Karlsruhe Institute of Technology

Transferring Scientific Results into Engineering Correlations

HySafe Research Priorities Workshop

Dr.-Ing. Thomas Jordan | Berlin, 16th of October 2012

Motivation or the Gap(?)

"Hierarchy" of Tools for Hydrogen Risk Assessment

Experiments
Δt, €, $

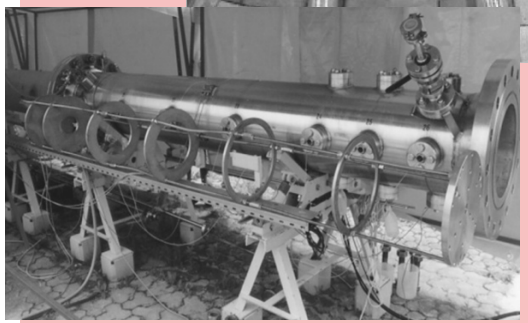
⇨

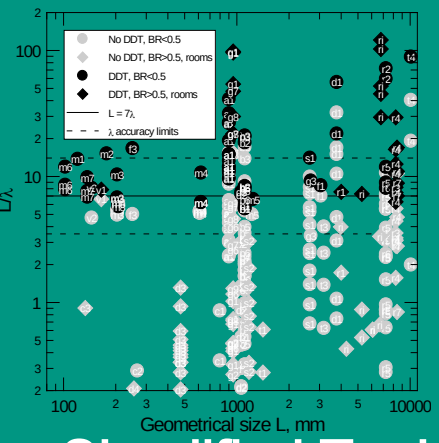
Engineering Correlations

⇦

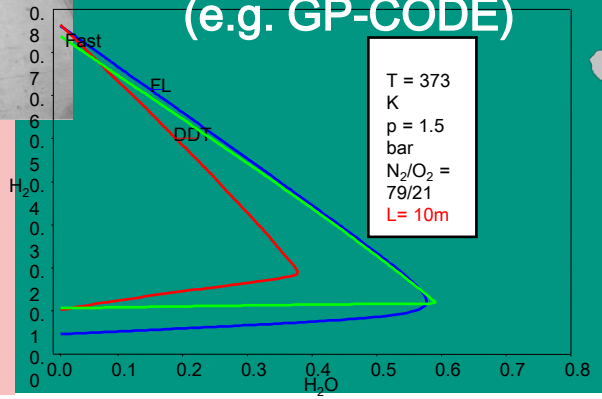
Theory and Software
Δt, €, $

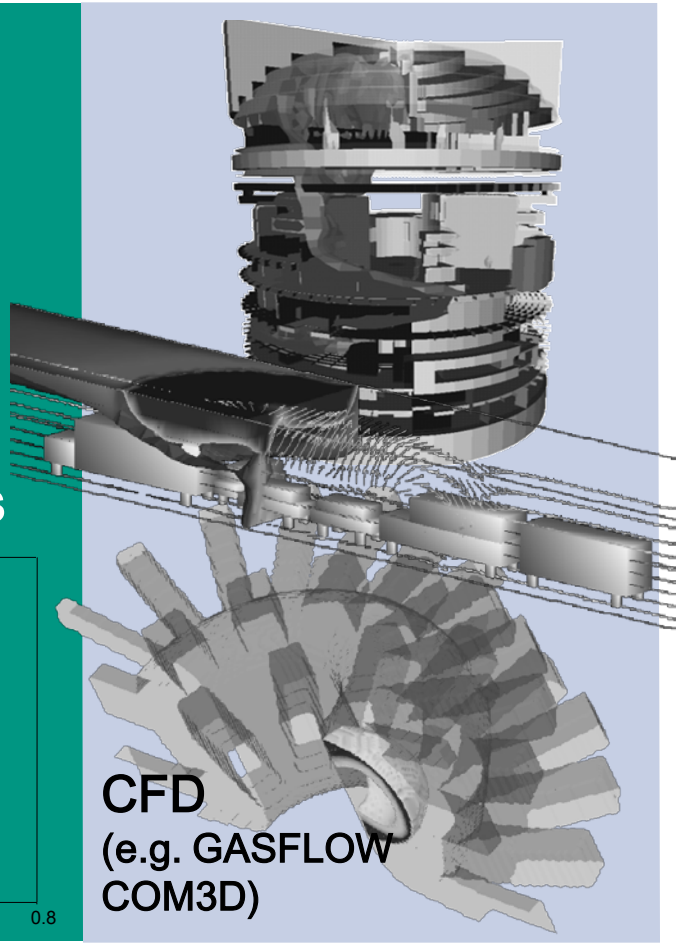
e.g.
HyKa





Simplified Tools
(e.g. GP-CODE)





CFD
(e.g. GASFLOW COM3D)

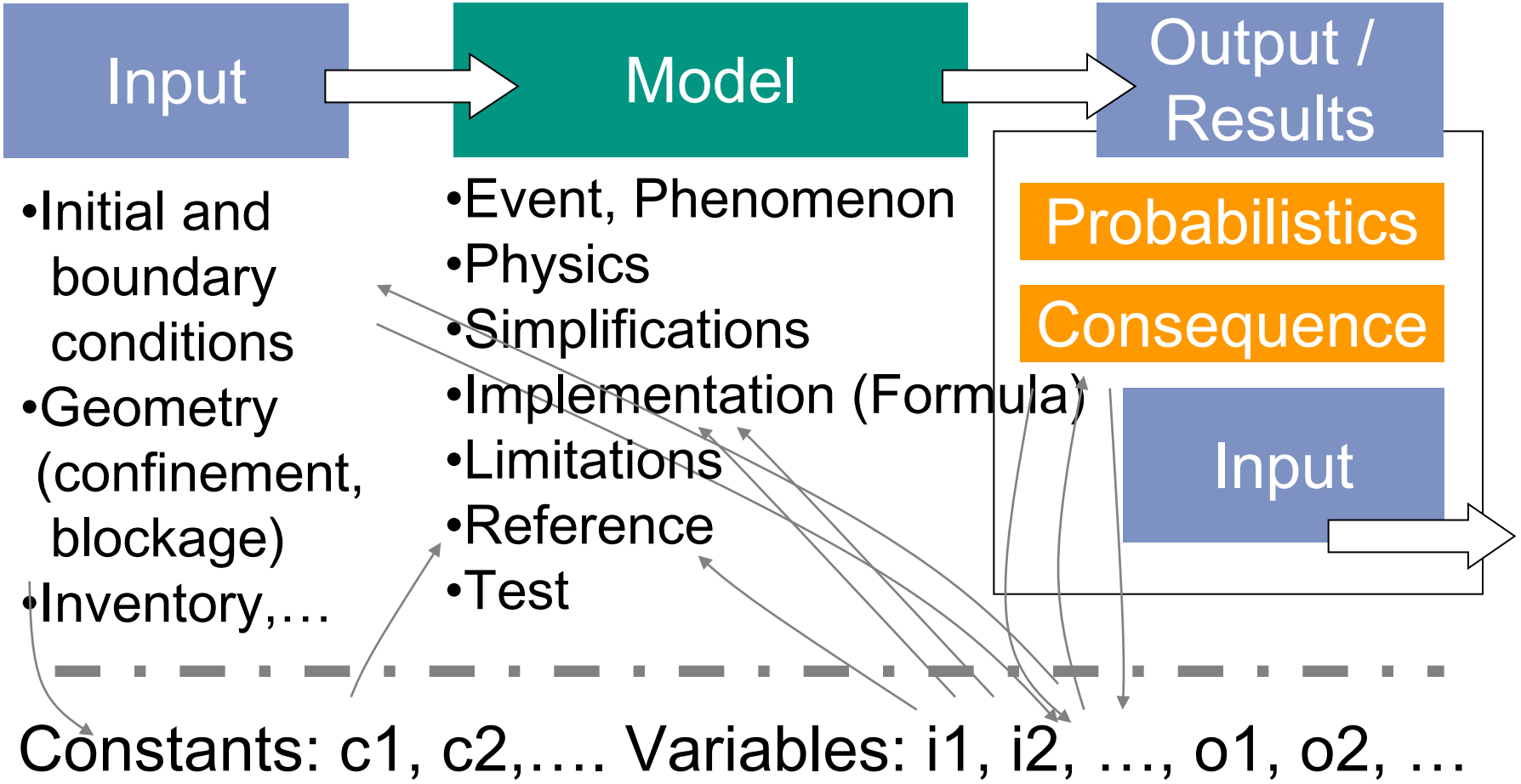
Basic Concept of the Toolbox

- Free and open set/collection of tools for risk assessment
- Based on robust, published state-of-the-art engineering correlations, statistics, criteria
- Highly modular „dispatched“ design
- Fast response times
- Easy to use, via command line or GUI, on- and offline
- Well documented, quality assured

