

MECHANISTIC SAFETY ANALYSIS OF HYDROGEN BASED ENERGY SYSTEMS

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CONTENT OF PRESENTATION



• Presentation consists of two topics which are treated in parallel





OUR EXAMPLE FOR HYDROGEN ANALYSIS

• Oil peak behind us, hydrogen fueled cars in widespread use • Returned from a trip late at night • There was some small collision but apperently no domage to LH₂-system • Park car in private garage • But at night the questions come . What could be the consequences? What would happen in case of a hydrogen leak? What would be Could they be How fast could the pressure flammable? loads? the burn be? What mixtures could develop? KIT - die Kooperation von Forschungszentrum Karlsruhe HELMHOLTZ Forschungszentrum Karlsruhe GmbH in der Helmholtz-Gemeinschaft 3 und Universität Karlsruhe (TH)

GENERIC ARCHITECTURE OF AN LH₂-TANK SYSTEM





Source: EU-Project EIHP-2, Final Report 2004

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INVESTIGATED GARAGE SCENARIOS

- A thermal energy deposition of 1 Watt into a cryogenic LH₂-tank leads to a boil-off of 170 g of gaseous hydrogen per day
- Assume here 5 release pulses per day, 34 g H_2 each, with two different release rates

GEOM	ETRY	HYDROGEN SOURCE							
Garage Volume (m ³)	Vent Openings	H ₂ -Rate (g/s)	Duration (s)	Total Mass (g)	Release Temp. (K)	Release Location	Nr.		
	Two times	3.40	10	34	22.3	under-neath	1		
70.2	10 x 20 cm ²	0.34	100	34	22.3	trunk	2		

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WHAT ARE THE IMPORTANT RISK DETERMINING PARAMETERS?



- Large spectrum of events possible, ranging from zero risk to destruction of garage
- What are the parameters influencing the outcome of such a leak scenario?

 Obvious first step is to understand mixture generation, defines initial and boundary conditions for further accident development

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AN INITIAL ESTIMATE ON HYDROGEN CONCENTRATION



• We can make a first estimate on the hydrogen concentration in the garage by using a single volume approach

volume fraction $H_2 \approx \frac{\text{volume } H_2 \text{ released}}{\text{volume of garage}}$	$=\frac{34\mathrm{g}\mathrm{H_{2}}\cdot22.4\mathrm{I}/2\mathrm{g}\mathrm{H_{2}}}{70\mathrm{m}^{3}}\approx0.5\%$
Any risk?	
Why is result independent of release rate?	
Obviously the real situation is more complex	
Next approach is a CFD model	

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Physical models of 3d code GASFLOW (1)



Rekos

- Conservation equations of fluid flow (fully compressible, 3-dim. Navier- Stokes)
- Thermophysical properties of components (JANAF) (internal energy, specific heats, 25 components including two-phase water)
- Molecular transport coefficients (CHEMKIN) (thermal conductivity, dynamic viscosity, binary diffusion coefficients)
- Convective and radiative heat transfer between gas and structure
- Heat conduction within structures
- Condensation and vaporization of water (film, droplets, sump)

IRWST

T>1000K

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Physical models of 3d code GASFLOW (2)

- Lumped- parameter sump model
- Boundary layer model for wall shear stress
- Turbulence modeling (algebraic, k-ε) (effects on molecular transport coefficients)
- Accident mitigation measures (Recombiner and igniter models, containment inertisation)
- Ventilation systems (1-dim. ducts, pipes, junctions, blowers, dampers, valves, filters, etc)



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GASFLOW EQUATIONS



Fully compressible Navier-Stokes, expressed in integral form for finite volume discretisation



J.R. Travis et al, Report FZKA-5994 (1998)

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GASFLOW VERIFICATION

• 3d code GASFLOW used and developed at FZK for hydrogen distribution simulation. Large verification matrix:

