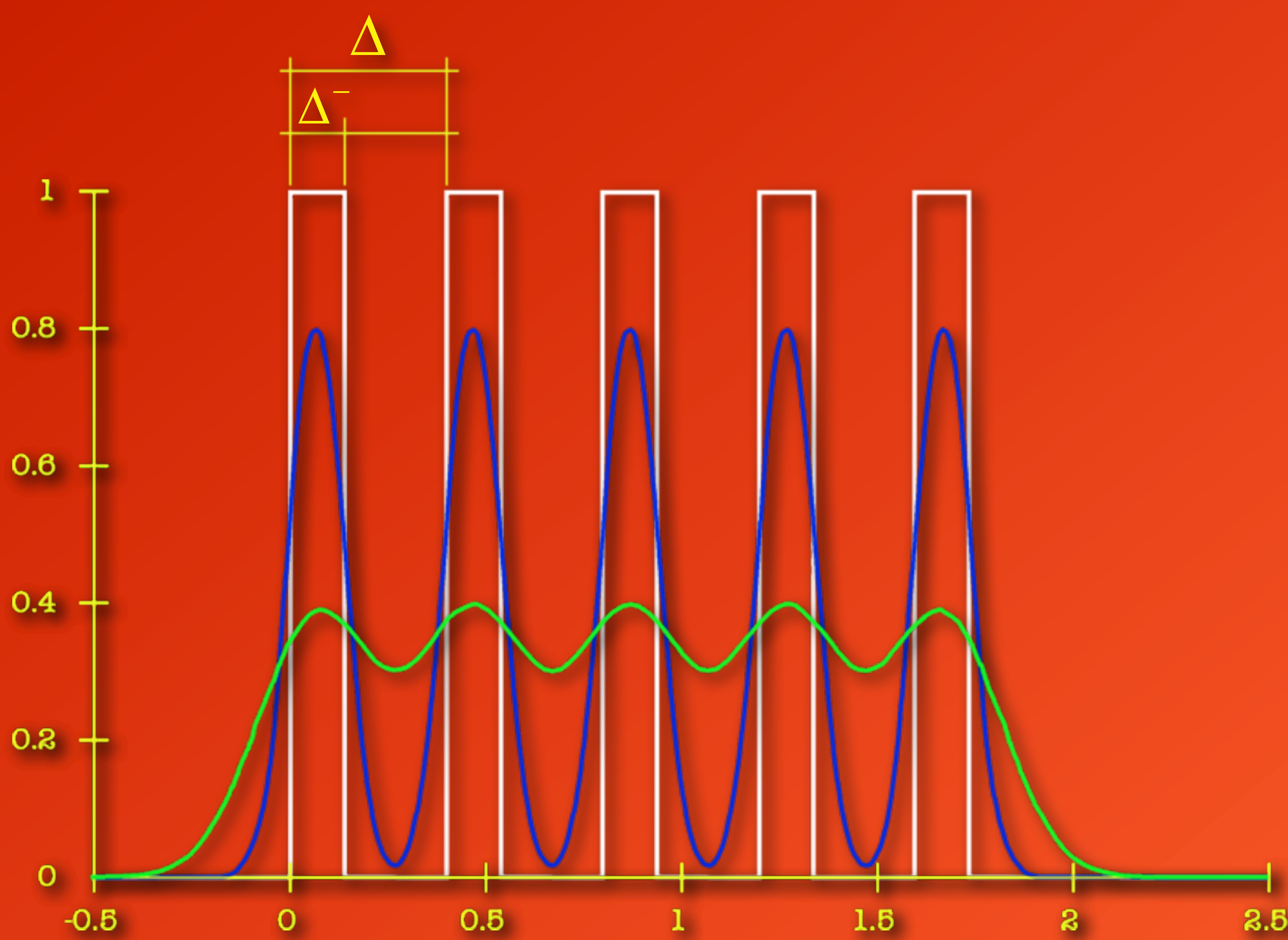
multiple layer



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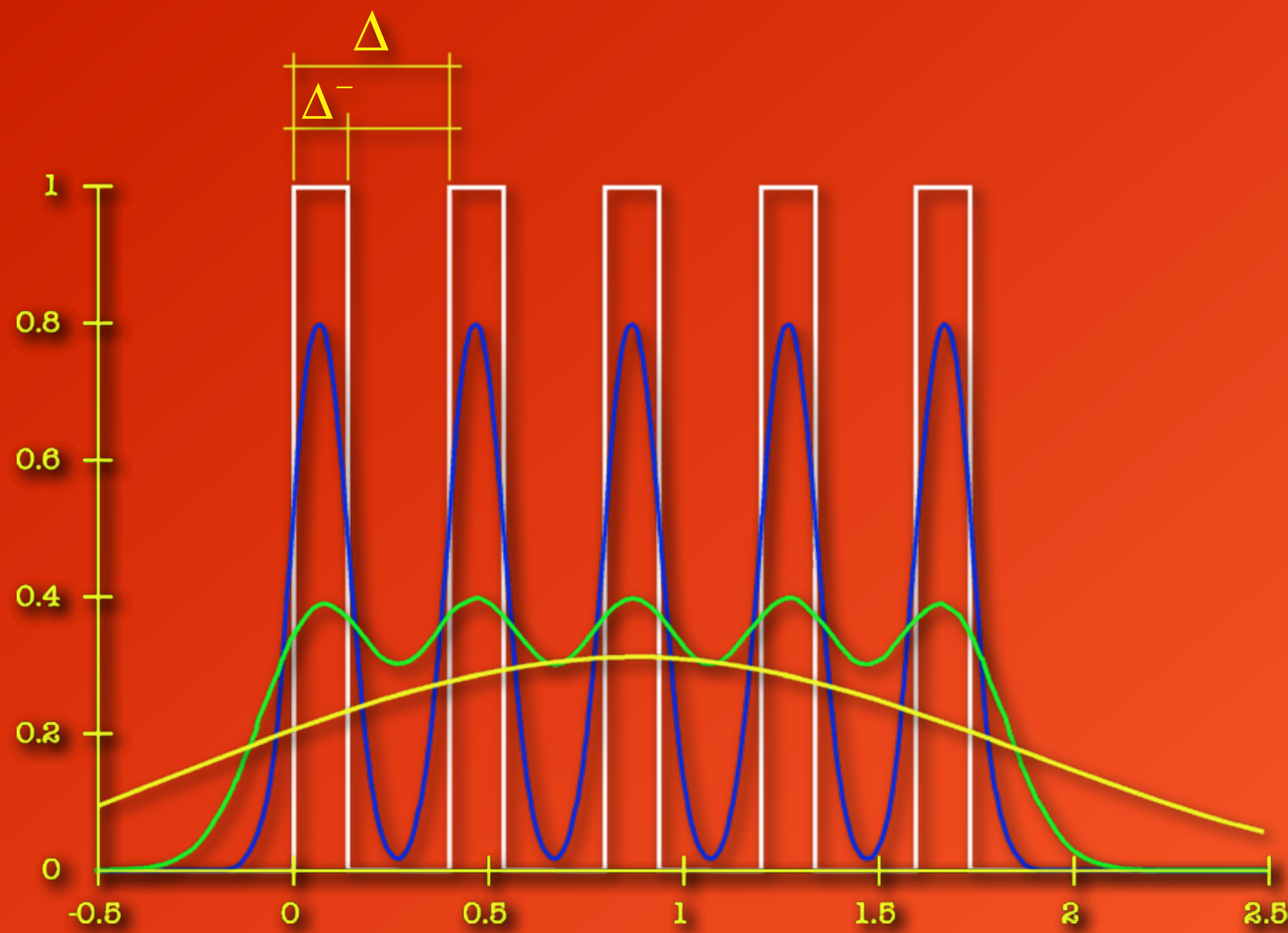
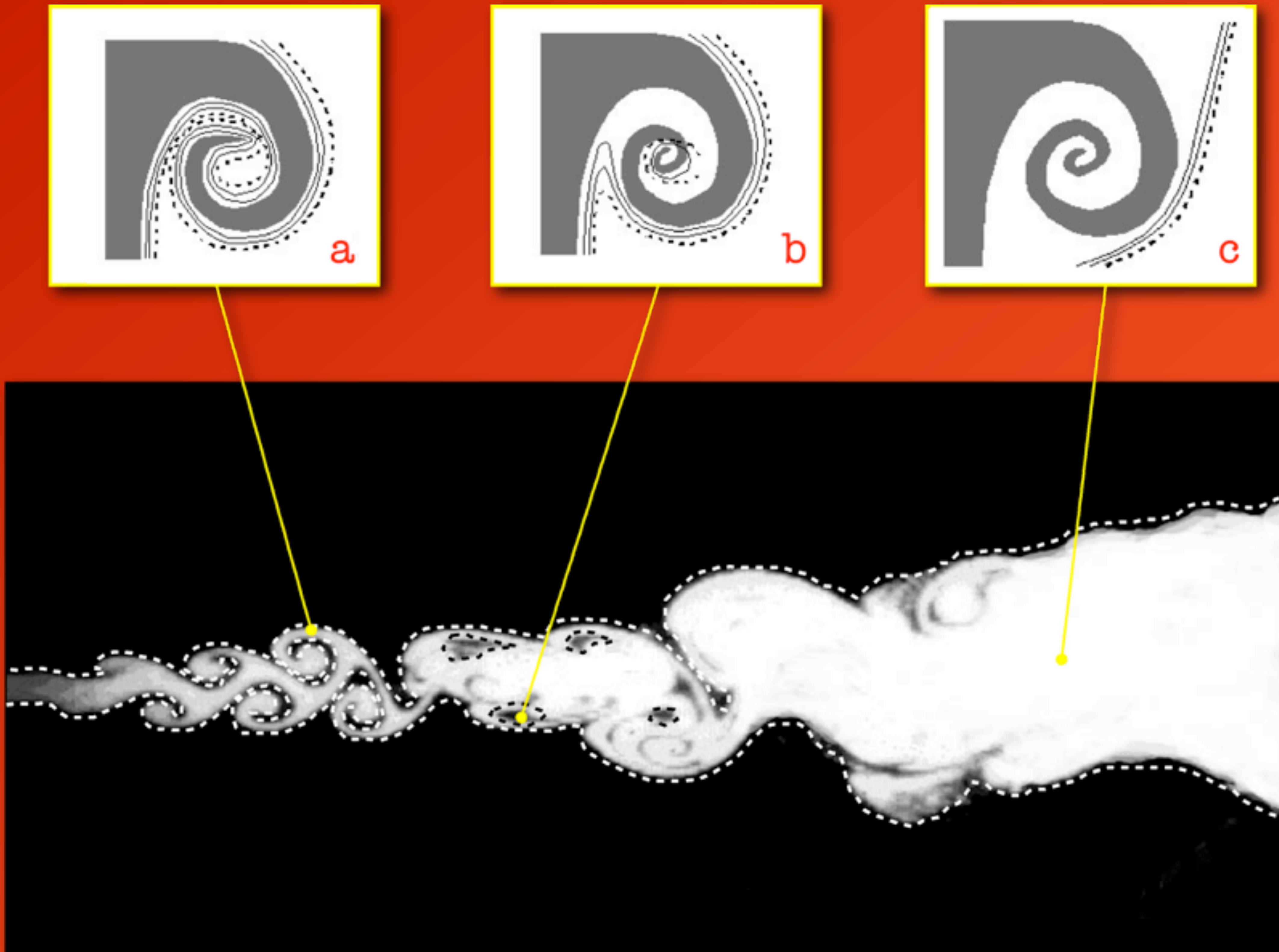
multiple layer