- Commonly defined and developed

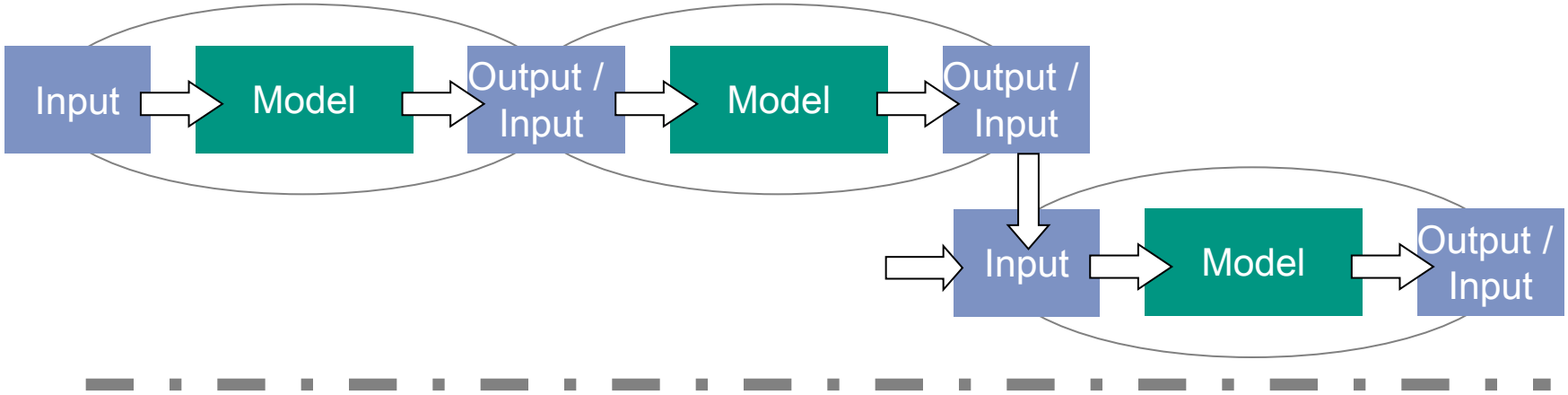
⇨ **HySafe + IEA HIA Task 31**
= perfect platforms

Basic Concept: Model



Basic Concept: Super-Model

- Every model provides a function:
  Output = Model(Input) where
  with „Output“ and „Input“ are sets of variables
- „Super-Models“ are composed of several models →
- Recursion



Constants: c1, c2,…. Variables: i1, i2, …, o1, o2, …

Phenomena Addressed 1/2

Major Phenomena	*Phenomena*	*Sub-Phenomena*	*Further Simplifications*
Thermodynamics / State			
	Equilibrium of State		ideal gas simplifications
	Equilibrium of State		ideal gas simplifications
	Equilibrium of State		ideal gas simplifications
	Equilibrium of State		real gas model
	Equilibrium of State		real gas model
	Equilibrium of State		real gas model
Release / Mixing			
	Permeation		
	Diffusion		
	Loss of Containment		
	Loss of Containment	Pipe failure	
	Loss of Containment	Failure of sealing	
	Inventory	Premixed Gas Cloud	
	Inventory	Liquid Pool Size	
	LH2 Pool Evaporation		
	Release into Secondary Vessel (Refuelling)		
	Release into Free Environment		
	Jet Release		
	Jet Release	Free Jet	
	Jet Release	Buoyant Jet	
	Jet Release	Wall Attached Jet	
	Jet Release	Impinging Jet	
	Release into Unventilated Box	Natural Ventilation	
	Release into Unventilated Box	Forced Ventilation	
Ignition /			

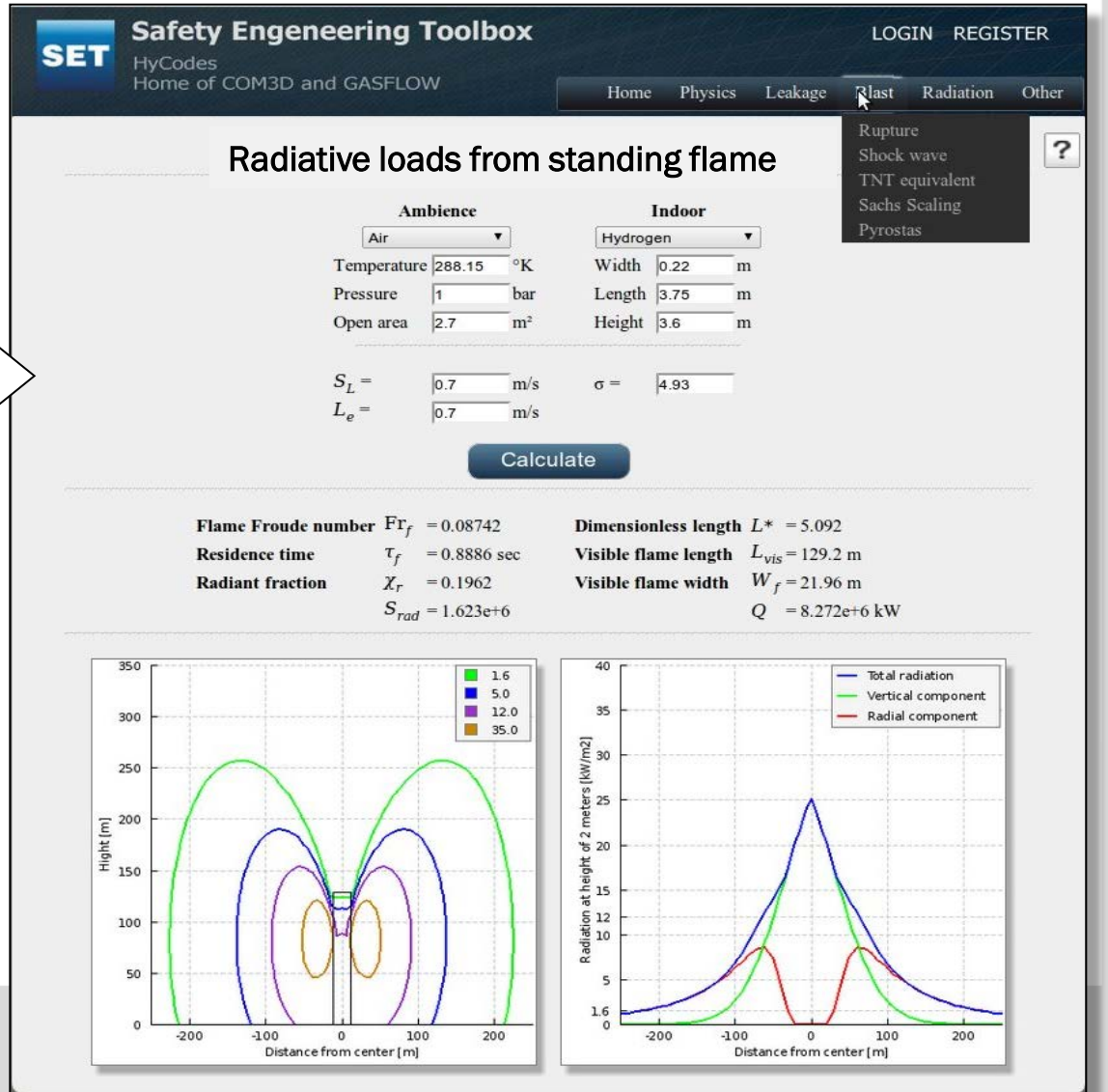
Phenomena Addressed 2/2

Ignition / Combustion		
	Ignition	Minimum Ignition Energy
	Ignition	Ignition Location
	Ignition	Ignition Time
	Ignition	Ignition Probability
	Flammability Limits	
	Flammability Limits	
	Laminar Flame Speed	
	Diffusion/Jet Flame	
	Diffusion/Jet Flame	
	Diffusion/Jet Flame	
	Diffusion/Jet Flame	
	Diffusion/Jet Flame	
	Pool Fire	
	Flash Fire	
	Fire Ball	
	Flame Acceleration	
	Flame Acceleration	
	Flame Acceleration	
	Flame Acceleration	
	DDT	
	DDT	Detonation Cell Size
Structural Response / Damage		
	Thermal Loads	Human Limits
	Thermal Loads	Structural Limits
	Pressure Loads	Human Limits
	Pressure Loads	Structural Limits