PHYSICAL PROCESS	MODEL	VERIFICATION																
		Analytical solution				Sin	igle e	effec	t te	sts				lr	ntegra	al ex	perin	nents
Distribution, GASFLOW			5.5	5.6	5.8		5.7	5.9	5.13	2	5.	11		5.12	5.13	5	.14	5.15
- geometry	 3d, cylindrical, cartesian graphical input 	Abb.	C/B1	I BMC	DAT	HET /	AECL	C/B2	2 HDI 1	R BN	IC PA	sco	BMC L	HDR T31.	5 E11	R ТІ 1.2	HAI F F	PHEBUS
 flow and transport 	 Navier-Stokes, 3d, vollkompressible 	 laminar channel flow 	Ì	1			1	1			1	•	•			• •		1
thermophys. properties	JANAF Tables																	
molekular transport	CHEMKIN	 diffusion, 1d 																
- turbulence	- k/ε		•	Jx7			÷							•)	• •		•
 turbulent heat transfer gas/wall 	 wall function 	 1D channel, theory 			•	•												
 heat conduction in struct 	 Fourier equation, 1d 	 1D Probleme 												•	, ,	•	•	•
 radiation 	 Momentum approximation 	• 1D, 2D										٠						
 vaporation/condensation 	 homogeneous equil. Model 							٠						•		• •		ė
 critcal flowl 	 analyt. Orifice solutions 																	
Mitigation:									6.	26	3 6.5	6.	4					
 rekombiners a) Siemens 	- 1-cell model								E11	.8.1		G	x4,6					
b) NIS	- 1-cell model									мс	3							
- igniter	- 1-cell model												Gx7					
 sump vaporization 	 homogeneous Sump model 									F	x4,5							

Report FZKA-7085 (2005), www.fzk.de/hbm

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EXAMPLE FOR RECENT GASFLOW VERIFICATION

- German national benchmark, test TH7 in Thai facility with condensation
- Blind pressure prediction of CFD codes

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GASFLOW SIMULATION OF GARAGE SCENARIO

• Case 1: release rate 3.4 g H_2 / s for 10 seconds



Isosurface with 4 vol% H₂, depicts flammable mixture in garage

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GASFLOW SIMULATION OF GARAGE SCENARIO

• Case 2: release rate 0.34 g H_2 / s for 100 seconds



Isosurface with 4 vol% H_2 , depicts flammable mixture in garage

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RESULTING HYDROGEN CLOUD IN GARAGE

- Computed dimension of combustible H₂-air cloud in garage (4...75% H₂)
- Characteristic size of combustible cloud expressed as $d_{CC} = (V_{cc})^{1/3}$
- Combustible cloud size strongly dependent on release rate, is result of balance between source strength and sinks, or release rate and mixing mechanisms



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WHAT IS RISK FROM COMBUSTIBLE CLOUD?

- How would you judge the hazard in both cases?
- Who would switch on lights in the garage?
- What physical quantities determine hazard potential of a combustible H₂-air cloud?



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COMBUSTION REGIMES

• H₂ – air mixtures can burn in different modes / combustion regimes









Inert, no stable flame propagation $v_{fl} = 0$

Laminar deflagration $v_{fl} \approx 1$ m/s, Ma << 1

Fast turbulent deflagration $v_{fl} \approx 300 \text{ m/s}, \text{ Ma} \approx 1$

Detonation $v_{fl} \approx 1500$ m/s, Ma >> 1

• Change of mode possible by transition process



Ignition



Flame acceleration

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Deflagration-to-detonation transition (DDT)

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PEAK OVERPRESSURES FROM HYDROGEN-AIR FLAMES





Maximum acceptable static load for typical inner containment structures (1 ton / m²)

- The maximum flame speed generally governs the damage potential
- Which combustion regime develops for given mixture and geometry?
- How fast can it burn?