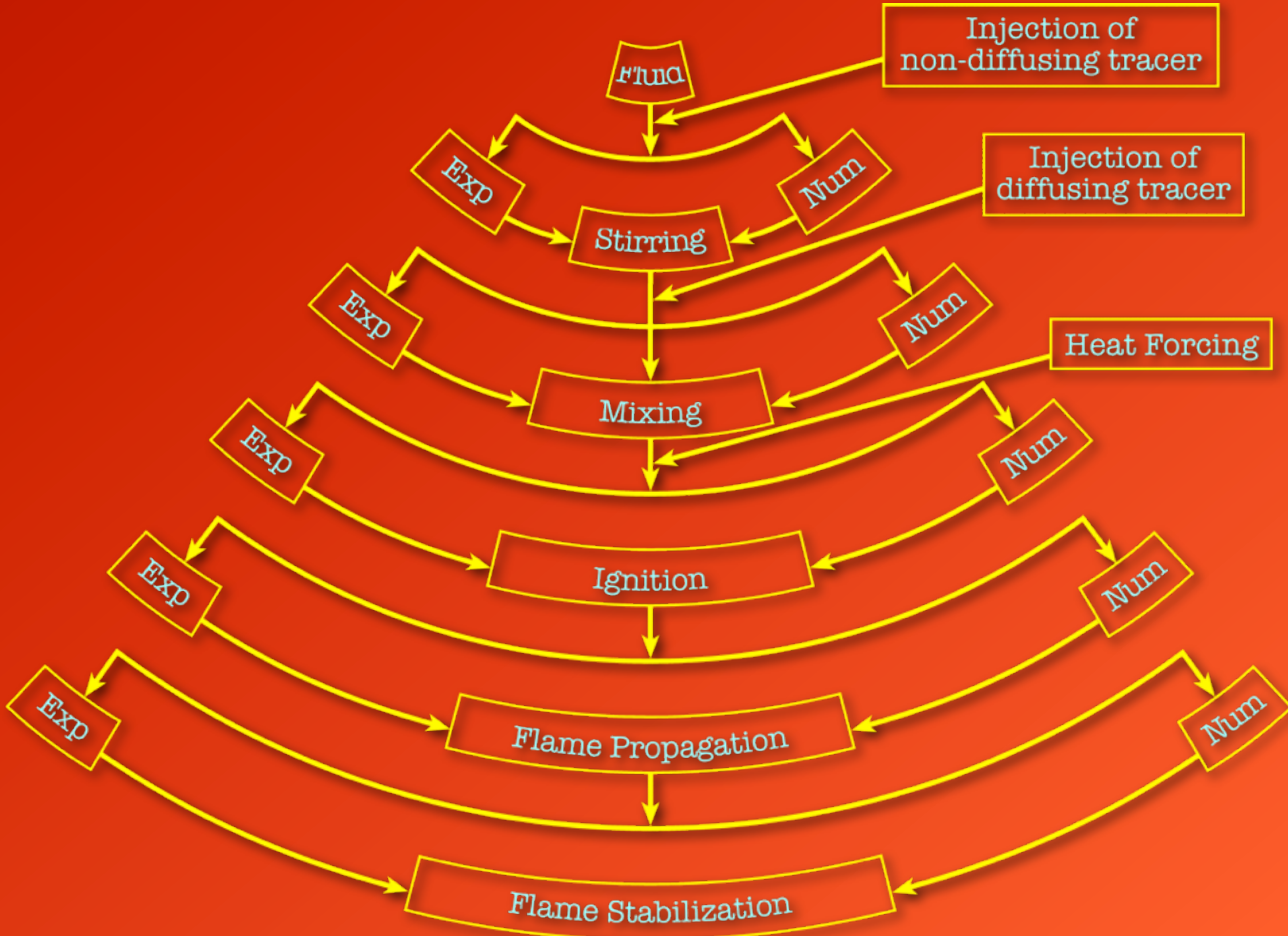


$n = 4$

$$Z = \sum_{i=0}^{n} \frac{1}{2}\left[erf\left(\frac{x - n\Delta - \Delta^{-}}{\delta} \right) - erf\left(\frac{x - n\Delta}{\delta} \right) \right]$$

Example of interface sequence showing a single vortex convolution

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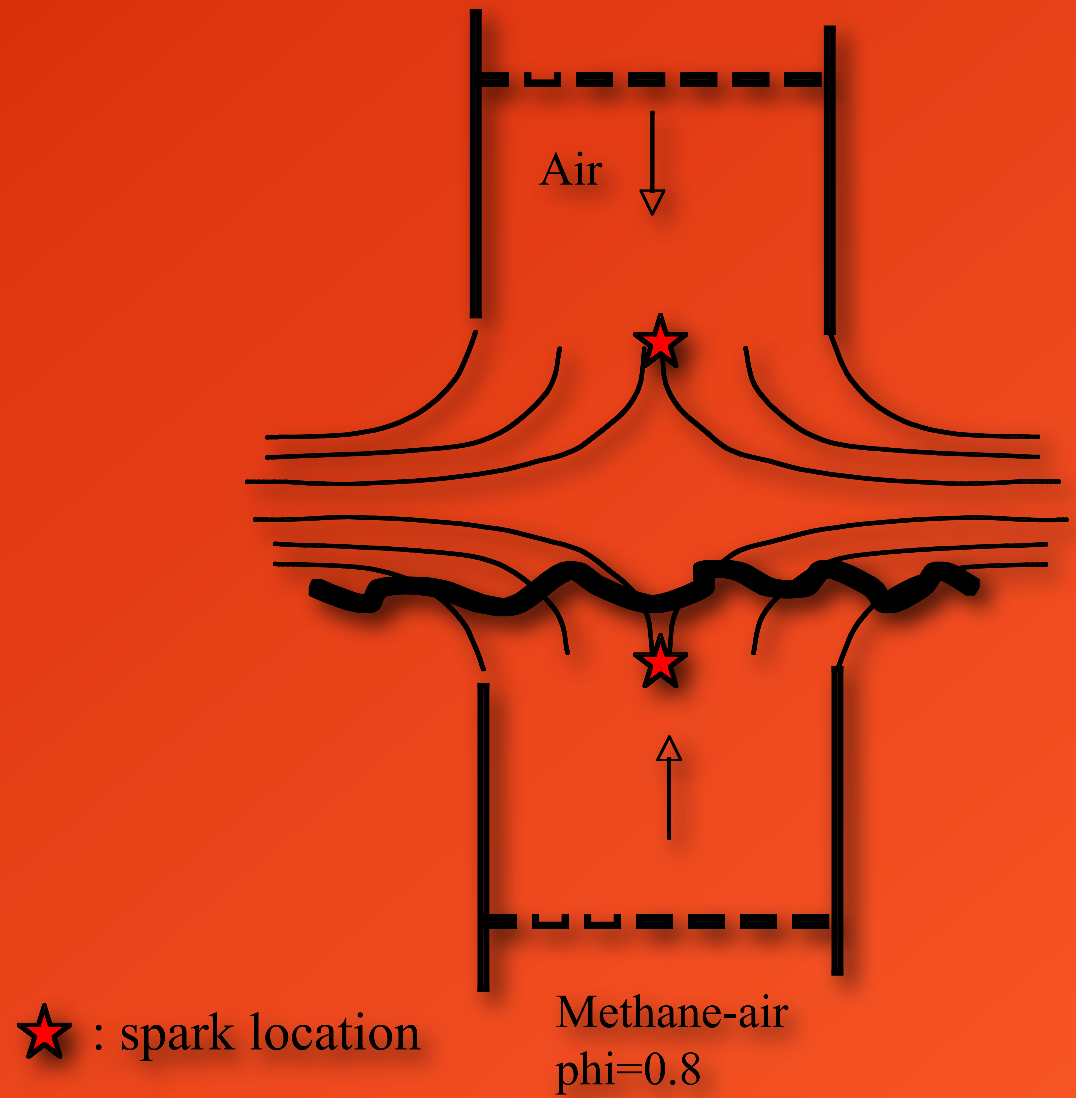
Exp
Num
Flame Propagation
Exp
Num
Flame Stabilization