FIRST IMPLEMENTATION OF THIS WEB-BASED TOOLBOX

Example: Flame Radiation (Houf, Hankinson,…)

Ignition / Combustion	
	Ignition
	Ignition
	Ignition
	Ignition
	Flammability Limits
	Flammability Limits
	Laminar Flame Speed
	Diffusion/Jet Flame
	Diffusion/Jet Flame
	Diffusion/Jet Flame
	Diffusion/Jet Flame
	Flame Acceleration
	Flame Acceleration
	Flame Acceleration
	Flame Acceleration
	DDT
	DDT
Structural Response / Damage	
	Thermal Loads
	Thermal Loads
	Pressure Loads
	Pressure Loads



FIRST IMPLEMENTATION OF THIS WEB-BASED TOOLBOX

Flame Radiation as a Super-Model

```
#
# STEP 1: CALCULATE DENSITY OF AIR AND FLAME FROUDE NUMBER
#

  Fr_f = (u_j * fs**1.5) / (rho_j / rho)**0.25 / ((Tmax/T - 1.0) * g * d_j)**0.5

#
# STEP 2: DETERMINE DIMENSIONLESS (SCALED) VISISBLE LENGTH  L_star/1
#
  if ( Fr_f < 5 ) L_star = 13.5 * Fr_f**0.4 / ( 1.0 + 0.07 * Fr_f**2)**0.2; else L_star = 23

#
# STEP 3: DETERMINE VISIBLE FLAME LENGTH  L_vis/m
#
  L_vis_H2 = L_star * d_j * sqrt(rho_j / rho) / fs

#
# STEP 4: DETERMINE VISIBLE FLAME WIDTH  W_f/m
#
  W_f_H2 = 0.17 * L_vis_H2

#
# STEP 5: DETERMINE RESIDENCE TIME t_f/s
#
  rho_f = Rho(p, Mpro, Tmax)
  t_f = rho_f * W_f_H2**2 * L_vis_H2 * fs / ( 3.0 * rho_j * d_j**2 * u_j )

#
# STEP 6: DETERMINE RADIANT FRACTION (ESCAPING THE FLAME)
#
  X_r_H2 = X_r(t_f, alfa_H2, Tmax_H2)
  S_rad_H2 = X_r_H2 * mfuel * Hu
```

Froude

L*

L_vis

W_f

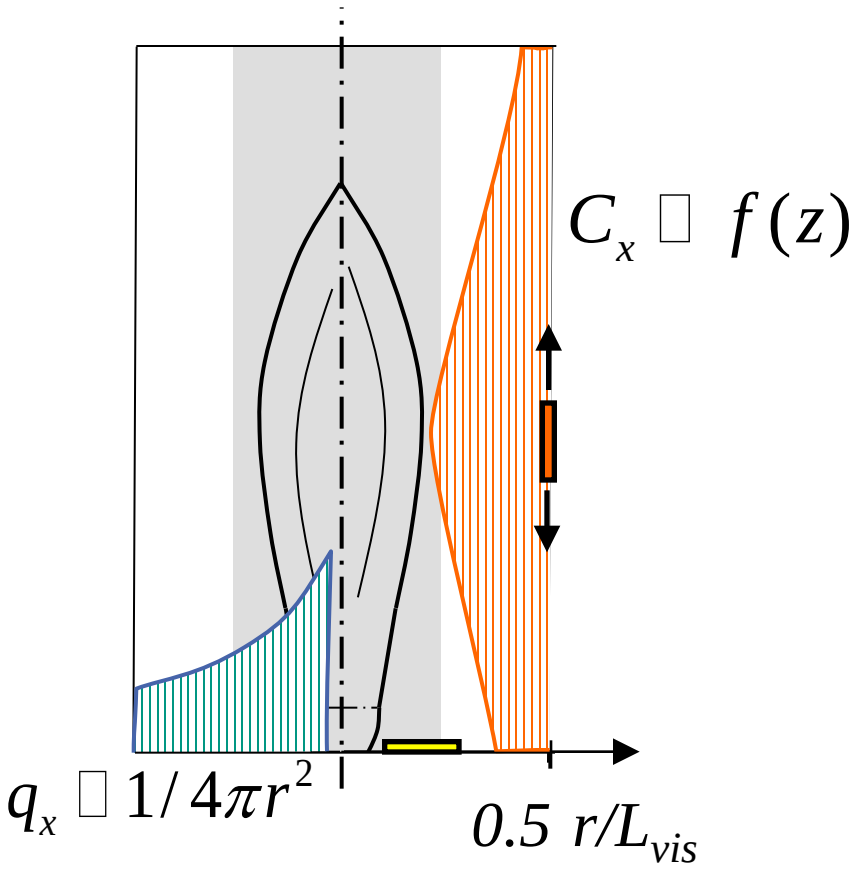
Rho_f

S_rad

IMPLEMENTED: HYDROGEN FLAME RADIATION (Houf, Molina, SNL)

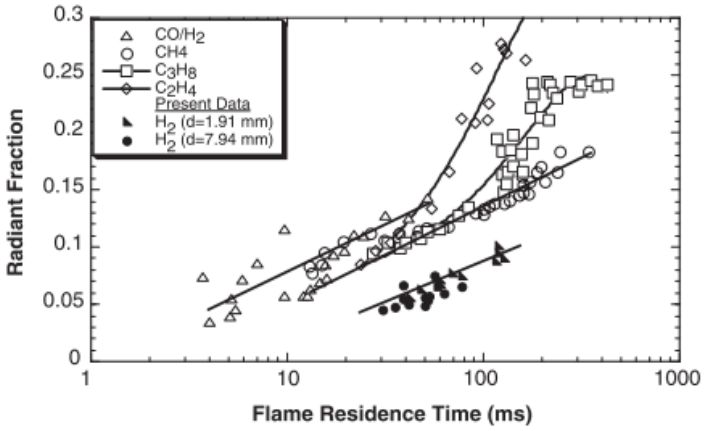
„Super-Model“ composed of a flame length model, etc.

- Referring to experimental data measuring radiation at radial distance of 0.5 of flame length
- Receiver parallel to flame axis
- Simplified approach for the component aligned to the axis
- Form functions for radial and axial variations
- Superpositioning for total radiation power
- Accounts for optical properties
- Limitation: near field



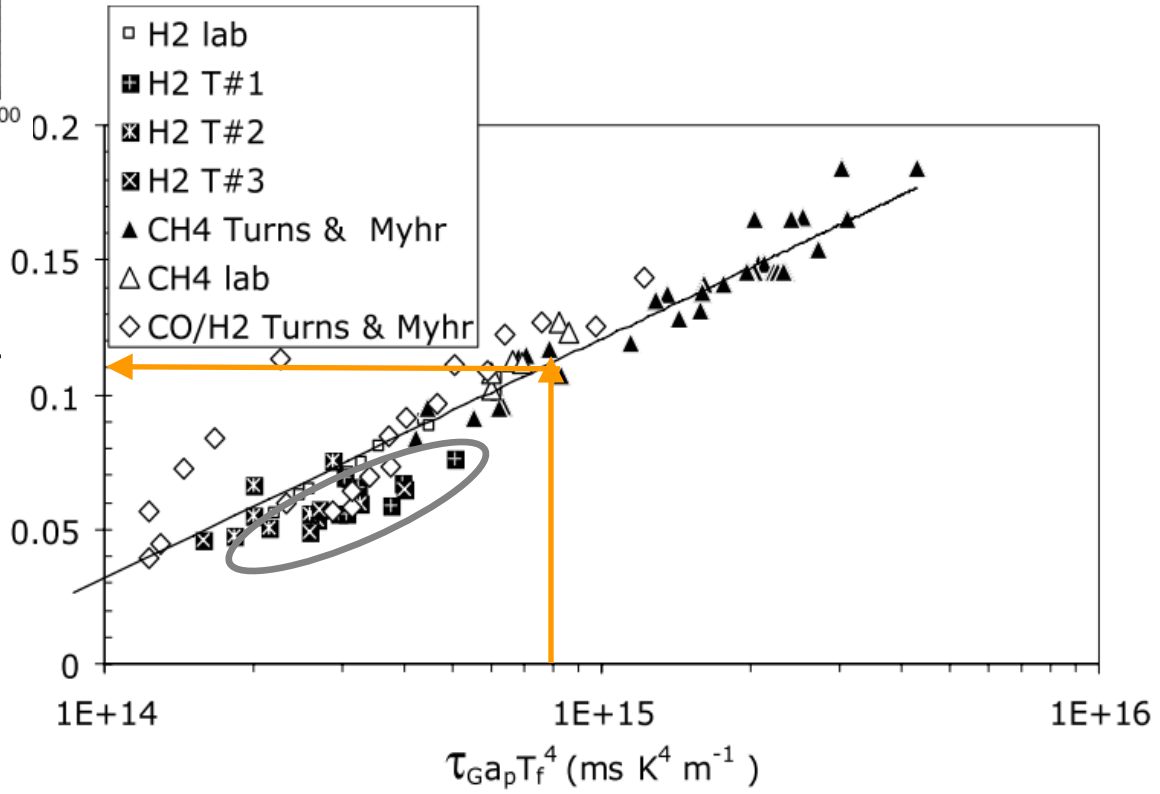
$$\Rightarrow q_x(r,z) \approx S_{rad} C_x(z) / 4\pi r^2$$

