HEALTH & SAFETY LABORATORY

Mathematical Modelling of Health & Safety Related Flows – Future Direction

Stefan Ledin
Health & Safety Laboratory, UK

Content

- Where is modelling used?
- Real Life Scenarios
- Flows of Interest
- Evolution in Mathematical Modelling
  - Turbulence Modelling
  - Combustion Modelling
  - Radiation Modelling
- Quality and Trust
- Future

Applications of Models

- Basic Research
- Consequence modelling to support
  - COMAH
  - Safety Cases
  - Land Use Planning applications
- Incident investigations
- Risk Assessments
  - Simplified Approaches
  - Quantified Risk Assessments (QRA)

Examples : HSL

HEALTH & SAFETY LABORATORY

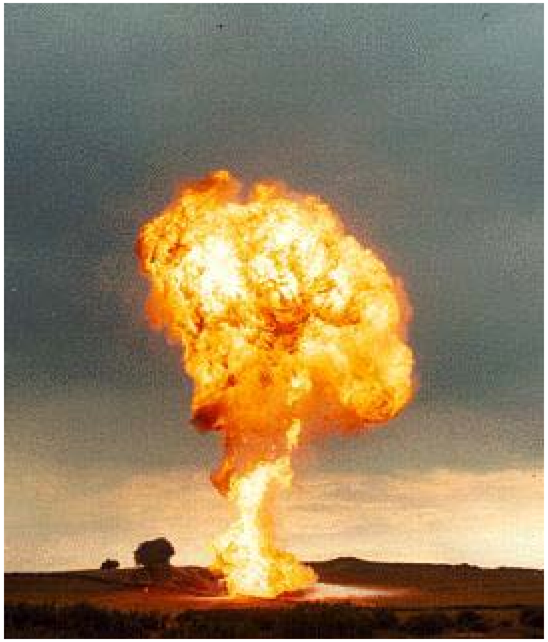
- Airflows through human airways
- Atmospheric dispersion modelling LNG dispersion / source terms
- Blast waves
- Fluid structure interaction (FSI)
- Gas leaks in enclosed spaces
- Gas dispersion in gas turbine enclosures
- Hydrogen Safety
- Natural ventilation on offshore platforms
- Smoke movement

Real Life Scenarios – 1

Buncefield:
Aerial photograph of the Buncefield incident

Buncefield:
Northgate Building, located to the West of the HOSL site

Real Life Scenarios – 2



BLEVE: 2 ton LPG tank

Didcot Power Station: Turbine Hall

Real Life Scenarios – 3

Burner based on a Rolls Royce Tay can combustor, operating at P > 4.0 MPa

High pressure jet of combustion products impacting on a flat plate (pre-test)