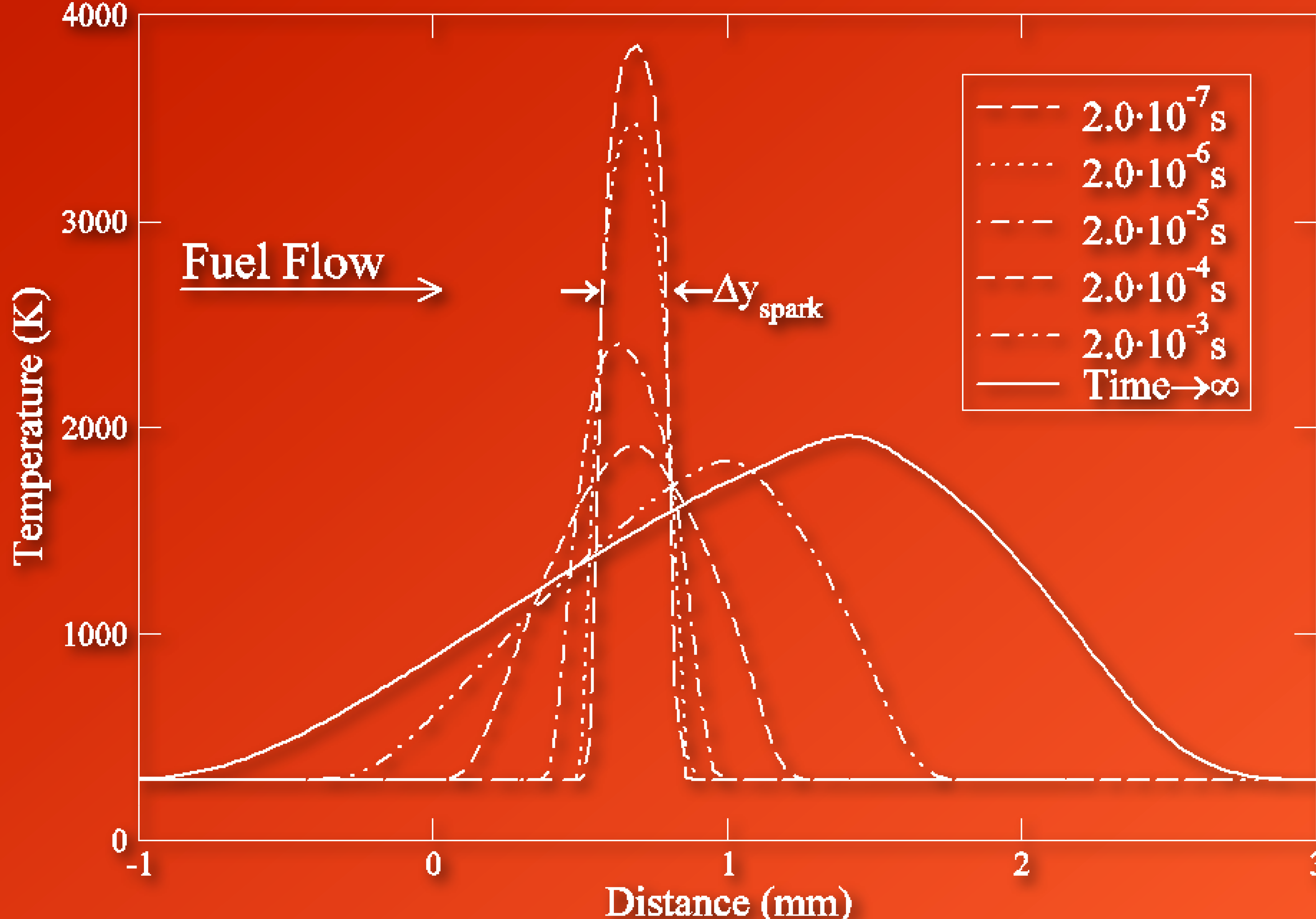
Spark-ignition of counterflow flames

Turbulent conterflow flames are:

- one dimensional
- easy to visualize and model theoretically
- well charcterized in literature

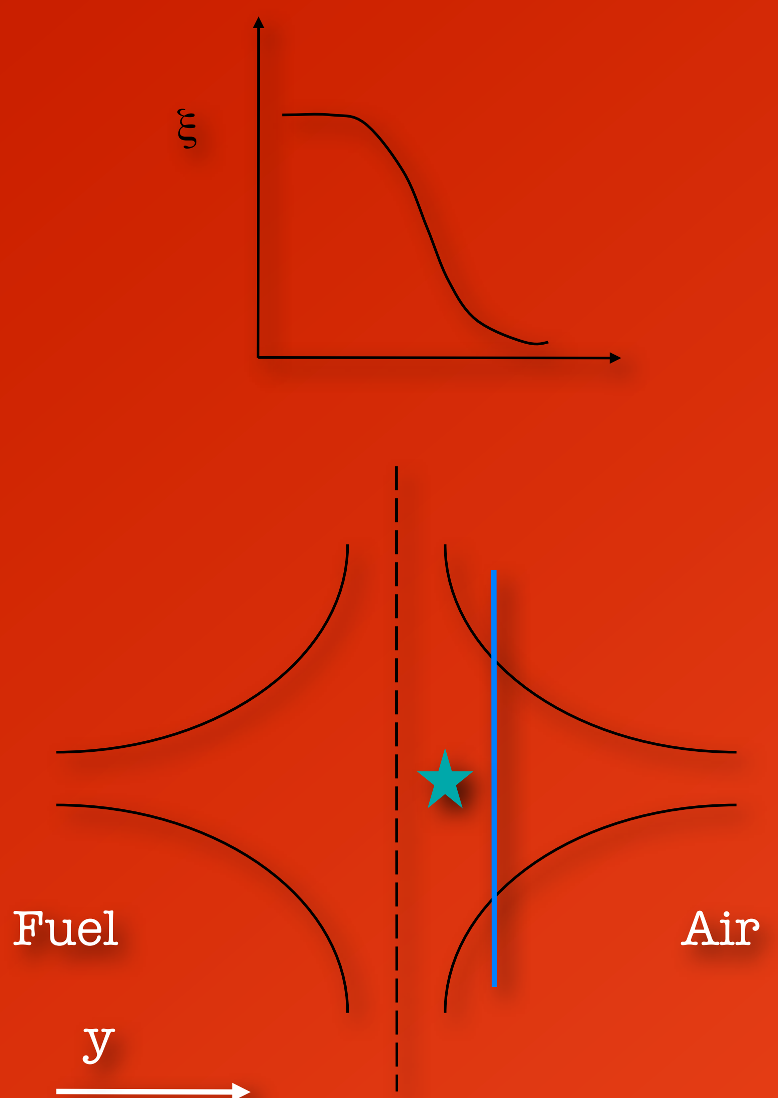


acknowledgement: Mastorakos Epaminondas
Hopkinson Laboratory Univ Cambridge

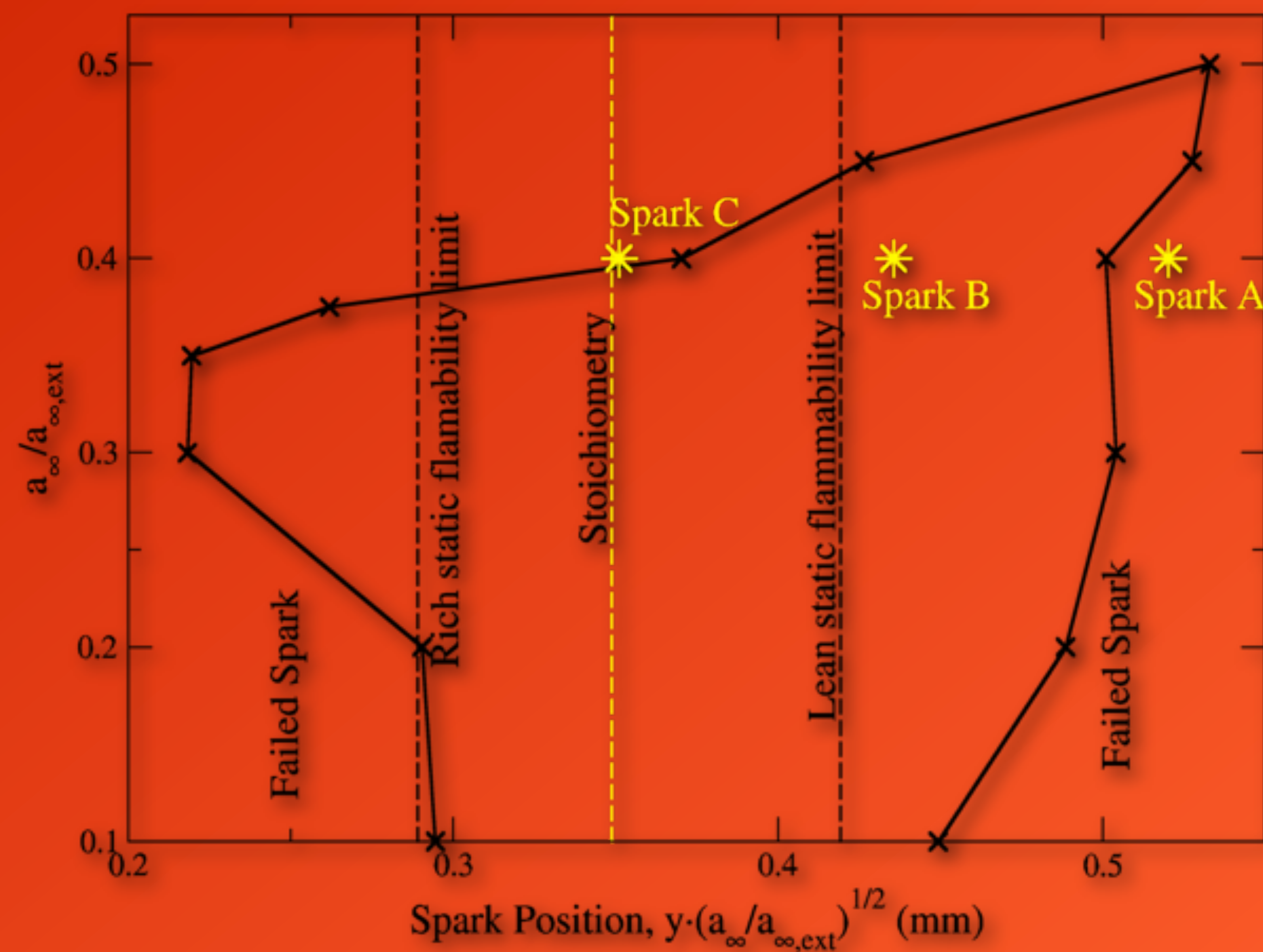


by Richardson E.S. and Mastorakos E.: " Numerical investigation on forced ignition in laminar counterflow non-premixed methane-air flames." Comb Sci. Tech. in printing 2006

...on local scalar dissipation rate.