State-of-the-Art Empirical Approach

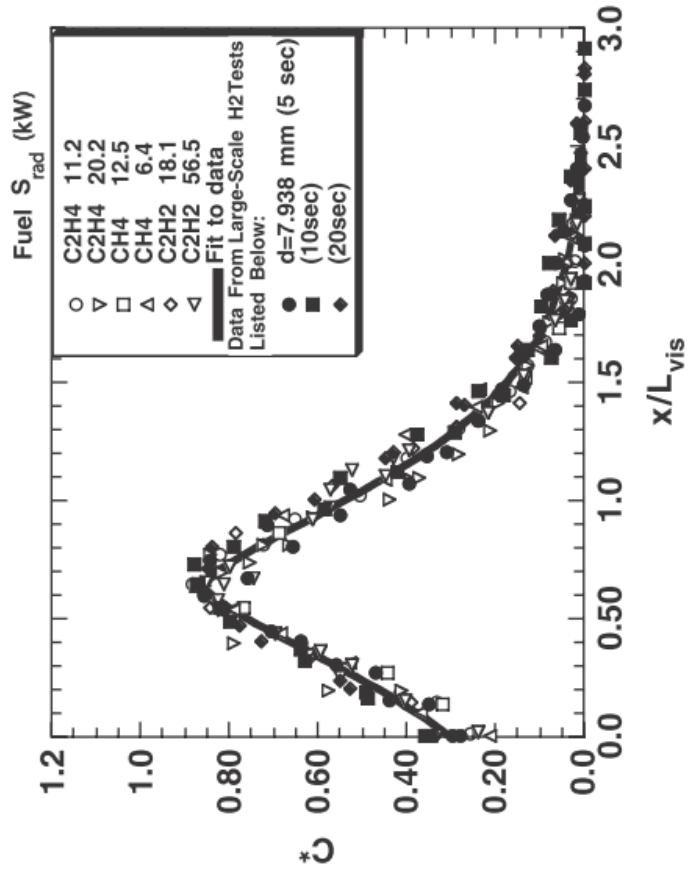


←
Radiation Fraction correlated with residance time (Schefer 2006)

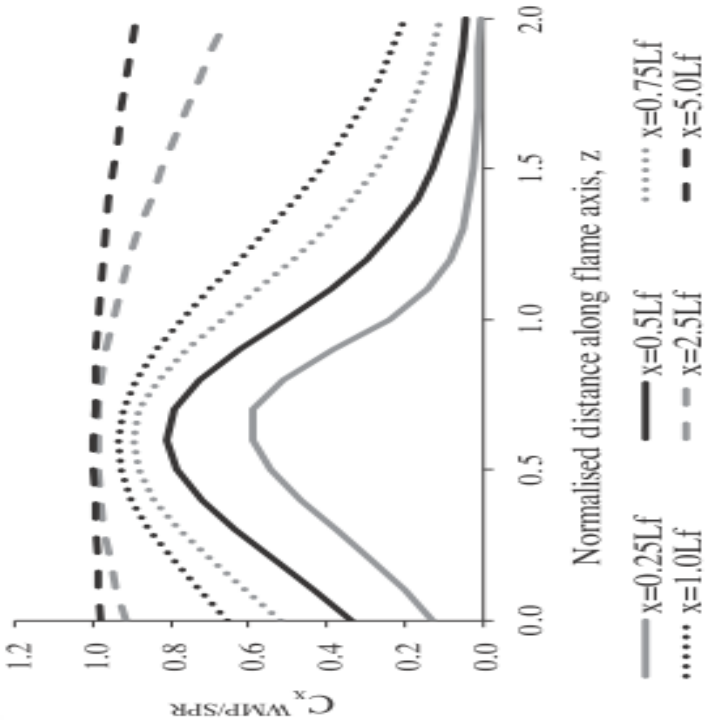
→
Unified correlation additionally accounting for T_f and optics; conservative for large flames
(Molina 2007)



Form Functions

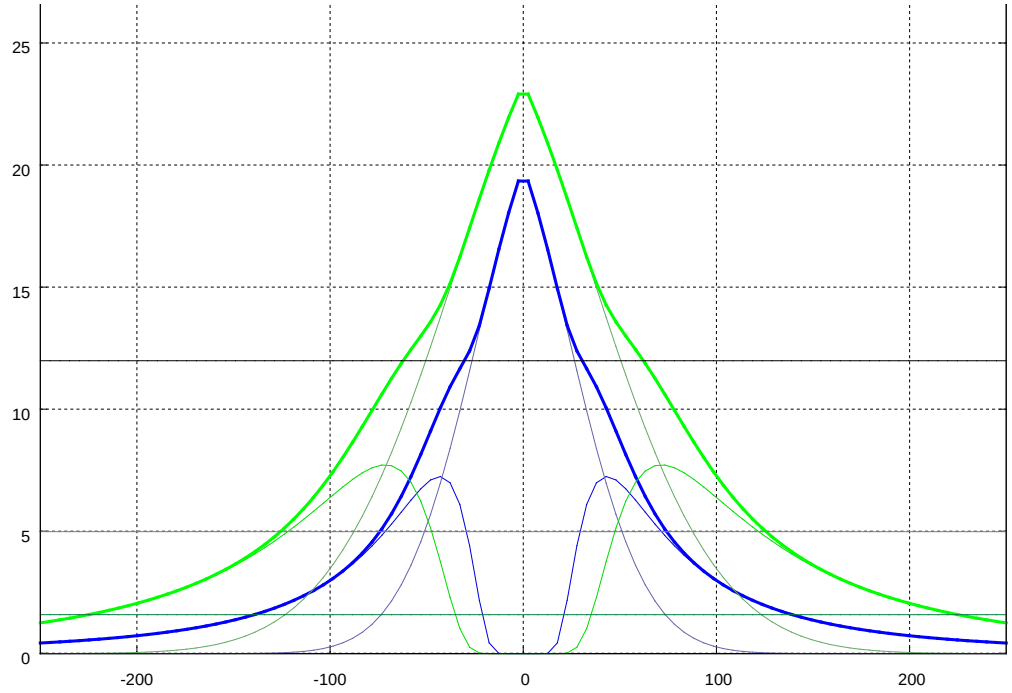


Based on measurements of radial component at $r=0.5L_{vis}$ (Houf und Schefer 2008)



Modifications for different r (Hankinson 2011)

Result at t=1d



Radiation load
/ kW/m2
at 2m height

H2
NG

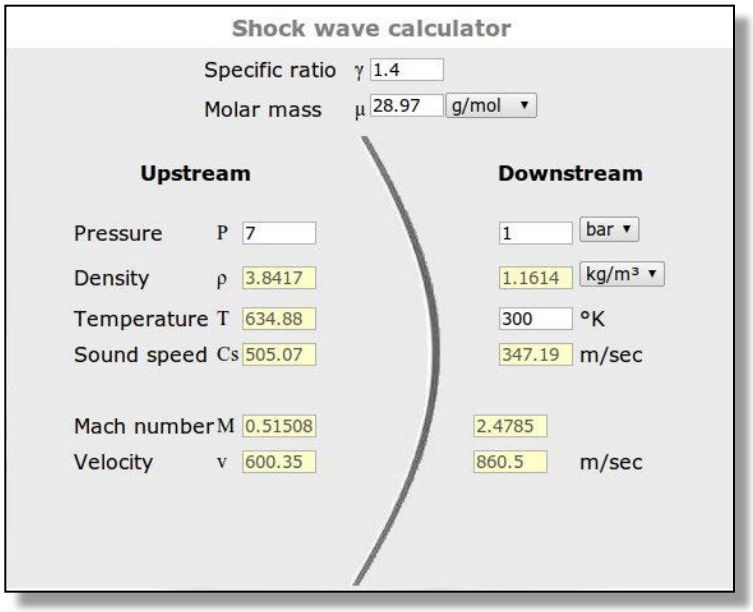
- General smaller load (no CO2) and
- Factor 3 faster decay (sound speed) with H2 in comparison to NG