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IGNITION

- Combustion requires an ignition source and a burnable mixture
- Many potential ignition sources exist
- More than 90% of incidents with GH₂ lead to ignition, cause often unknown
- Ignition difficult to exclude in a hydrogen safety analysis, conservatively the presence of an ignition source may be assumed
- Controlling factor is then flammability of mixture, well known for H₂-air



Kreiser et al, Report Univ. Stuttgart IKE 2-116 (1994)

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FLAME ACCELERATION

 Conservative conditions for flame acceleration in hydrogen mixtures were investigated in closed obstructed tubes, e.g. FZK 12m-tube



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RESULTS OF FLAME ACCELERATION EXPERIMENTS



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FLAME ACCELERATION CRITERION

- Summary of experiments with different H₂-O₂- dilutend (N₂, Ar, He) mixtures in obstructed tubes of different scales
- Each point represents one experiment
- Results of data evaluation: expansion ratio σ is mixture property which governs flame acceleration limit
- No flame acceleration for σ < 3.75 ± 0.1 (10.5% H₂ in dry air)



In lecture notes

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DEFLAGRATION-TO DETONATION TRANSITION



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- Two different modes of DDT have been observed
 - shock focussing
 - detonation on-set in turbulent flame brush
- Present here one example for DDT with pressure wave emitted from an obstructed region and focussed in a conus



• Shock tube with conus (idealized mode A)



Partially obstructed tube with conus (prototypic mode A)



• Fully obstructed tube (prototypic mode B)



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TURBULENT DEFLAGRATION EXPERIMENT WITHOUT DDT



• Partially obstructed tube with conus, 15 % hydrogen in air



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TURBULENT DEFLAGRATION EXPERIMENT WITH DDT



• Partially obstructed tube with conus, 16.5 % hydrogen in air



• Result: focussing of pressure waves emitted from a fast turbulent flame can trigger a detonation on other parts of the system

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CRITERION FOR DDT

- Experiments on DDT in differently sized and shaped facilities have shown that a certain minimum scale is required for DDT
- Correlation of all experimental data with given definitions of D and detonation cell size data shows that detonations are only possible for $D/\lambda > 7$
- Current uncertainty in detonation cell size $\lambda \approx$ factor 2

• In accident scenarios D/λ can vary by orders of magnitude, criterion has therefore predictive capability



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DETONATION CELL SIZES

Detonation cell sizes (in cm) of H₂-air-steam mixtures at 375 K and 1 bar initial pressure. Dry hydrogen concentration is defined as H₂ / (H₂ + air)



State of the Art Report by a Group of Experts "Flame Acceleration and Deflagration – to – Detonation Transition in Nuclear Safety", Nuclear Safety NEA/CSNI/R(2000)7, August 2000

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SUMMARY OF CRITERIA



 Criteria for possible occurrence of fast combustion regimes were evaluated from many experiments with various H₂-mixturs on different scales



- Transition phenomena cannot be modeled numerically on large building scale
- Criteria allow selection of fastest possible combustion mode from computed H₂-air cloud composition and scale

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COMPUTED HAZARD PARAMETERS FOR GARAGE SCENARIOS





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HAZARD POTENTIAL FOR GARAGE SCENARIOS

• Risk parameters show strong dependence on H₂ release rate

- Case 1: (3.4 g H ₂ /s)	 Continuous potential for slow deflagration (≈ 20 g of 34 g) potential for supersonic combustion regimes (and ignition) during the release period high release rate not tolerable without mitigation measures
- Case 2: (0.34 g H ₂ /s)	 only small potential for slow deflagrations, natural mixing processes sufficient release rate (and mass) seems tolerable for present garage design

• Only **Case 1** followed in further safety analysis





COMBUSTION EXPERIMENTS FOR CASE 1

- Up to 20 g of hydrogen would be in burnable concentrations
- A significant part of this could potentially burn with high flame speeds
- What would be pressure loads and consequences from a local explosion in the garage?
- Outcome uncertain, experiments performed in test chamber simulating the garage

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COMBUSTION UNITS



- To obtain conservative pressure loads, combustion units were developed providing the fastest possible flame speed for a given H₂ mass
- Cubes were made for 0.5, 1, 2, 4, 8 and 16 g of H₂, which can be inserted into each other
- Wire grids 6.5 x 0.65 mm, 12 layers between cubes

Hydrogen injection device

cubes covered with plastic, filled with stoichiometric H_2 - air mixture





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UNCONFINED TEST OF COMBUSTION UNIT



FLAME SPEEDS IN COMBUSTION UNITS



- The flame acceleration inside the combustion units was measured with photodiodes
- For 8 and 16 g H₂ detonation speeds are obtained at the outer edge of the cube