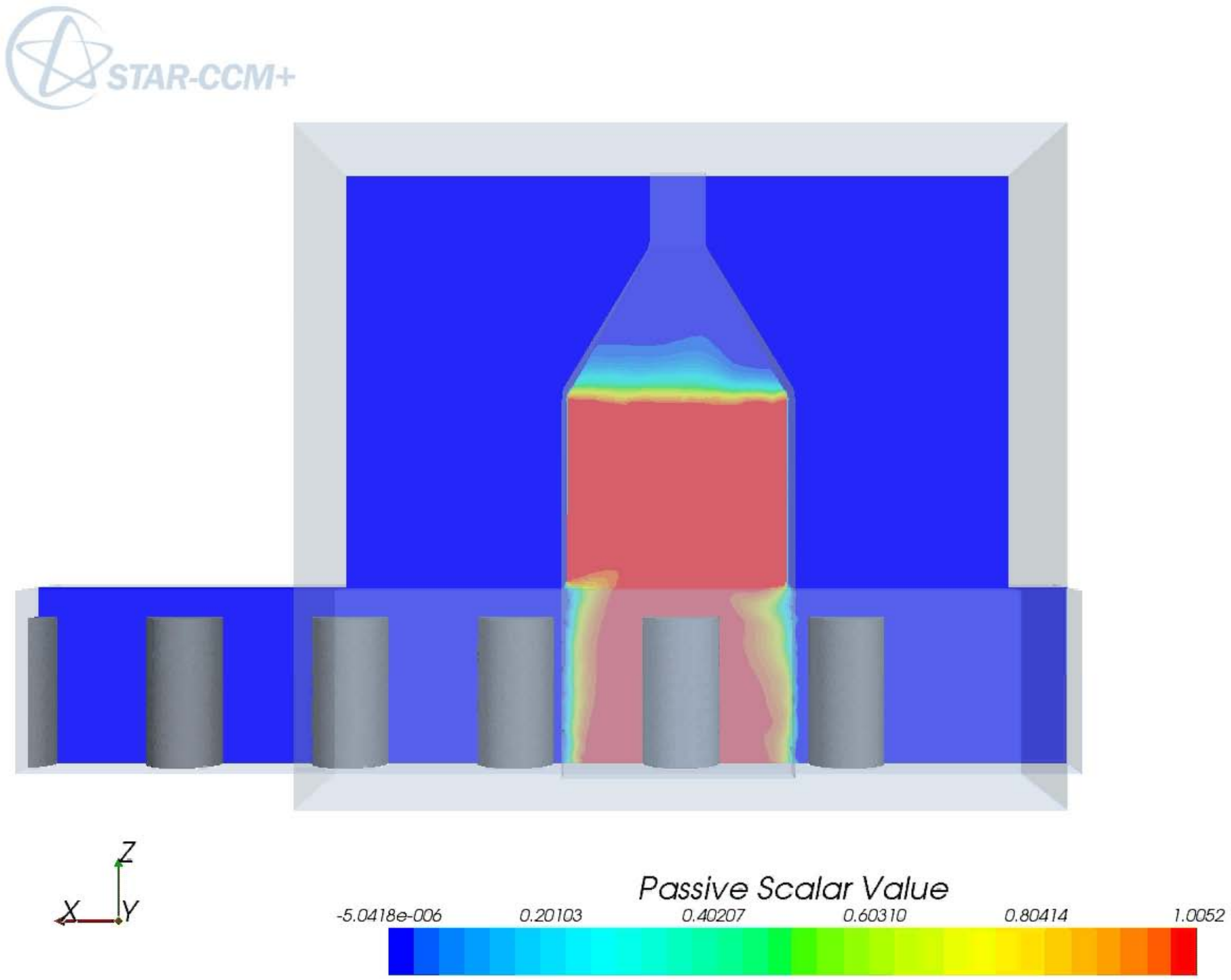
Real Life Scenarios – 4

HEALTH & SAFETY LABORATORY

Family of offshore installations in the North Sea

Velocity measurements in one of the process modules. Note the congestion

Drum Filling

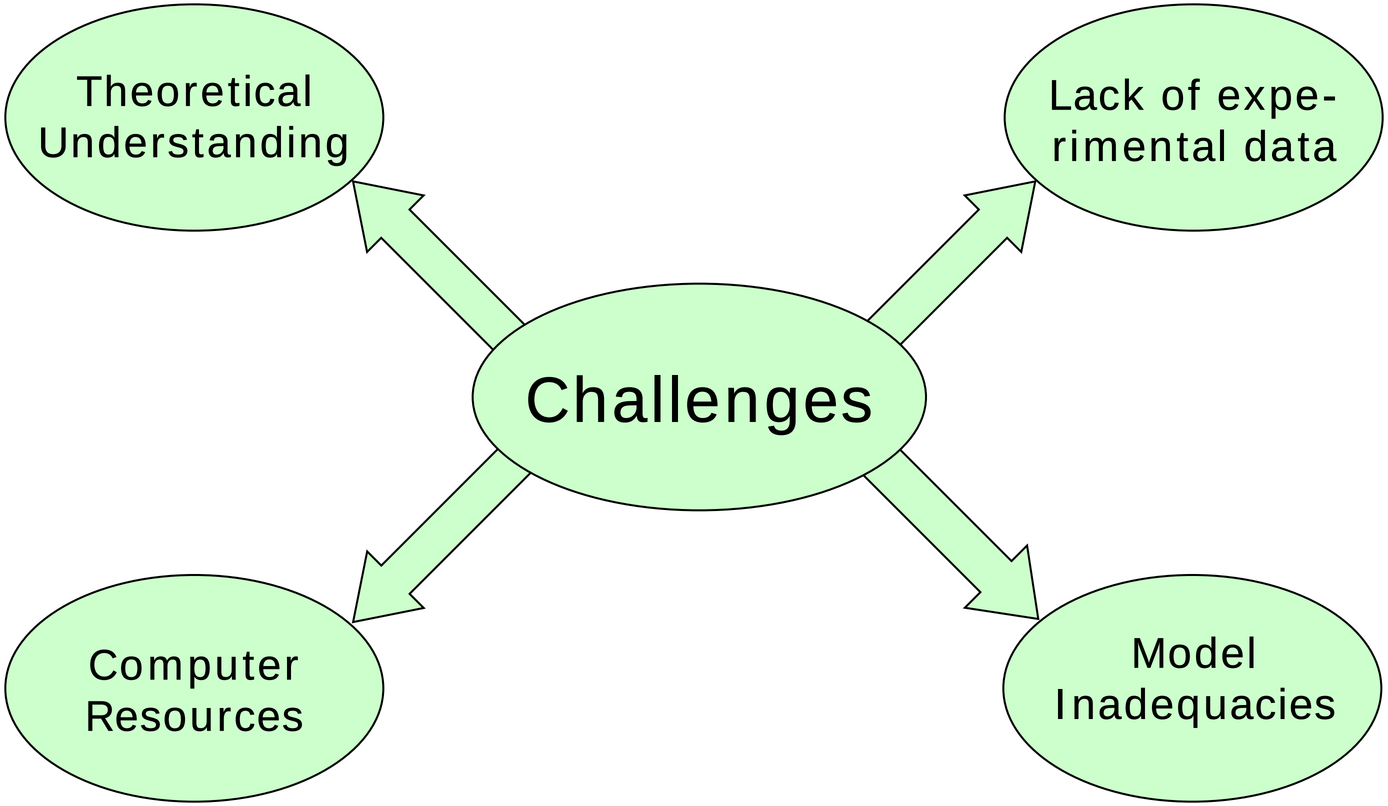


N.B. There are no experimental data available for this scenario.
It is a proof-of-concept exercise

Flows of Interest

- Dispersion
  - Biologically active substances
  - Flammable substances
  - Toxic substances
- Combustion
  - Deflagration
    - Explosions
    - Fires
  - Detonation, Deflagration to Detonation Transition (DDT)
  - Ignition
- Cryogenic liquids
- Supercritical fluids
- Free surface flows
- Free or impacting high-momentum jet
  - Combusting
  - Non-combusting
- Nano-particle laden flows
  - Occupational Health
  - Explosion
- Fluid-Structure Interaction – CFD and FEA
- Two-phase/multi-phase flows
- Phase transition