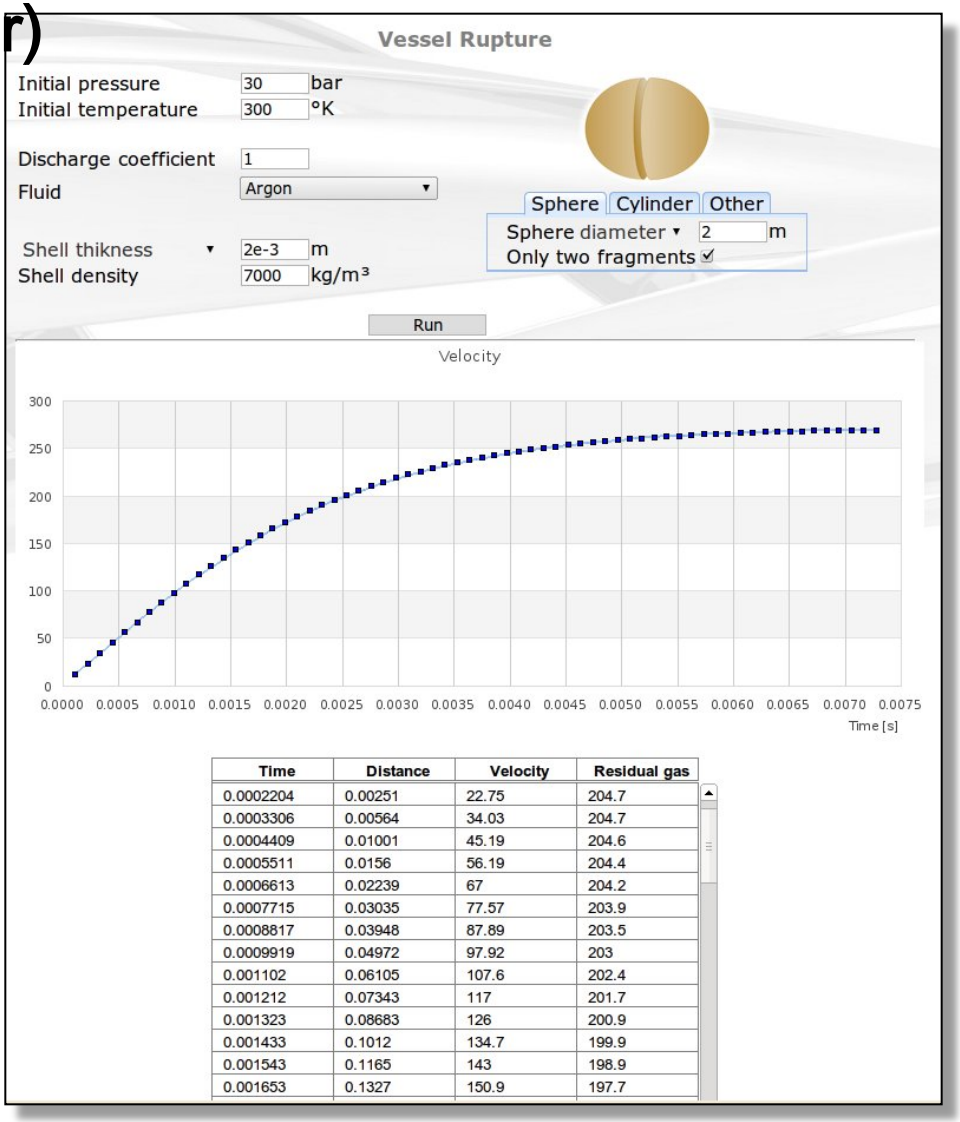
Open Points:
- Validation at large scale
- Axial component
- Late ignition scenario

FURTHER IMPLEMENTED EXAMPLES

Vessel fragmentation (Baker)

- Theory of the phenomena
- Description of the approach
- Instructions for the use
- Limitations of the model
- References
- Test



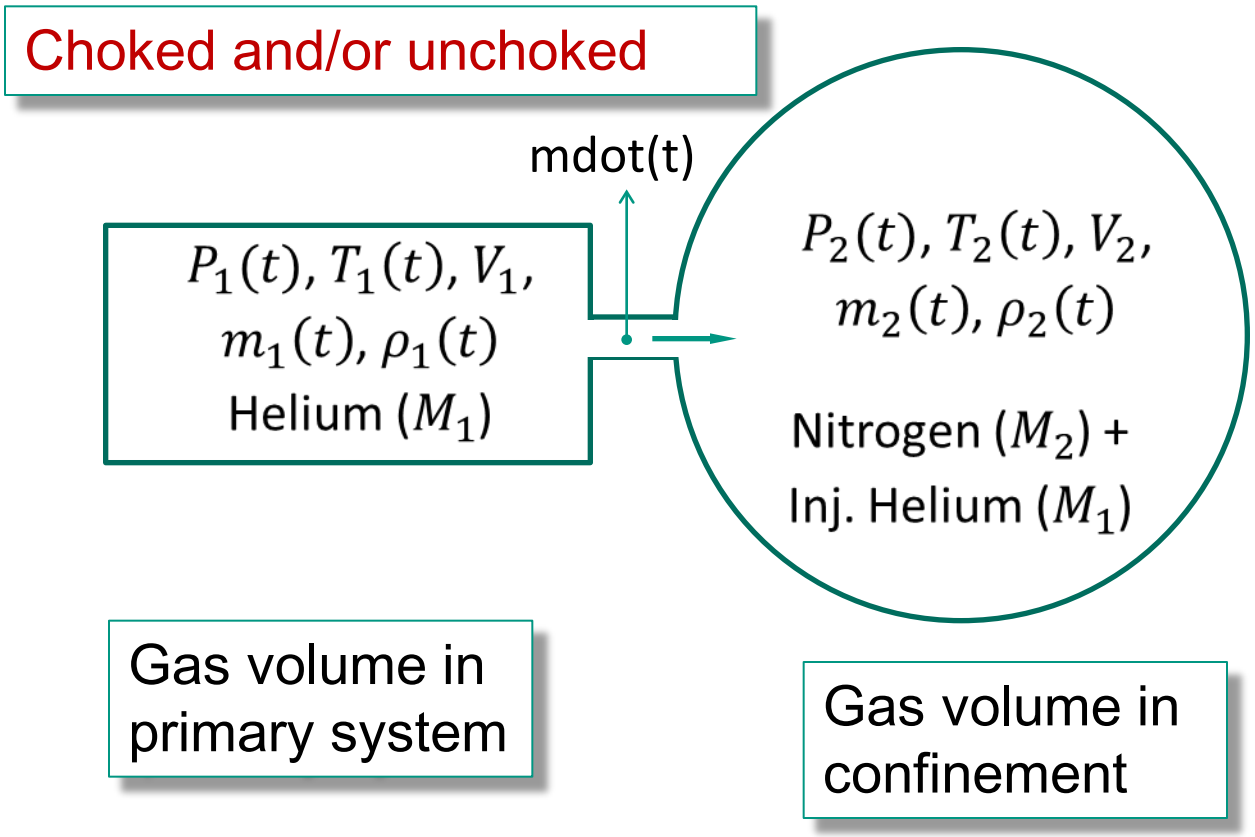


Time	Distance	Velocity	Residual gas
0.0002204	0.00251	22.75	204.7
0.0003306	0.00564	34.03	204.7
0.0004409	0.01001	45.19	204.6
0.0005511	0.0156	56.19	204.4
0.0006613	0.02239	67	204.2
0.0007715	0.03035	77.57	203.9
0.0008817	0.03948	87.89	203.5
0.0009919	0.04972	97.92	203
0.001102	0.06105	107.6	202.4
0.001212	0.07343	117	201.7
0.001323	0.08683	126	200.9
0.001433	0.1012	134.7	199.9
0.001543	0.1165	143	198.9
0.001653	0.1327	150.9	197.7

EXAMPLE PLANNED FOR RELEASE

KIT Tool: Release into Secondary Vessel „Injection Source“ (XU, KIT)

Theoretical solution on the injection source term from the primary loop into the confinement