a: strain rate



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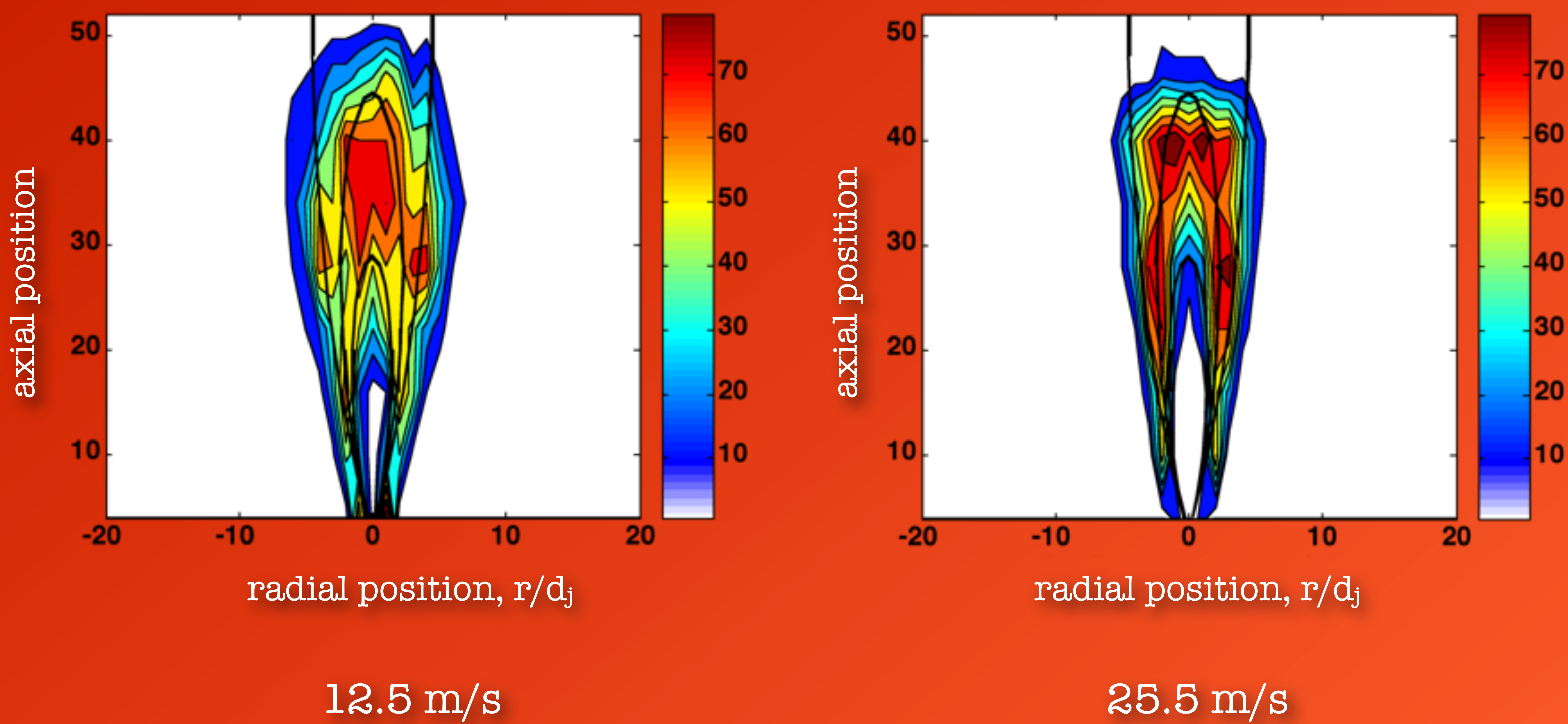
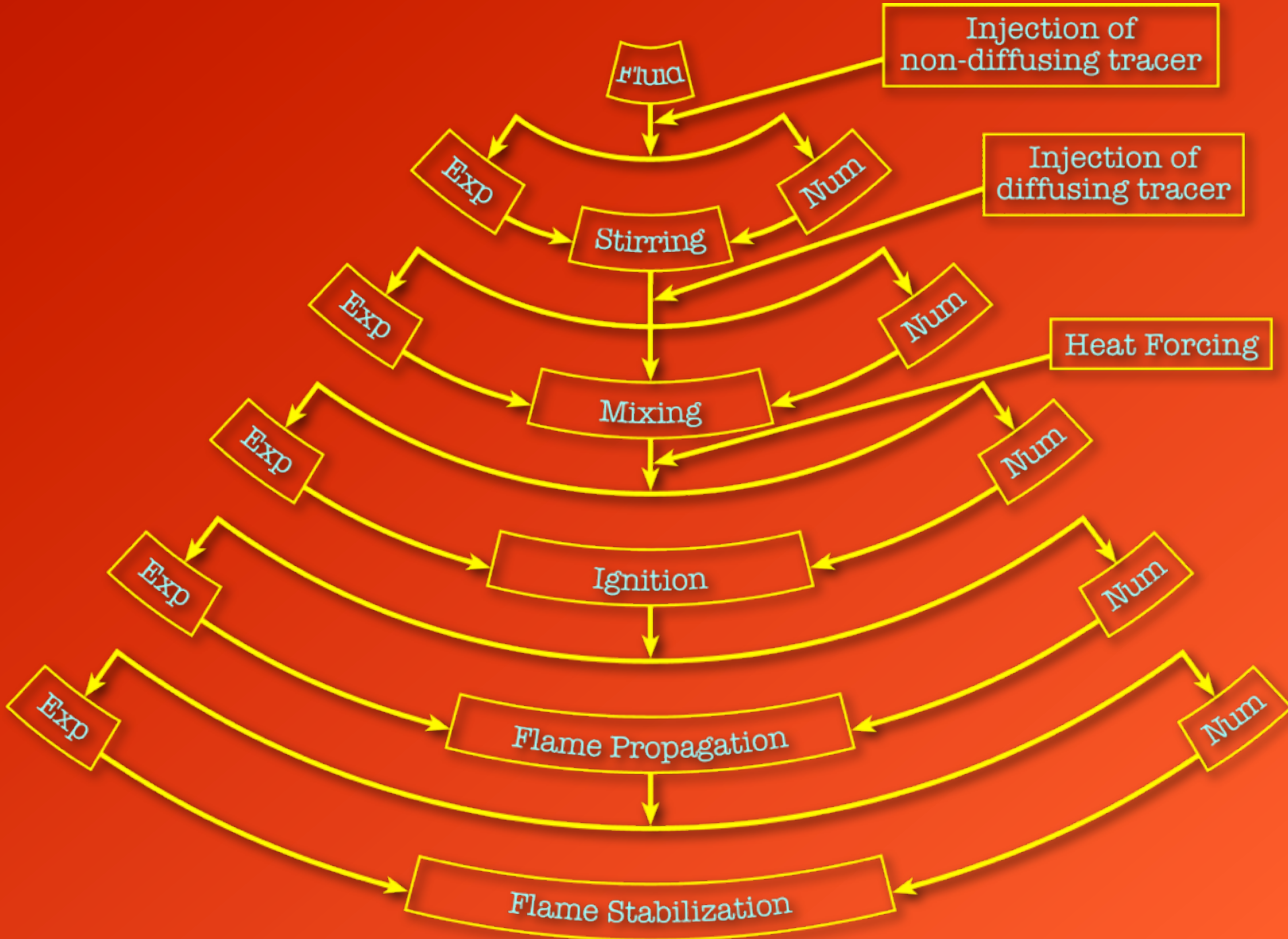
Ignition probability



by Ahmed S.F. and Mastorakos E: "Spark-ignition of lifted turbulent jet flames"
Combustion and Flame in printing 2006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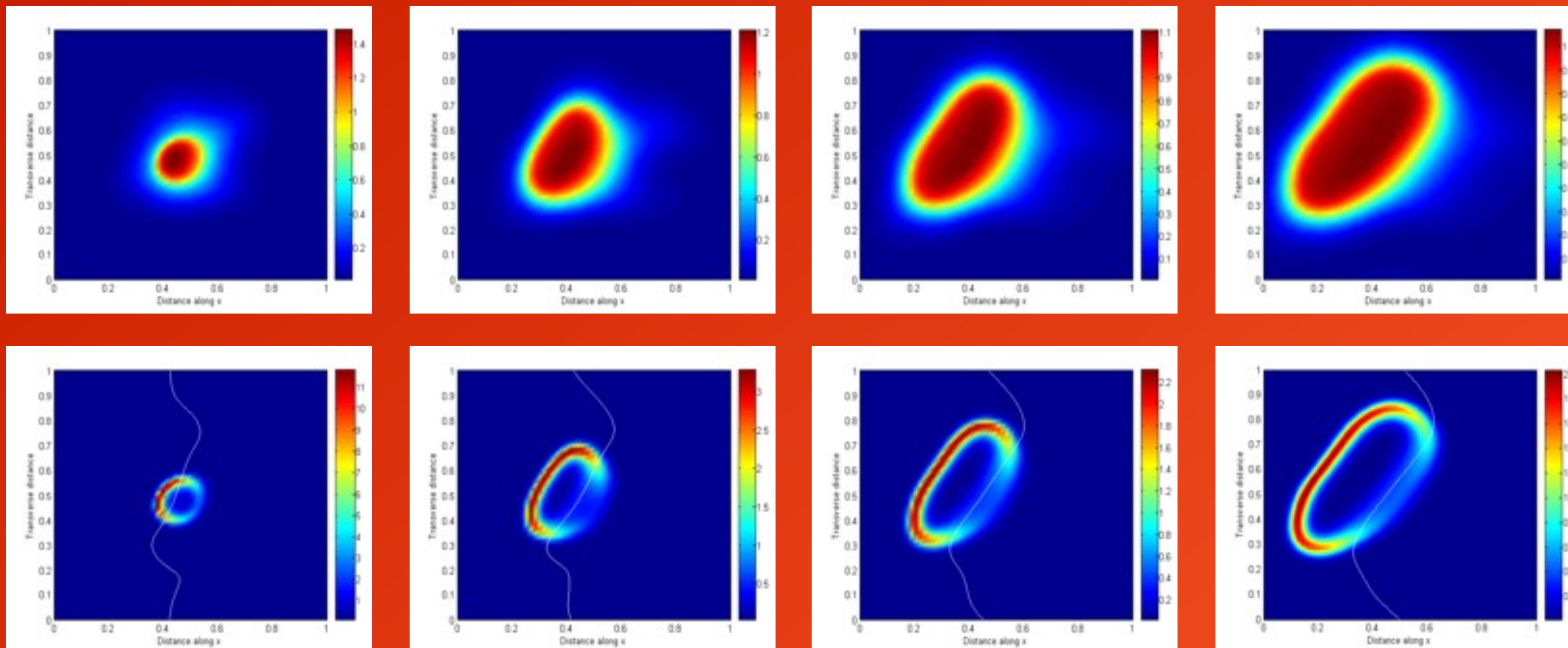
DNS of spark-ignition of non-premixed flames