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- Measured peak overpressures Δp^+ in unconfined tests with combustion units of 0.5 to 16 g H₂
- Data are well reproducible



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IMPULSE VS DISTANCE









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SCALED PEAK OVERPRESSURES VS DISTANCE



- Use of Sachs scaling collapses measured peak overpressures to universal correlation for \geq 1 g H₂, E = total energy of explosive charge
- Combustion units provide conservative and well defined overpressures



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TEST CELL FOR GARAGE SIMULATION

- Dimensions 5.5 x 8.5 x 3.4 m, about 160 m^3
- Air flow ≤ 24.000 m³/h, up to 1 air exchange in 24s
- Controlled air flows in chamber possible
- All ventilation systems
 explosion protected
- Test cell used for simulation of garage /confined volume





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INSTRUMENTATION OF GARAGE

• The instrumentation included pressure and acceleration sensors at different locations, covering flat surfaces, (2d) edges and (3d) corners



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LOCAL HYDROGEN EXPLOSIONS IN A GARAGE

- H₂ mass:
- 1g
- 2g
- 4g
- 8g - 16g



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REPRODUCIBILITY OF MEASURED DATA

- The experiment with 1 g H₂ was performed three times
- Acceleration and pressure sensors show very good reproducibility of measured signals
- Complex, but reproducible pressure waves are created in confined local explosions of H₂-air mixtures





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COMPARISON OF OVERPRESSURES



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 Pressure sensor 2 B, floor near combustion unit Pressure sensor 8 A, back wall, half wall height

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 Pressure signals very consistent in timing, amplitudes increase systemarically with H₂ mass, reproducible pattern of reflected pressure waves in confined volume.





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TURBULENT DEFLAGRATION REGIMES



COM3D EQUATIONS



Hydrodynamic equations

The set of conservation laws for mass, momentum, energy and species reads as

$$\begin{split} (\rho)_t &+ (\rho u_j)_{x_j} = 0, \\ (\rho u_j)_t &+ (\rho u_i u_j)_{x_j} = \rho g_i - p_{x_i} + M_{ij;x_j}, \quad i = 1, 2, 3 \\ (\rho e)_t &+ ((\rho e + p)u_j)_{x_j} = \\ &\rho g_j u_j + u_i M_{ij;x_j} + (\frac{\mu_{tur}}{C_h} (e - \frac{1}{2} u_i u_i + \frac{p}{\rho})_{x_j})_{x_j} + B + \rho \epsilon, \\ (\rho f_\alpha)_t &+ (\rho f_\alpha u_j)_{x_j} = \overline{w}_\alpha + (\frac{\mu_{tur}}{C_{f\alpha}} f_{\alpha;x_j})_{x_j}, \end{split}$$
here

$$e = \sum_{\alpha=1}^{N} \frac{f_{\alpha}}{\mu_{\alpha}} \left(h_{\alpha} + \Delta h_{\alpha}^{0} - RT \right) + \frac{1}{2} u_{j} u_{j}, \quad f_{\alpha} = \frac{\rho_{\alpha}}{\rho},$$
$$M_{ij} = -\frac{2}{3} \delta_{ij} (\rho k + \mu_{tur} u_{r,xr}) + \mu_{tur} (u_{i,xj} + u_{j,x_i}).$$

Closure of the equation depends on the knowledge of the following variables: μ_{tur}, k, ϵ (theory of turbulence) and \dot{w}_{α} (combustion model).

• COM3D under development at FZK for simulation of turbulent deflagration

RNG k-e model

$$\begin{aligned} (\rho k)_t + (\rho u_j k)_{x_j} &= S - \rho \epsilon + (\frac{\mu_{tur}}{C_k} k_{x_j})_{x_j}, \\ (\rho \epsilon)_t + (\rho u_j \epsilon)_{x_j} &= \frac{\epsilon}{k} [(C_1 - C_\eta) S - C_2 \rho \epsilon] + (\frac{\mu_{tur}}{C_\epsilon} \epsilon_{x_j})_{x_j} + \\ &+ [C_3 - \frac{2}{3} C_\eta (C_\mu \frac{k}{\epsilon} u_{j;x_j} + 1)] \rho u_{j;x_j} \epsilon. \end{aligned}$$