INJECTION SOURCE: KEY EQUATIONS

– Choked phase

$$mdot(t)=A\left[\alpha\gamma P_1(t)\rho_1(t)\right]^{0.5}$$

$$P_1(t) = P_{10}{\rho_{10}}^{-\gamma}\left({\rho_{10}}^{\frac{1-\gamma}{2}} + \frac{\gamma-1}{2}kt\right)^{\frac{2\gamma}{1-\gamma}}$$

$$T_1(t) = \frac{M_1}{R}P_{10}{\rho_{10}}^{-\gamma}\left({\rho_{10}}^{\frac{1-\gamma}{2}} + \frac{\gamma-1}{2}kt\right)^{-2}$$

$$T_2(t) = \frac{\beta m_{20}T_{20} + m(t)T_1(t)}{\beta m_{20} + m(t)}$$ (Based on energy balance)

$$P_2(t) = \frac{RT_2(t)}{V_2}\left(\frac{m(t)}{M_1} + \frac{m_{20}}{M_2}\right)$$ (Based on EOS of ideal gas)

INJECTION SOURCE: KEY EQUATIONS

$$mdot(t)=A\left\{2P_1(t)\rho_1(t)\frac{\gamma}{\gamma-1}\left[\left(\frac{P_2(t)}{P_1(t)}\right)^{\frac{2}{\gamma}}-\left(\frac{P_2(t)}{P_1(t)}\right)^{\frac{\gamma+1}{\gamma}}\right]\right\}^{0.5}$$

$$\left[m_{21c}+\beta m_{22}+m(t)\right]T_2(t)=\left(m_{21c}+\beta m_{22}\right)T_{2c}+m(t)T_1(t)$$

(Energy balance)

$$T_1(t)=\frac{M_1V_1}{R[m_{1c}-m(t)]}P_1(t)$$

(EOS on volume V_1)

$$T_2(t)=\frac{V_2}{R\left[\frac{m_{21c}+m(t)}{M_1}+\frac{m_{22}}{M_2}\right]}P_2(t)$$

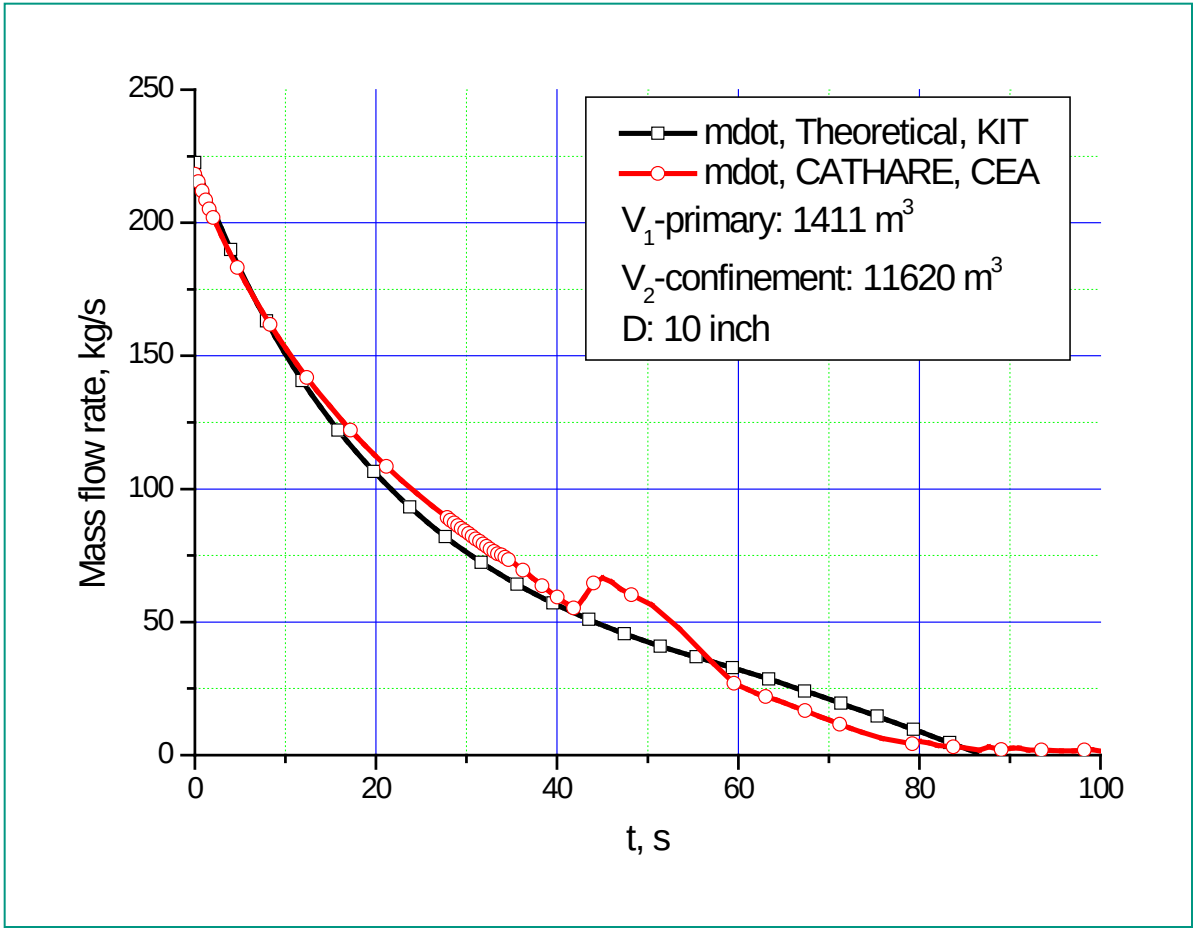
(EOS on volume V_2)

$$P_1(t)^{1-\gamma}T_1(t)^{\gamma}=P_{1c}{}^{1-\gamma}T_{1c}{}^{\gamma}$$

(Adiabatic condition)

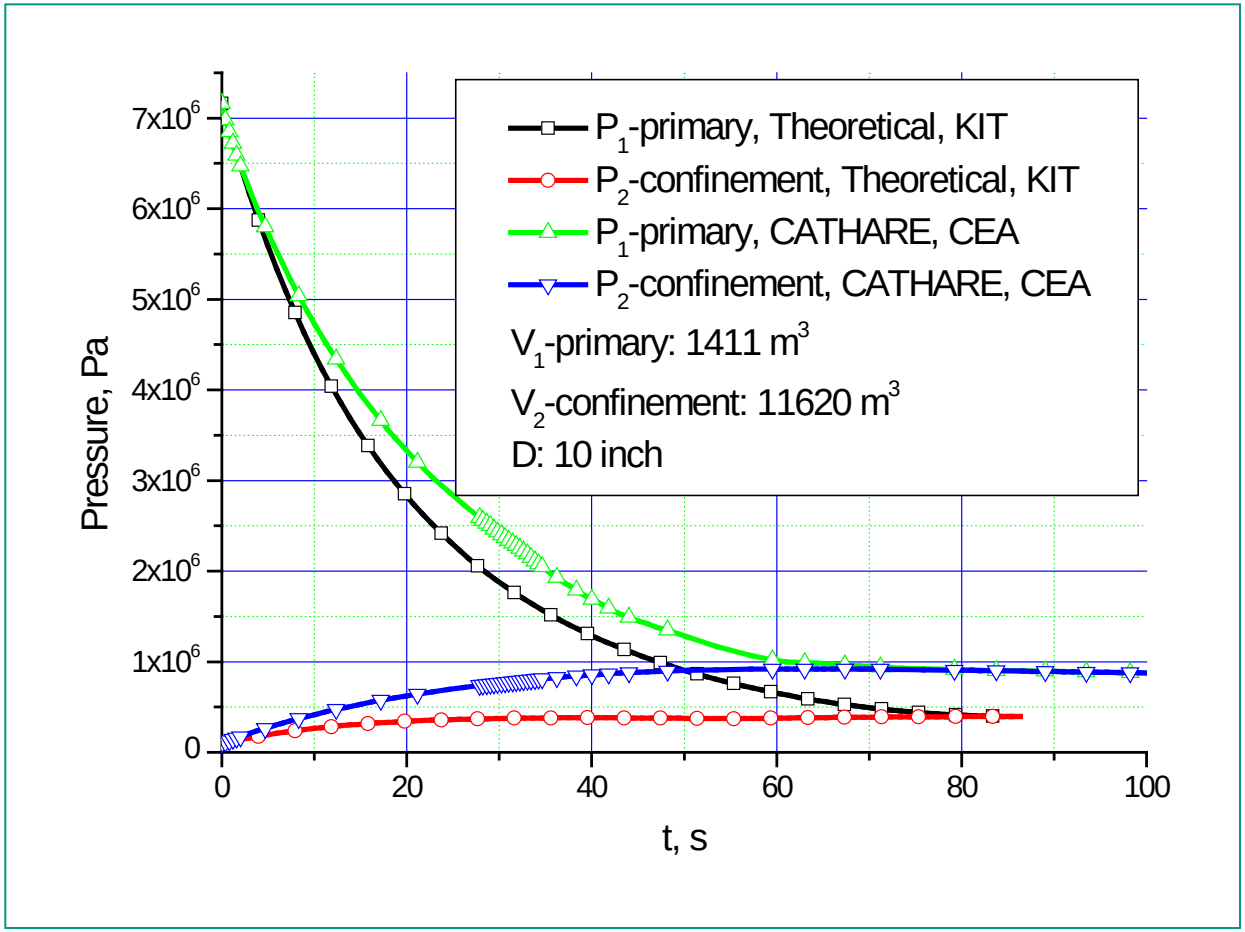
Validation
ANALITICAL SOLUTION VS. CATHARE