T

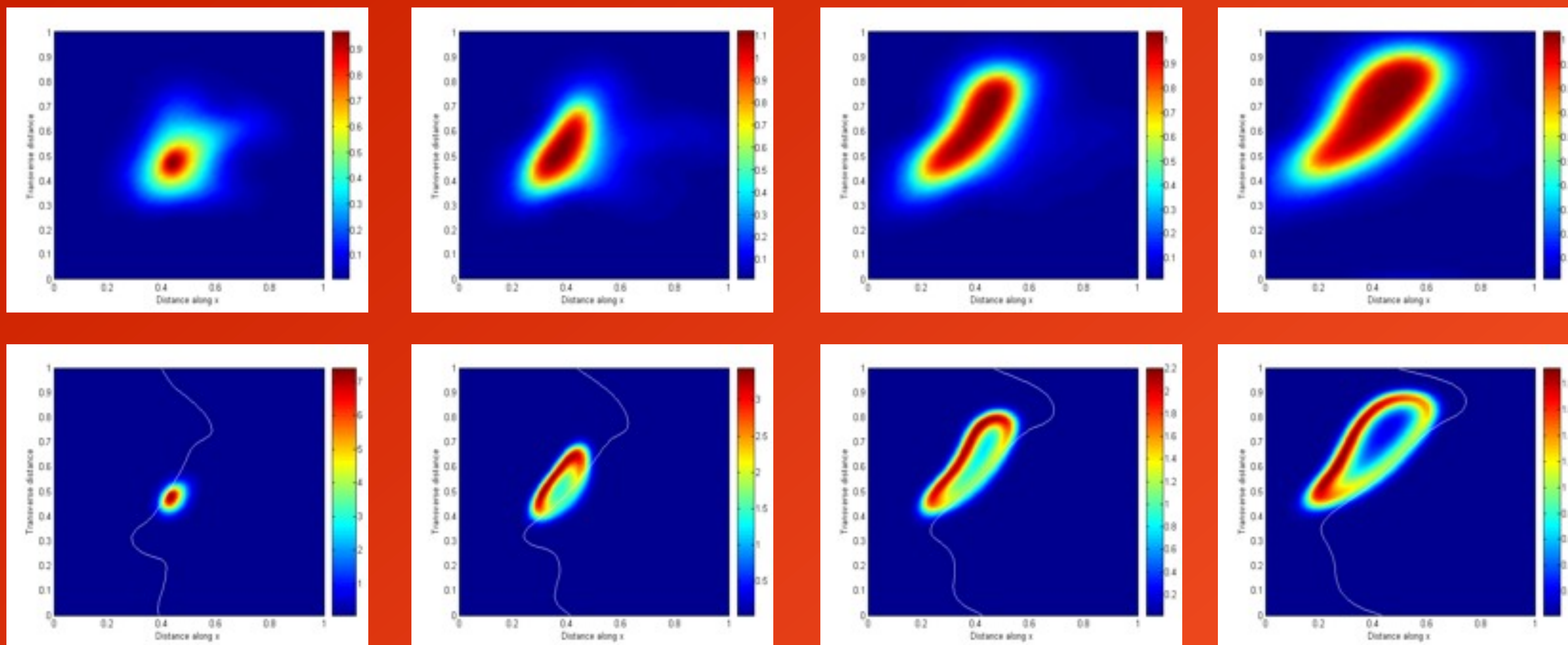
$\dot{W}$

$1.0\ t_{sp}$ $2.0\ t_{sp}$ $3.0\ t_{sp}$ $4.0\ t_{sp}$

$u'/S_L = 4$: Successful ignition, flame spreads

related to Richardson E.S. Chakrabirty N. Mastorakos E. “Analysis of DNS of ignition fronts in turbulent non-premixed flames in the context of ConditionalMomentClosure”31th Intern.Symp. onCombustion 2006

DNS of spark-ignition of non-premixed flames



T

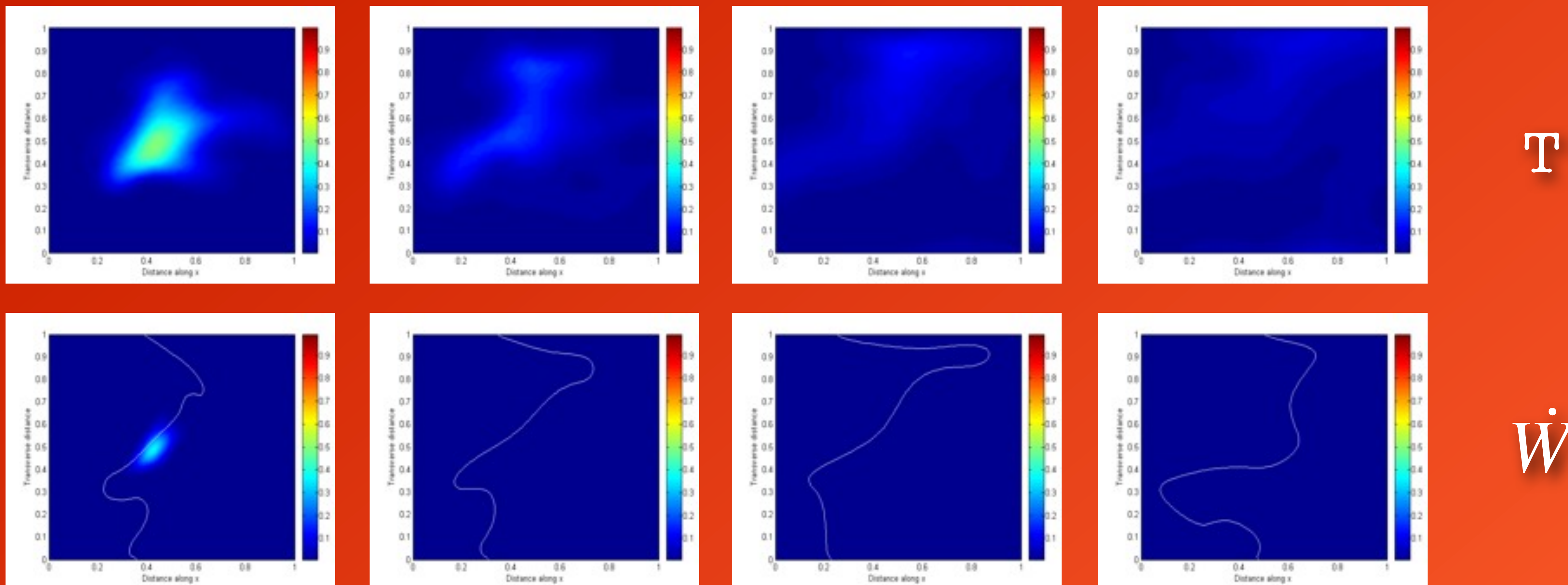
$\dot{W}$

$1.0\ t_{sp}$ $2.0\ t_{sp}$ $3.0\ t_{sp}$ $4.0\ t_{sp}$

$u'/S_L = 8$: Successful ignition, flame spreads but slower than before.

related to Richardson E.S. Chakrabirty N. Mastorakos E. “Analysis of DNS of ignition fronts in turbulent non-premixed flames in the context of ConditionalMomentClosure”31th Intern.Symp. onCombustion 2006

DNS of spark-ignition of non-premixed flames

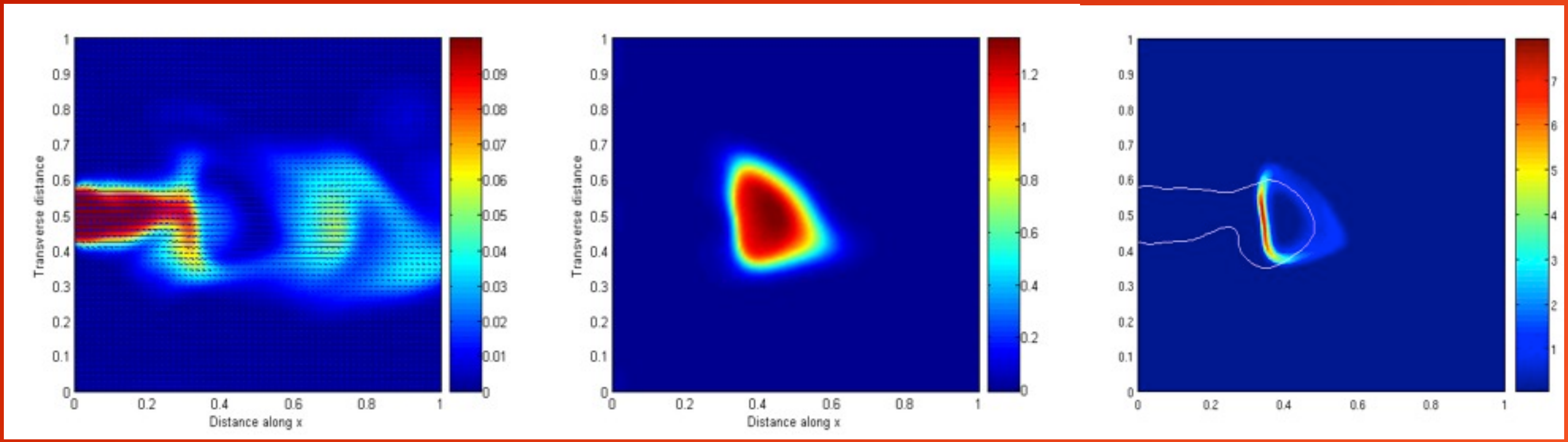


$1.0\ t_{sp}$ $2.0\ t_{sp}$ $3.0\ t_{sp}$ $4.0\ t_{sp}$

$u'/S_L = 12$: Failed ignition, flame does not spread.

related to Richardson E.S. Chakrabirty N. Mastorakos E. "Analysis of DNS of ignition fronts in turbulent non-premixed flames in the context of ConditionalMomentClosure"31th Intern.Symp. onCombustion 2006