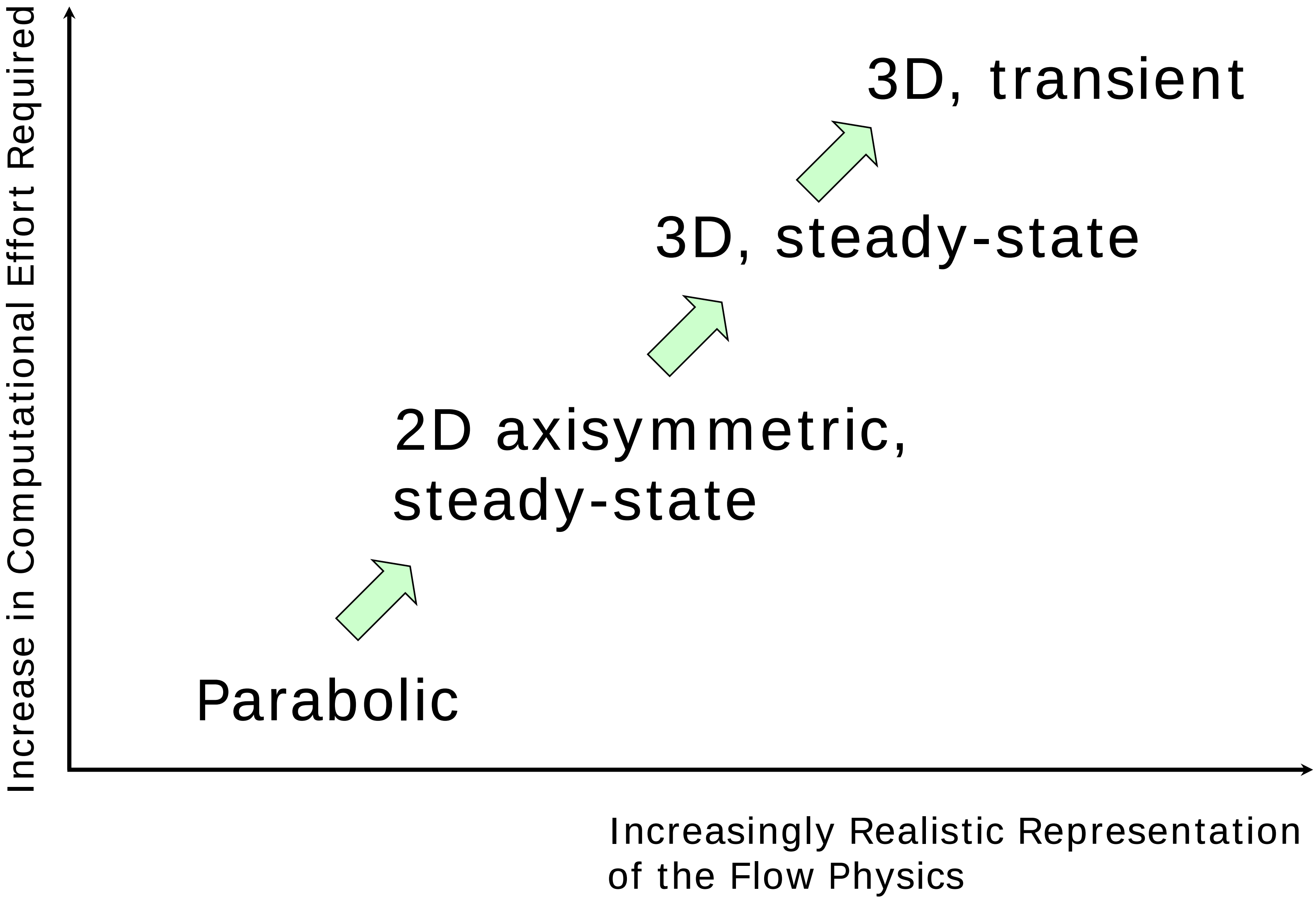
Challenges – 1



Challenges – 2

- DDT
- Deposition
- Deflagration
- Ignition
- Phase transition
- Two-phase and multi-phase flows
- And combinations of the above

Progression



Types of Models

- Empirical correlations – derived from a large number of experiments
- Simple models – may involve solving a set of ODEs for mass, momentum, etc.
- Statistical models
- CFD – realistic representation of the flow, but still broadly based on empirical data

Or Direct Numerical Simulation which means that all relevant length and time scales are resolved ⟹ No Modelling!!!

Turbulence Modelling

- k-ε model
  - Launder, Spalding, Harlow, … (1967-ish)
- k-ω
  - Wilcox (1985?)
  - Menter (1992)
- LES
  - Schumann (1975)
- RSTM
  - Hanjalic and Launder (1972, 1976)
  - Launder, Reece and Rodi (1975)

Evolution – Turbulence (1)

- 1989
  - Two-equation Eddy Viscosity models
    - Variations on the k-ε model theme
    - Variations on the k-ω model theme
  - Second moment closures (rarely)
    - Reynolds stress transport models
    - Algebraic Reynolds stress transport model
- 1999
  - Two-equation Eddy Viscosity models
    - Variations on the k-ε model theme
    - Variations on the k-ω model theme
  - Second moment closures (rarely)
    - Reynolds stress transport models
    - Algebraic Reynolds stress transport model

Evolution – Turbulence (2)

HEALTH & SAFETY LABORATORY

- 2009
  - Two-equation Eddy Viscosity models
    - Variations on the k-ε model theme
    - Variations on the k-ω model theme
  - Large Eddy Simulations (LES)
    - Standard/Dynamic Sub-Grid Scale model
    - Detached Eddy Simulation (DES)
    - Scale Adaptive Simulation (SAS)
  - Second moment closures (very rarely)
    - Reynolds stress transport models
    - Algebraic Reynolds stress transport model

Combustion Modelling – 1

- Eddy BreakUp model (P)
  - Spalding (1972)
- Eddy Dissipation Concept Model (NP)
  - Magnussen and Hjertager (1976)
- Laminar Flamelets – Non-Premixed
  - Bilger and others (late 1970s)
- Laminar Flamelets – Premixed
  - Moss, Bray and Libby and others (late 1970s)