Here C_η is defined by

and

$$C_{\eta} = rac{\eta(1-\eta/\eta_0)}{1+eta\eta^3}, \qquad \eta_0 = 4.38$$

$$\eta = \frac{k}{\epsilon} \left(\frac{1}{2} (u_{i,x_j} + u_{j,x_i}) (u_{i,x_j} + u_{j,x_i}) \right)^{1/2},$$

$$C_3 = \frac{-1 + 2C_1 - 3m(\gamma - 1) + (-1)^{\delta} \sqrt{6} C_{\mu} C_{\eta} \eta}{3}.$$

Turbulence model constants $C\mu$ C_1 C_2 C_k C_{ϵ} β 1.42 0.719 0.719 RNG k-e 0.0845 1.680.0121.44 1.92 Standard k- ϵ 0.09 1.0 1.3

Turbulence and reaction model

The standard k- ϵ model (semi-empirical character: the constants C_{α} are calibrated against turbulent tube experiments)

$$(\rho k)_t + (\rho k u_j)_{x_j} = S - \rho \epsilon + (\frac{\mu_{tur}}{C_k} k_{x_j})_{x_j},$$

$$(\rho \epsilon)_t + (\rho \epsilon u_j)_{x_j} = \frac{\epsilon}{k} (C_1 S - C_2 \rho \epsilon) + (\frac{\mu_{tur}}{C_k} \epsilon_{x_j})_{x_j}.$$

Where

$$S = u_{i,x_j} M_{ij} - B; \ B = rac{\mu_{tur}}{C_{
ho}} rac{1}{
ho^2}
ho_{x_T} p_{x_T}; \ \mu_{tur} = \mu + C_{\mu}
ho rac{k^2}{\epsilon}.$$

Limiting regimes of turbulent combustion $D_a = \tau_{turb} / \tau_{chem}$:

- low turbulence intensities / fast chemical reaction

- high turbulence intensities / slcw chemical reactions

$$\dot{\omega} = \begin{cases} -C'_f \frac{\epsilon}{k} \omega(1-\omega); & D_a > 1\\ -K_{chem} \omega \exp(-E_a/T); & D_a < 1 \end{cases}$$

$$\tau_{turb} = \frac{k}{\epsilon}; \quad \tau_{chem} = \frac{1}{K_{chem}\omega \exp(-E_a/T)}$$

and (Said & Borghi)

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$$C_f' = C_f \left(1 + \frac{4.4}{1 + 3.2 \frac{k^{1/2}}{S_L}} \right)$$

A. Kotchourko, IKET

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COM3D VERIFICATION (1)

- Large scale experiments performed in RUT facility near Moscow (FZK, CEA, partly NRC), H₂-air, H₂-air-steam
 - Total length 62 m
 - Total volume 480 m³
 - First channel with obstacles
 - Second part without obstacles





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COM3D VERIFICATION (2)



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- Numerical simulation of large scale RUT experiments with hydrogen-air and hydrogen-air steam mixtures. Standard k-ε and Eddy-Break-up model.
- Venting in experiments, no venting in simulation



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SIMULATION OF UNCONFINED TESTS

- The unconfined tests with different combustion units were simulated with COM3D
- The COM3D combustion model was fitted to the measured flame speed in the combustion units



• The calculated peak overpressures agree with the experimental values and follow Sachs scaling

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COM3D COMBUSTION SIMULATION

- 3d pressure field, calculated isosurface for 1.1 bar
- Isosurface 110000 Pa • Test with 8g H₂ Préssure 200000 180000 160000 140600 120600 CALLS SHELLING William. 100000 1.1185-15 80000 60000 40000 20000 0 Test Cell COM3D v.2.2.5 KIT – die Kooperation von HELMHOLTZ Forschungszentrum Karlsruhe GmbH

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COMPARISON OF OVERPRESSURES



 Good agreement, remaining differences are due to geometry simplification and rigid wall model in simulation









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STRUCTURAL RESPONSE



• What are effects of blast loads on the structure?