DNS of spark-ignition of non-premixed flames: with shear

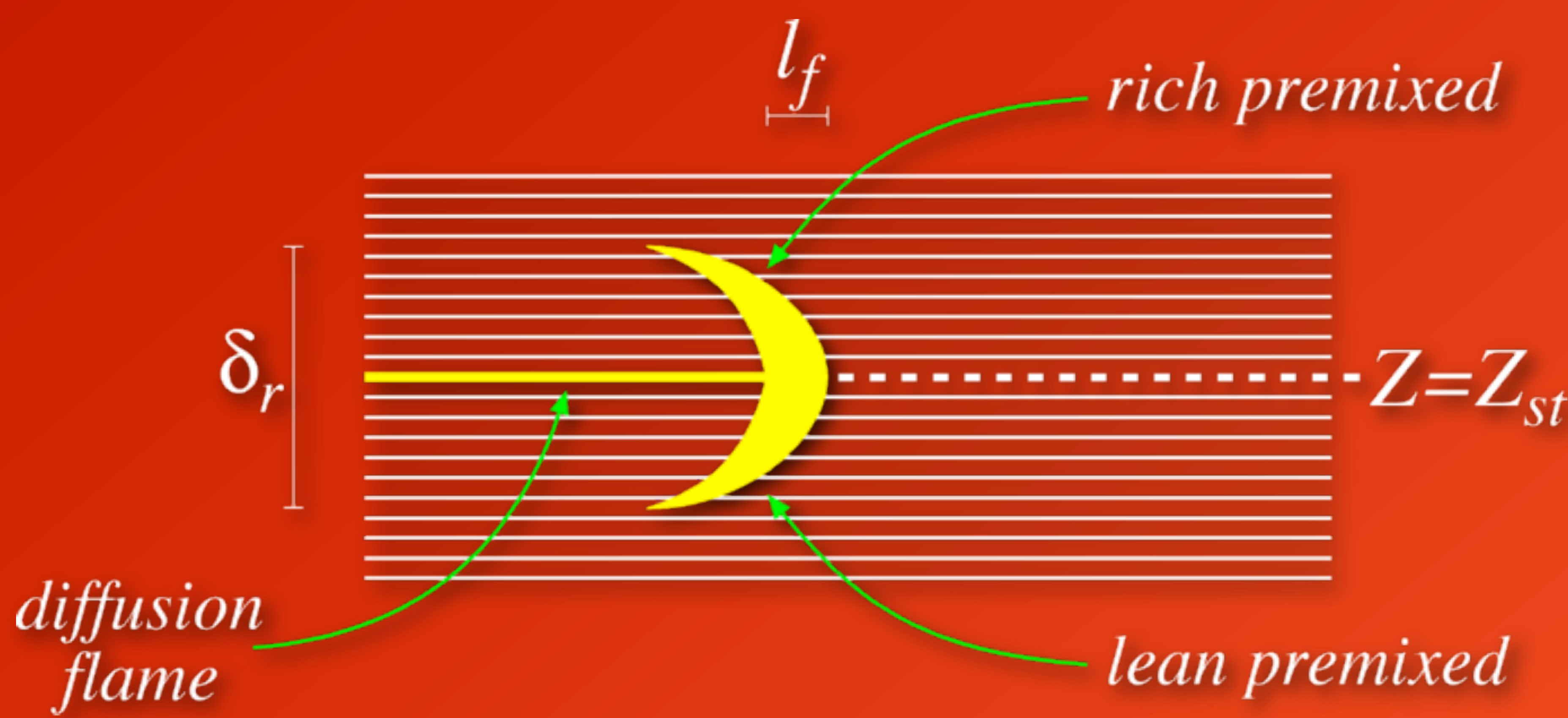


Y_{fu} T $\dot{W}$

u'/ S_L = 8: Successful ignition, flame kernel distorted, flame spreads.

related to Richardson E.S. Chakrabirty N. Mastorakos E. "Analysis of DNS of ignition fronts in turbulent non-premixed flames in the context of ConditionalMomentClosure"31th Intern.Symp. onCombustion 2006

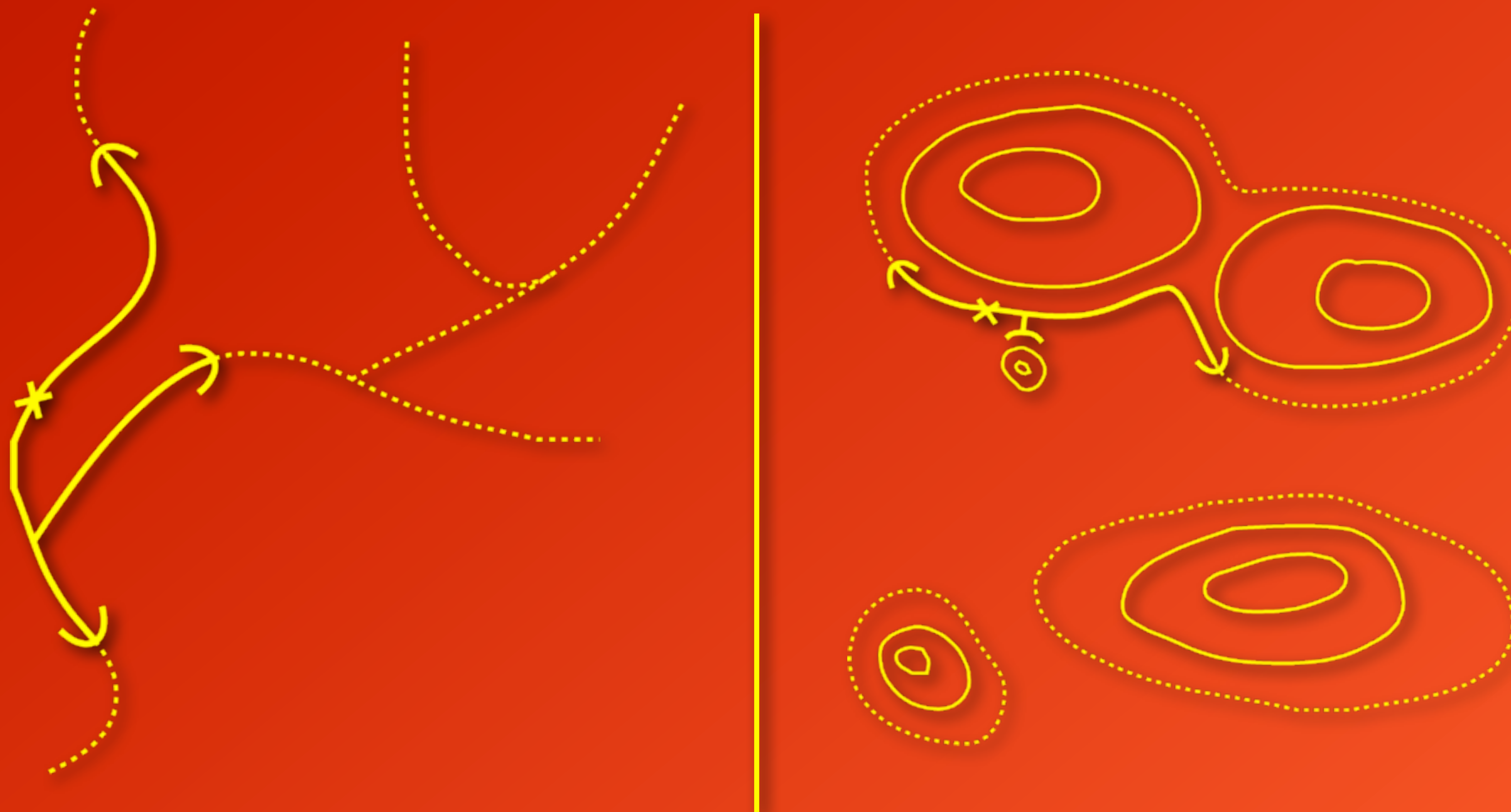
Schematic of triple flames



$$B = \frac{l_f}{\delta_r}$$

$$l_f \propto \frac{\alpha}{v_f}$$

$$\delta_r \propto \delta_m = \gamma \delta_m^{ns}$$

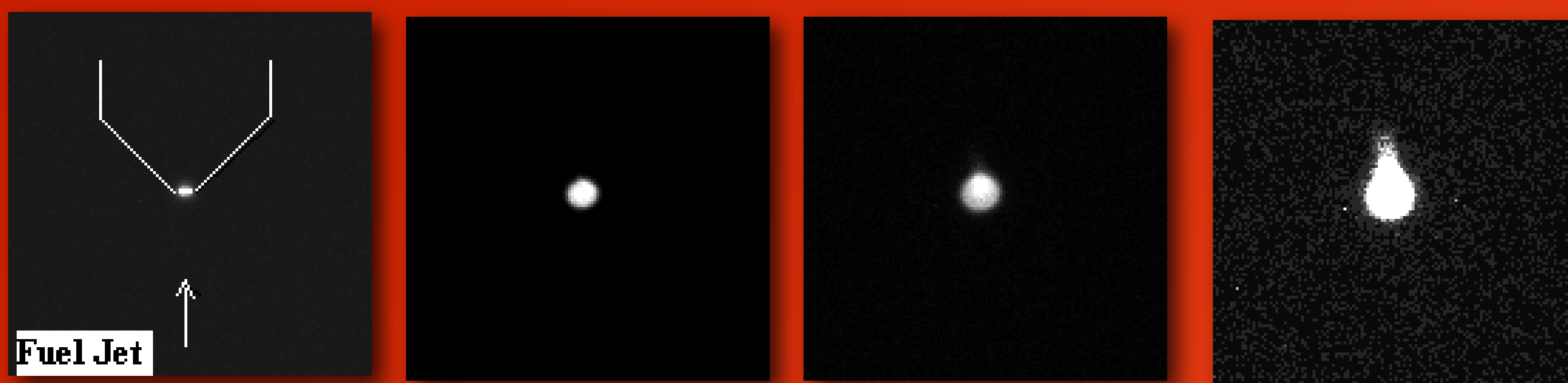


Sketches of non steady triple flame propagation along open and closed isosurfaces.