Test:
Mass flow rate



Validation
ANALITICAL SOLUTION VS. CATHARE

Test:
Pressure

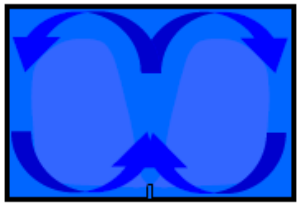
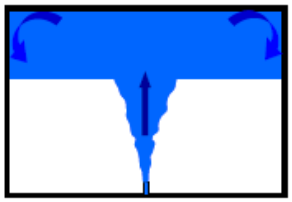
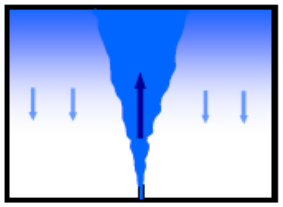


EXAMPLE PLANNED FOR DISTRIBUTION

H_2 DISTRIBUTION IN A CLOSED UNVENTILATED BOX

(Jallais, AirLiquide, CEA) not yet published ← HyInDoor

The main governing dimensionless number is : $Ri_v = \frac{V^{1/3} g'_0}{U_0^2}$

R_{iv}	Regime		Model
R_{iv}< 2.5E-3	Homogenous		Cleaver
2.5E-3 < R_{iv} < 3	Stratified with a homogenous layer		Cleaver
R_{iv} > 3	Stratified without homogenous layer : • Parabolic shape • Linear shape		Worster and Huppert with α function of R_{i0} for the larger source diameter (20 mm and more) **or** Linear correlation for the smaller source diameter (5 mm and less)

Limit between the 2 regimes is unclear (d ?? or a dimensional number ?)

Only empirical correlation

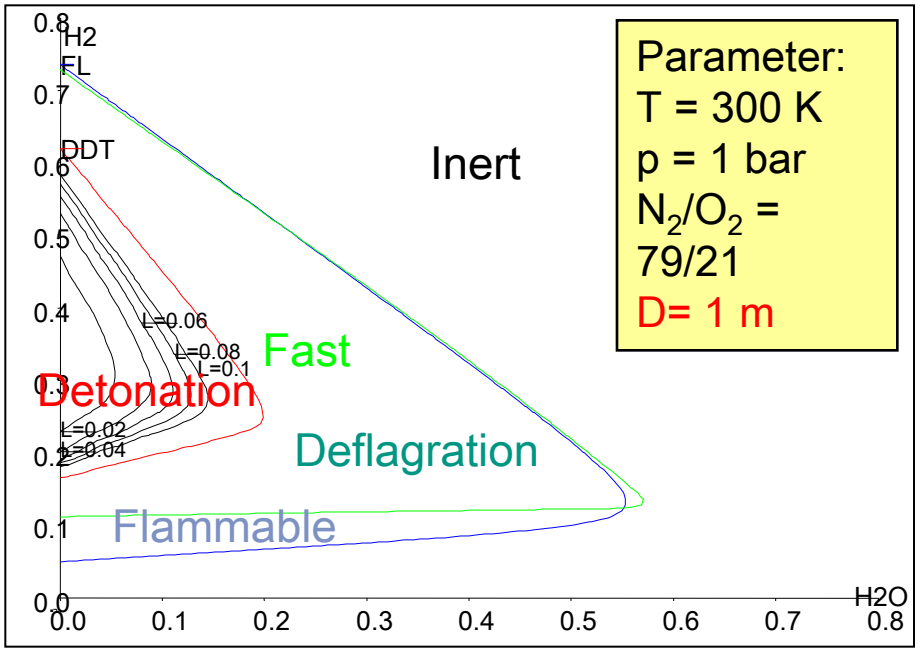
EXAMPLE PLANNED FOR RISK POTENTIAL

Flame Acceleration and DDT Criteria (Dorofeev)

GP Program to be integrated → limits/regions of flammability flame acceleration FA, and deflagration-detonation transition DDT for all H_2-O_2-N_2-steam mixtures

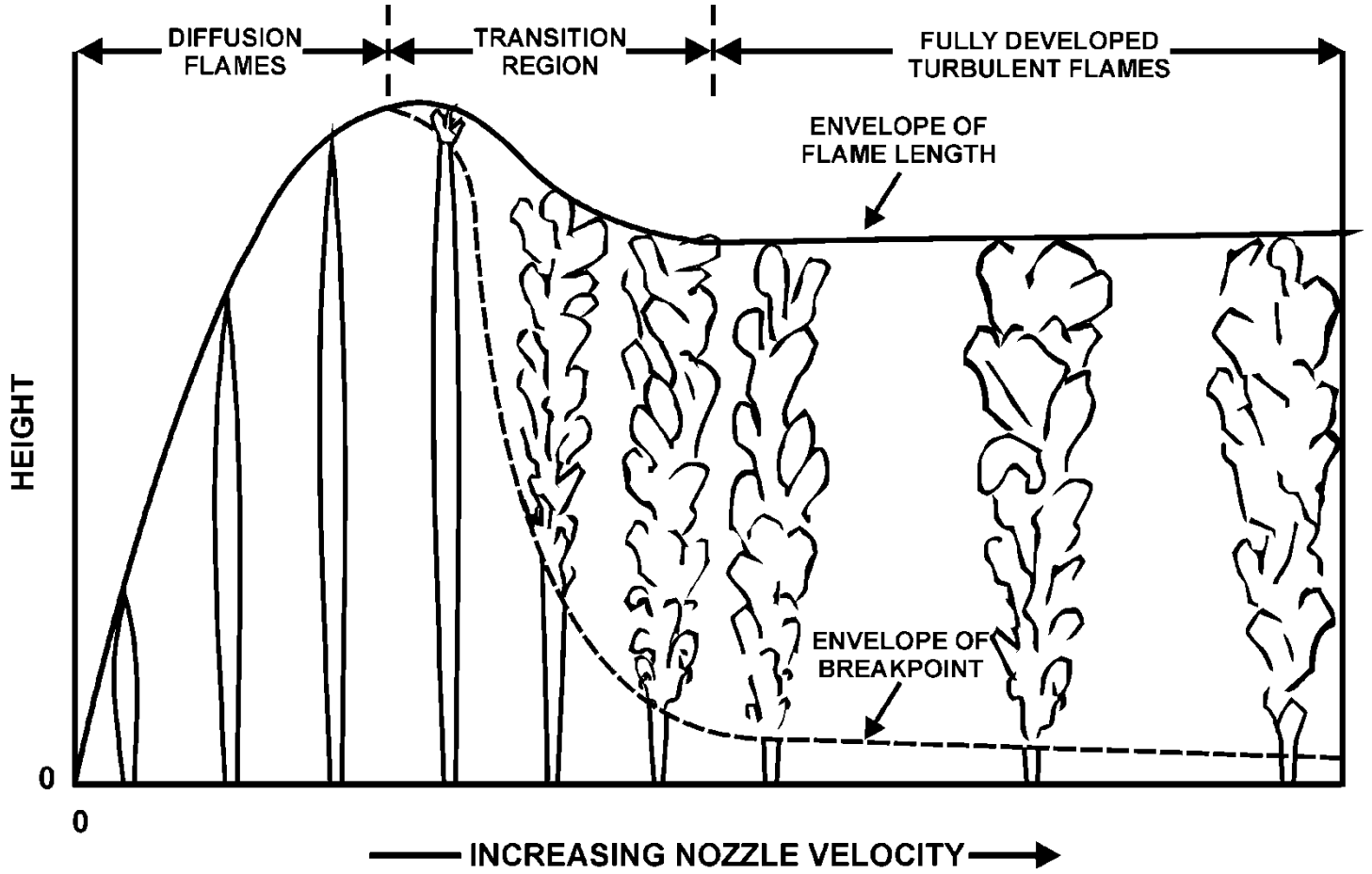
σ-Criterion for FA

7λ-Criterion for DDT



EAMPLE PLANNED FOR FLAME LENGTH

Unified correlation for expanded and under-expanded jet flame length (Molkov, UU)