Definitions – NP: Non-Premixed, P: Premixed, pP: Partially Premixed

Combustion Modelling – 2

HEALTH & SAFETY LABORATORY

- Flame speed correlations (P)
  - Bradley and others (late 1970s)
- Transported PDF (Detailed/Reduced Chemical Kinetics) (NP)
  - Pope, Jones and Kollmann, and others (mid-1980s)
- Transported PDF (Detailed/Reduced Chemical Kinetics) (P)
  - Pope and others (late 1990s)

Definitions – NP: Non-Premixed, P: Premixed, pP: Partially Premixed

Evolution – Combustion (1)

- 1989
  - Eddy Break-Up/Eddy Dissipation models (P/NP)
  - Laminar flamelets with prescribed PDF (P/PN)
  - Conditional Moment Closure (NP)
  - Reduced kinetics with transported PDF (NP)
- 1999
  - Eddy Break-Up/Eddy Dissipation models (P/NP)
  - Flame speed correlations (P)
  - Laminar flamelets with prescribed PDF (P/NP)
  - Conditional Moment Closure (NP)
  - Reduced kinetics with transported PDF (P/NP)

Definitions – NP: Non-Premixed, P: Premixed, pP: Partially Premixed

Evolution – Combustion (2)

- 2009
  - Eddy Break-Up/Eddy Dissipation models (P/NP)
  - Flame speed correlations (P)
  - Zimont model (pP)
  - Detailed kinetics with transported PDF (P/NP)
  - Conditional Moment Closure [CMC] (NP)

The combustion models used in academia are usually more advanced than those used routinely in industry

Definitions – NP: Non-Premixed, P: Premixed, pP: Partially Premixed

Evolution – Radiation (1)

- 1989
  - Optically thin / Optically thick assumption
  - P1
  - Four-flux and six-flux model
  - Discrete Ordinate model
  - Discrete Transfer model
- 1999
  - Optically thin / Optically thick assumption
  - P1
  - Four-flux and six-flux model
  - Discrete Ordinate model
  - Discrete Transfer model

Evolution – Radiation (2)

- 2009
  - Discrete Ordinate model
  - Discrete Transfer model
  - Monte Carlo
  - Optically thin / Optically thick assumption
  - P1
  - Four-flux and six-flux model
  - With grey gas, mixed grey gas or narrow-band model

Quality and Trust

- Verification
  - Models
    - Right equations
    - Right terms
  - Coding
- Validation
- Application of appropriate mathematical tools
  - Include all important physical processes
  - Right models
- Degree of uncertainty
  - Uncertainties in the input
  - Uncertainties in the modelling
- Best Practice Guidance
  - Generic
  - Application specific
- Training
  - Academic (MSc/PhD?)
  - Specific training on using the mathematical tools
- Proper documentation of the simulations
  - Assumptions
  - Parameter settings, mesh
- Sensitivity analysis
  - Mesh resolution
  - Time step
  - Ray/photon dependence

Future Direction – 1

HEALTH & SAFETY LABORATORY

- Turbulence models
  - Two-equation turbulence models, such as the *k*-ω and the *k*-ε models will find continued extensive use
  - LES/DES/SAS will become more widely used, especially for fire modelling
  - Reynolds stress models (and algebraic Reynolds stress models) may be used to model specific scenarios
- Combustion models
  - Eddy Break-Up model and Eddy Dissipation Concept models will still be used
  - Laminar flamelets with prescribed or transported PDF are unlikely to replace EBU/EDC models
  - Detailed/Reduced kinetics with transported PDF
  - CMC – interesting for non-premixed combustion, but not making great inroads as yet

Future Direction – 2

- Radiation models
  - Discrete Transfer Model and Discrete Ordinate Model are sufficiently sophisticated in many situations
  - Monte Carlo method is applicable to all scenarios

Issues to Consider

- Characterisation of the source term
- Parameter values
- Boundary conditions
- Representing atmospheric conditions
  – Stable
  – Unstable
- Long transient simulations
- Experimental data
  – Lack of data
  – Uncertainty re. what was actually measured
  – Ambient and initial conditions

Other Remedies – 1

- Moore's Law – doubling of the number or transistors on a microchip every 2 years
  - Constraints by physics
  - Manufacture of chips more difficult
  - Cooling issues
  - Current projections are that Moore's Law will apply for another decade
- Parallel processing
  - Improved chip architecture
  - Better algorithms

Other Remedies – 2

- Adaptive Mesh Refinement and De-refinement

HEALTH & SAFETY LABORATORY

Thank You for your attention!

Any Questions?