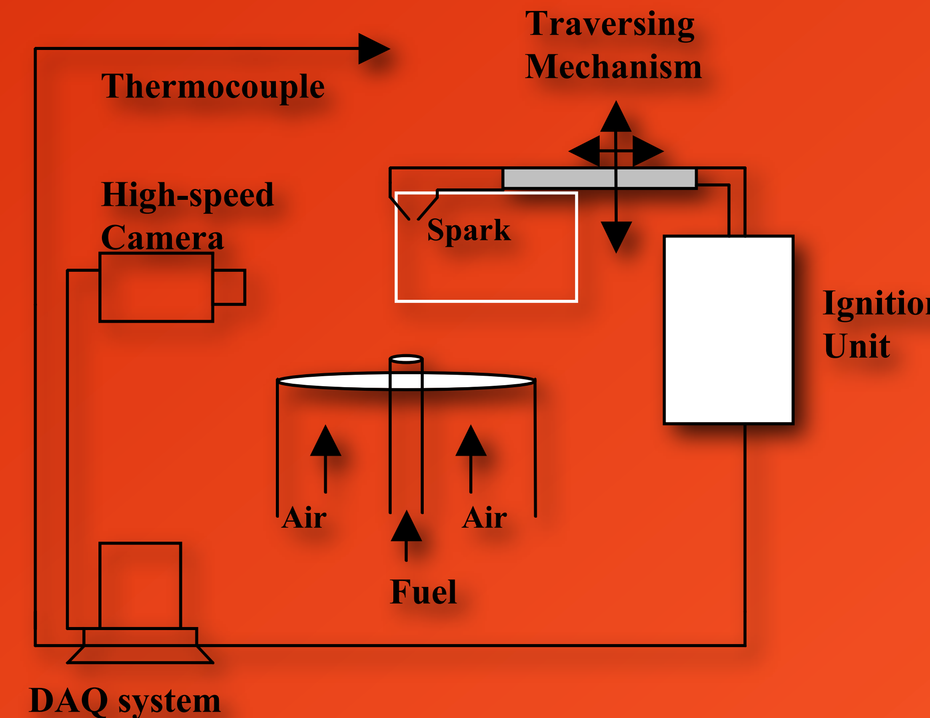
Dotted lines stand for stoichiometric surface. Solid line mark burned regions

Spark-ignition of turbulent jet flames

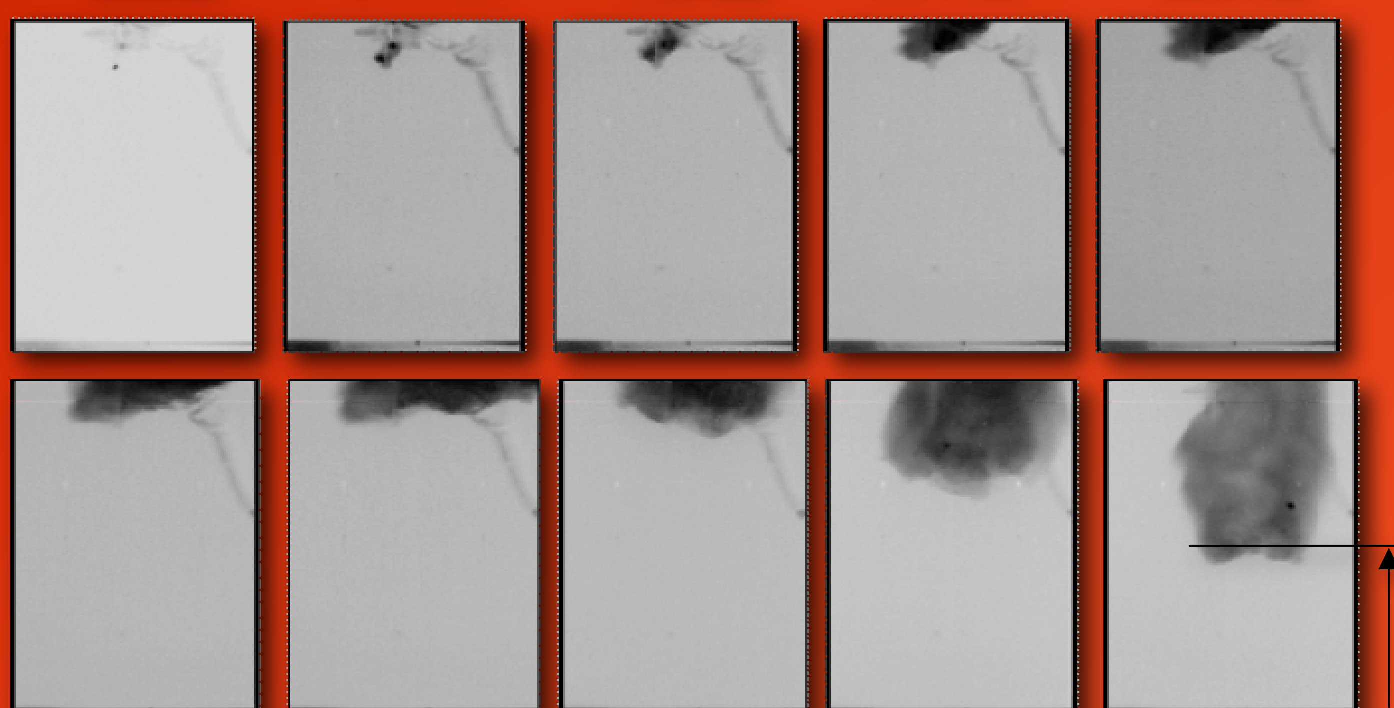
Turbulent jet of fuel/air into air
Sparker unit, fast Intensified CMOS, OH-PLIF



50 µs 350 µs 950 µs 1.45 ms

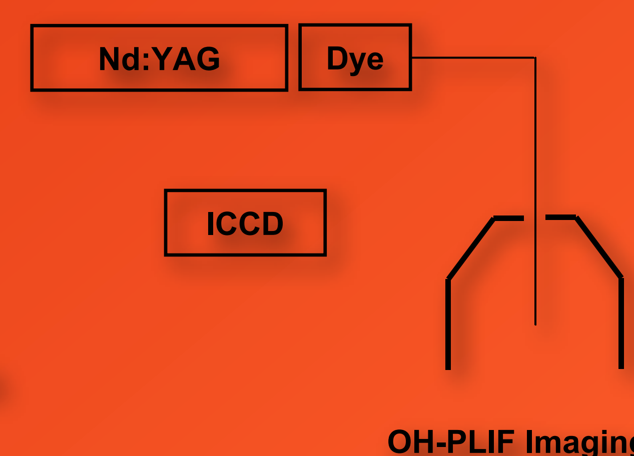


238 µs 4.76 ms 7.14 ms 11.9 ms 14.2 ms



Flame position

95,2 ms 238 ms 310 ms 405 ms 452 ms



by Ahmed S.F. and Mastorakos E: “Spark-ignition of lifted turbulent jet flames”
Combustion and Flame in printing 2006

Ignition at r/D=0, z/D=30//Fuel from below//v(jet)=25.5 m/sec

50 μs 350 μs 950 μs 1.45 ms

Fuel jet

by Ahmed S.F. and Mastorakos E: "Spark-ignition of lifted turbulent jet flames"
Combustion and Flame in printing 2006

Ignition at r/D=0, z/D=30//Fuel from below//v(jet)=25.5 m/sec

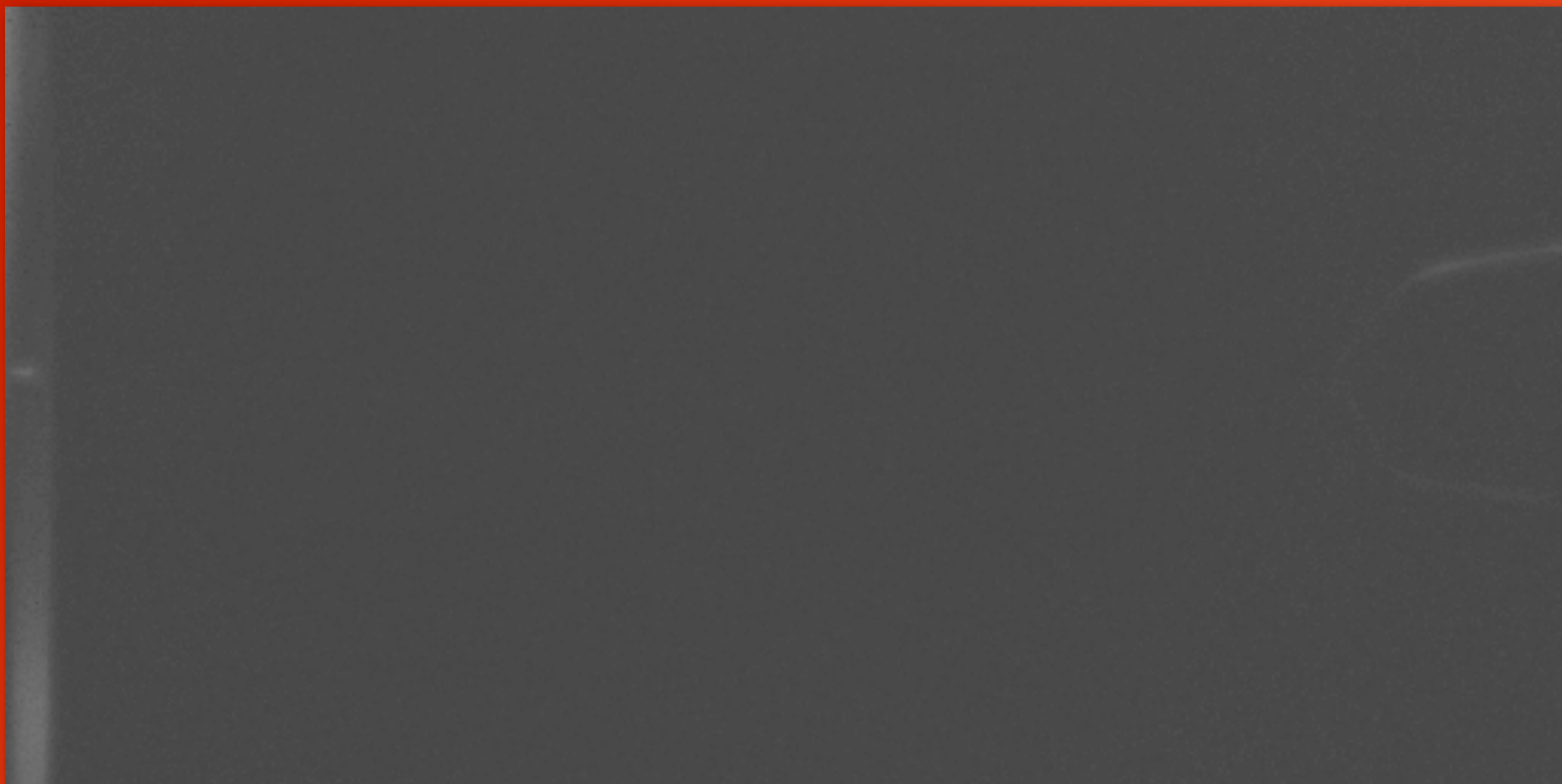
200 μs | 3.2 ms | 6.2 ms | 10.2 ms

Fuel jet

16.6 ms | 20.6 ms | 25.6 ms | 31.7 ms

by Ahmed S.F. and Mastorakos E: “Spark-ignition of lifted turbulent jet flames”
Combustion and Flame in printing 2006