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- Simplest model for structural response is SDO model
- Describes ground mode (first harmonic) of structural element which is represented by lumped values for mass, stiffness and damping of motion
- Tool to understand basic effects of transient pressure loads on global displacement of element
- In FEM analysis also higher modes included, but superposition of different effects, results not so transparent



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BLAST LOADED ELASTIC OSCILLATOR (1)



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- Damage is determined by maximum displacement x_{max}, can be found from solution by setting $\dot{x}(t) = 0$
- Scaled displacement = f(scaled loading time)

$$\frac{x_{max}}{\Delta p^+/k} = f(\omega T_{load})$$

0.0

0.1

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1.0

scaled loading time ωT

10

100

p*(t) = P*e^{-t/T}

1000



BLAST LOADED ELASTIC OSCILLATOR (2)

 Asymptotes for maximum deflection /deformation can be computed from energy balances Quasistatic loading realm (T load >>T osc) - strain energy = work on structure Scaled displacement $\frac{1}{2}$ kx²_{max} = $\Delta p^{+} \cdot x_{max}$ $\frac{x_{max}}{\Delta p^+/k} = 2$ dynamic maximum deflection is two times static deflection (DLF = 2) • Impulsive loading realm ($T_{load} \ll T_{osc}$) - initial kinetic energy = strain energy $\frac{1}{2}mv_0^2 = \frac{1}{2}kx_{max}^2$ $\frac{l^2}{2m} = \frac{1}{2}kx_{max}^2 \qquad l = \int_0^\infty \Delta p^+ e^{-t/T_{load}} = \Delta p^+ \cdot T_{load}$

 $\frac{\mathbf{x}_{\text{max}}}{\Delta \mathbf{p}^+/\mathbf{k}} = (\frac{\mathbf{k}}{\mathbf{m}})^{1/2} \mathbf{T}_{\text{load}} = \boldsymbol{\omega} \mathbf{T}_{\text{load}} \quad \text{or} \quad \mathbf{x}_{\text{max}} = (\frac{1}{\mathbf{k} \mathbf{m}^{1/2}}) \cdot \mathbf{I}$

maximum deformation is proportional to blast wave impulse I



Scaled loading time ωT

W.E. Baker, P.A. Cox, P.S. Westine, J.J. Kulesz, R.A. Strehlow; Explosion Hazards And Evaluation; Fundamental Studies in Engineerings, 5; Elsevier

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OSCILLATOR RESPONSE: ANOTHER VIEW

- Often oscillator response is presented with inverted ordinate and unscaled load parameters Δp^+ and T_{load}
- Quasistatic asymptote

$$\frac{\Delta p^{+}}{kx_{max}} = \frac{1}{2}$$
$$\Delta p^{+} = \frac{kx_{max}}{2}$$

Maximum deflagration x_{max} is only proportional to applied peak overpressure Δp^+ , independent of load duration

• Impulsive asymptote

$$\frac{\Delta p^{+}}{kx_{max}} = \frac{1}{\omega T_{load}}$$
$$\Delta p^{+} = (km)^{\frac{1}{2}} x_{max} \frac{1}{T_{load}}$$
$$\Delta p^{+} T_{load} = I \sim x_{max}$$

Maximum deflection x_{max} is proportional to applied impulse



log of positive overpressure duration $\mathsf{T}_{\mathsf{load}}$

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STRUCTURAL DAMAGE FROM CONFINED LOCAL H₂ EXPLOSIONS IN GARAGE



Results: - windows and light garage components (door) wold break

- damage to masonary walls only from nearly explosion of 16 g H₂
- wooden framework construction would be destroyed

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HUMAN EFFECTS FROM CONFINED LOCAL H₂ – EXPLOSIONS IN GARAGE



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SUMMARY OF MECHANISTIC SAFETY ANALYSIS OF HYDROGEN BASED ENERGY SYSTEMS

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PROCEDURE FOR HYDROGEN SAFETY ANALYSIS



• A complete, self-consistent and mechanistic analysis procedure has been developed which addresses all important physical phenomena of hydrogen behaviour in accidental release scenarios



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MITIGATION MEASURES

• The proposed analysis procedure allows identification of possible mitigation measures for risk reduction



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