EXAMPLE PLANNED FOR FLAME LENGTH

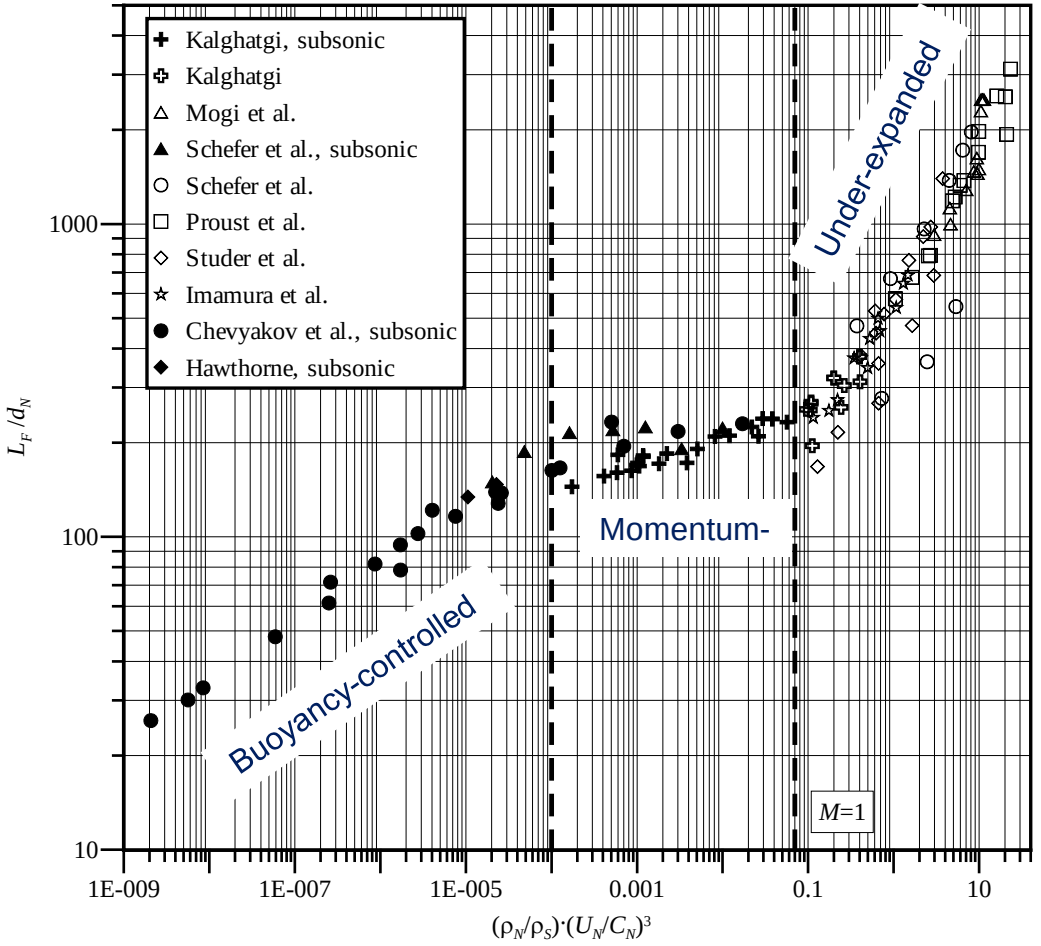
THE DIMENSIONLESS CORRELATION (MOLKOV, UU)

Validation:
***P* =0.1-90 MPa**
***d*=0.4-51.7 mm**
L/T; SS/S/SS

Line *M*=1
(choked flow)

***M* (*M*<1)-> (*Re, Fr*)**

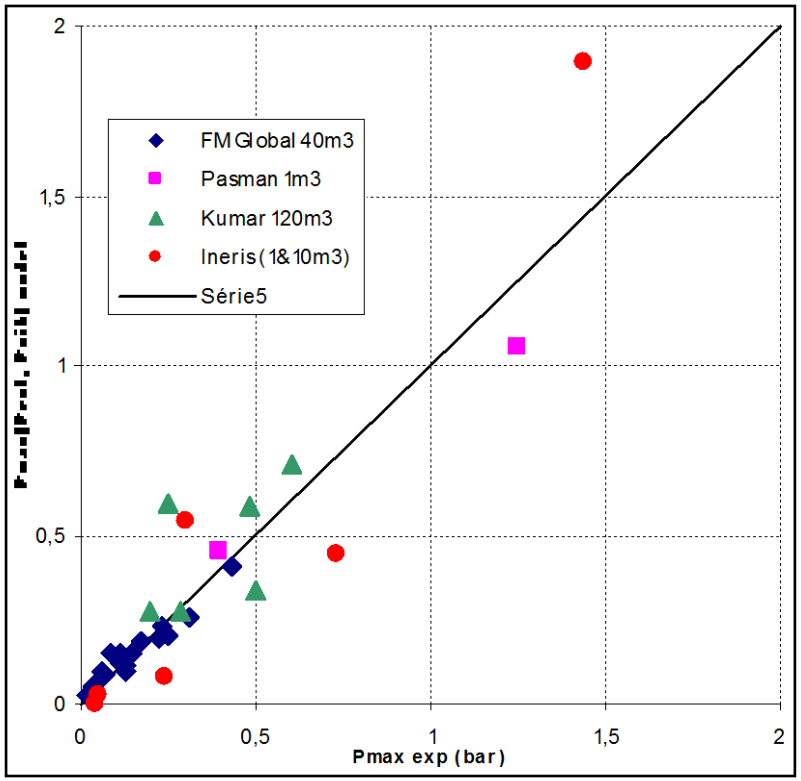
$$\frac{\rho_N}{\rho_S}\cdot\left(\frac{U_N}{C_N}\right)^3 = \frac{g\cdot\mu_N}{\rho_S\cdot C_N^3}\cdot \mathrm{Re}\cdot Fr$$



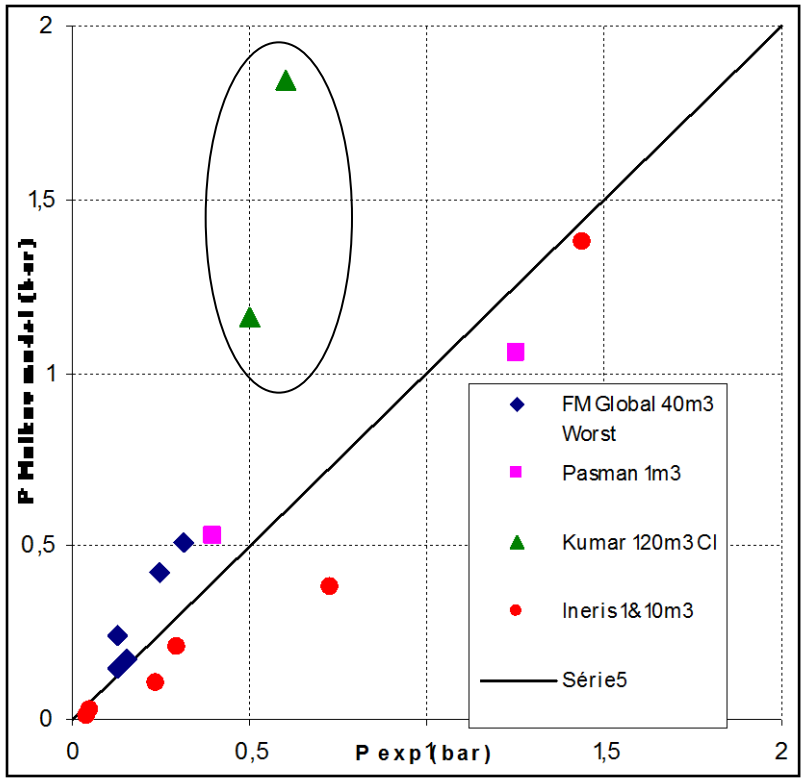
POSSIBLE CONTRIBUTIONS FROM RUNNING PROJECTS

HyInDoor → Vented Explosions

FM Global Model



Molkov Model



- **Relative good agreement of the 2 models**
  - **Molkov model seems to be conservative**
- **Validation needs to be extended with new exp. data**

Elements for Discussion

- *H2 & FC require innovations*
- *Standards and regulations based on conventional technologies tend to be over-conservative (at best)*
- *Experiments and simulations resolving physics in detail (e.g. CFD,…) are time consuming and costly → no practical solution for SMEs developing the innovative products*
- **Open, free toolset for simplified analysis** of risk relevant quantities fills this gap
- **Collaborative efforts** with a minimum continuity needed to extract/translate findings of research into these tools
- Certification?