Ignition at r/D=0, z/D=40//Fuel(methane) from left side //v(jet)=12.5 m/sec

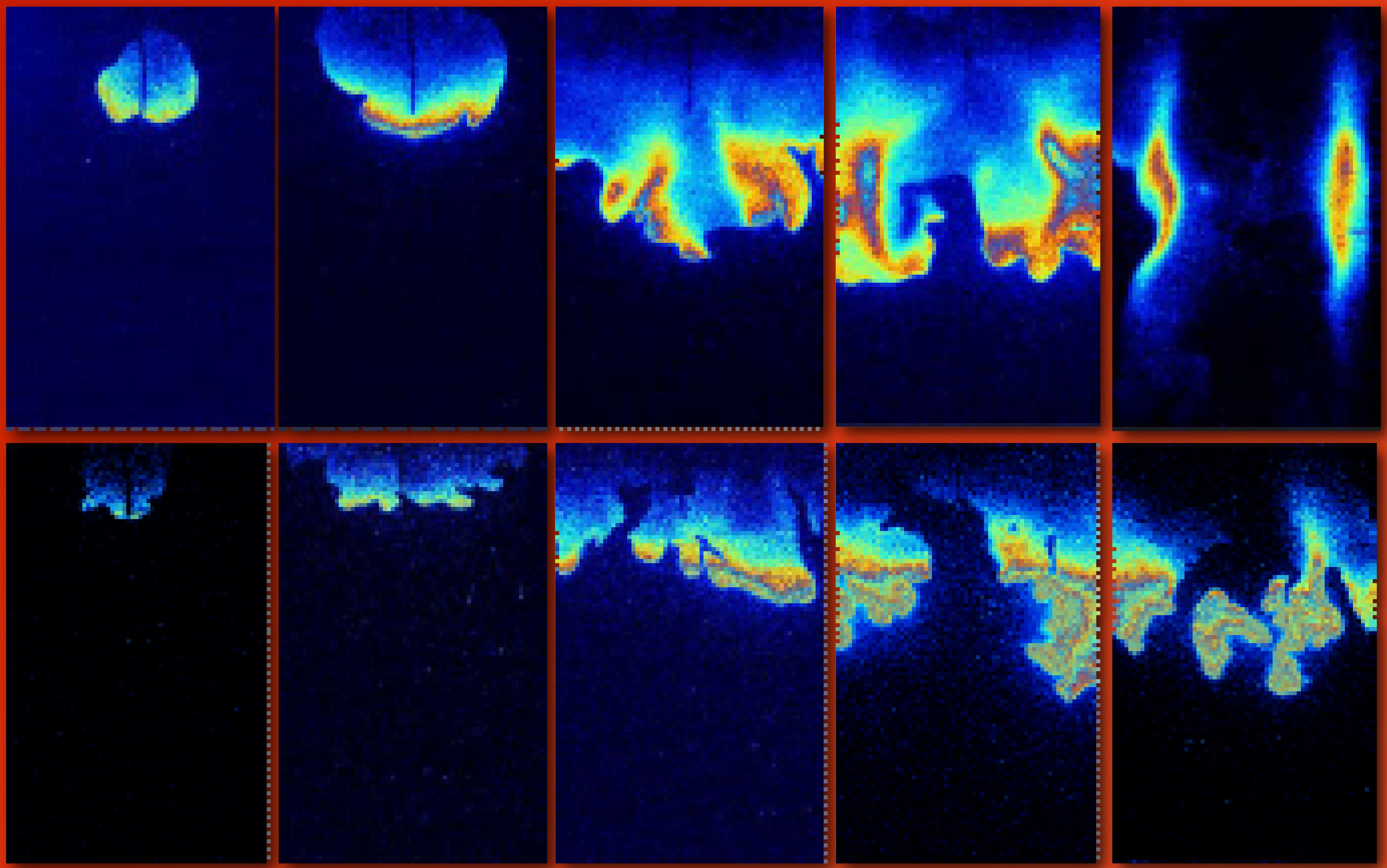


by Ahmed S.F. and Mastorakos E: “Spark-ignition of lifted turbulent jet flames” Combustion and Flame in printing 2006

Ignition at r/D=0, z/D=40//Fuel(methane) from left side //v(jet)=25.5 m/sec

by Ahmed S.F. and Mastorakos E: “Spark-ignition of lifted turbulent jet flames” Combustion and Flame in printing 2006

OH-PLIF images //Ignition at r/D=0, z/D=40//Fuel from below//Image region form z/D =24 to z/D=55

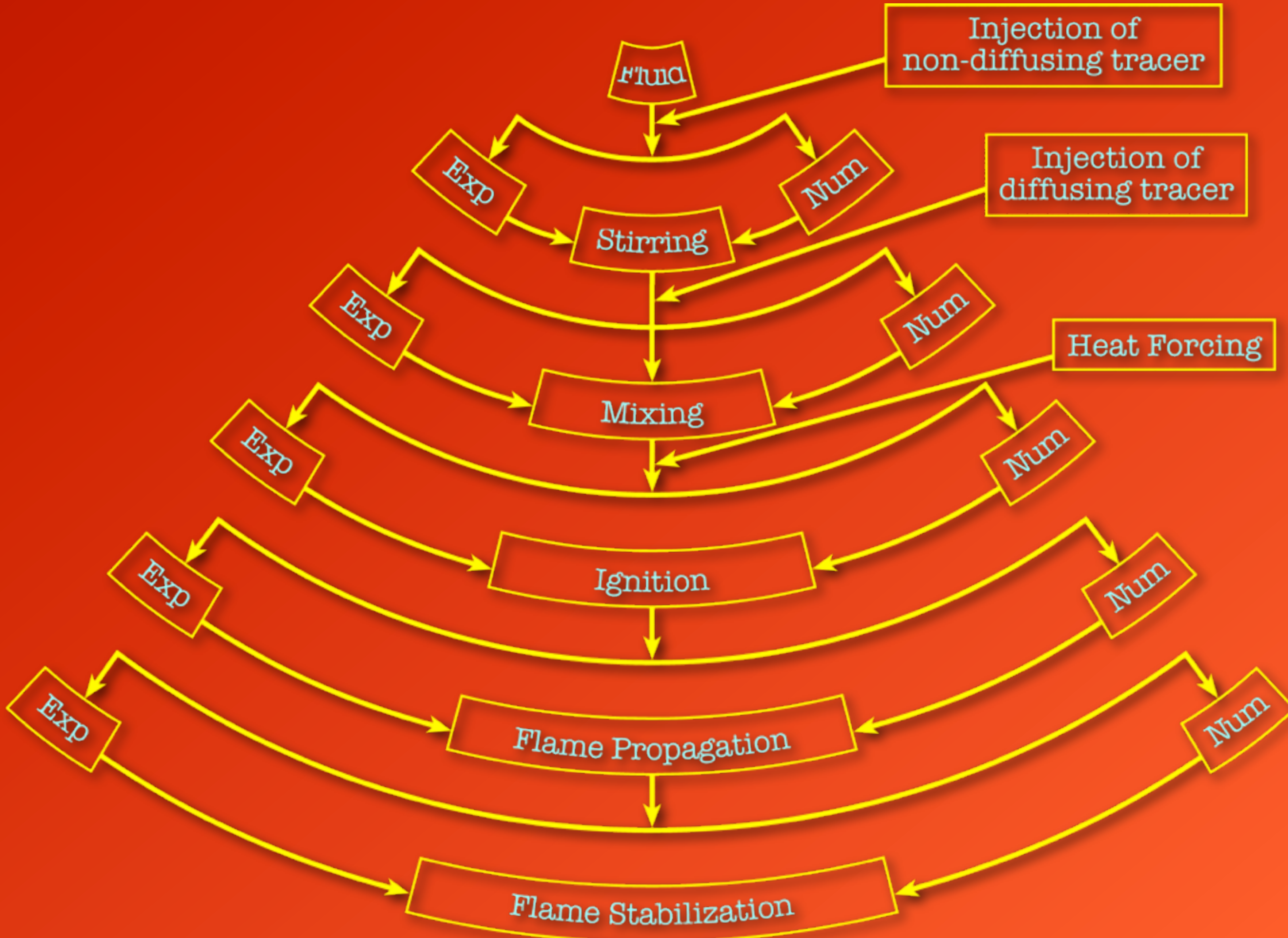


U_j=12.5 m/s

U_j=25.5 m/s

5 ms 10 ms 30 ms 60 ms 100 ms

by Ahmed S.F. and Mastorakos E: “Spark-ignition of lifted turbulent jet flames”
Combustion and Flame in printing 2006


Fluid
Injection of non-diffusing tracer
Exp
Num
Stirring
Injection of diffusing tracer
Exp
Num
Heat Forcing
Mixing
Exp
Num
Ignition
Exp
Num
Flame Propagation
Exp
Num
Flame Stabilization

- **If** there is **not segmentation** of the assessment of the different steps and if there is **not cooperative** generation information from both experimental and numerical side, there is no way to make effective in practice the procedure and the whole 3SEC strategy **looses its usefulness**.

- 3SEC procedures is at moment a **proposal**. It is based on steps, which can only partially be followed along the path way of previous work.
- At the moment it has to be evaluated for its **methodological aspects** rather than for the information on single pieces.
- It is **needed** in any case as a **comprehensive presentation** because it is a challenging enterprise and it can be substantiated during the years only by means of numerous ensemble of works which need in turn a reference framework, like the one presented here.

- **Combustion dynamics** can be the basis for a **3SEC Strategy**. In fact the single effect can be introduced in a process with higher level of complexity by changing boundary and initial conditions. Therefore the **"simpler" process develops along the time toward the more "complex" one**.

Sequential **E**nlargement **C**ombination of
Separated **E**ffects **C**ontributions for
Side-by-side **E**xp/num **C**hecking

Strategy for **E**valuation of **C**ombustion **P**rocesses

Possible acronyms could be:

4SEC Processes or

3SEC Strategy for Evaluation of Combustion Processes.