## **ATKINS**

# Dense gas dispersion for LNG plant

#### ... some recent findings

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#### **Overview**

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- Introduction
- Dense gas dispersion why is this unusual?
- What does "validation" mean ...
- How well does CFD model dense gas dispersion?
- Conclusions ... ending with a question

#### Introduction – context for this talk

- Liquefied Natural Gas (LNG) is a booming market now.
- Large numbers of LNG plant are in design & construction around the world.









- UKELG, 18/10/12, slide 3

#### Introduction – context for this talk

- Assessment is required of these plant to gauge hazards to:
  - personnel working on the plant
  - public beyond the plant perimeter
  - the plant itself
- Wide range of consequence modelling is undertaken:
  - typically with integral or "box models"
  - ... but increasingly with CFD.





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#### Introduction – context for this talk

- **NTKINS**
- In an LNG plant, there are large inventories of cold and heavy gases
- So many of the accidental releases are dense vapours:

Material	Temperature	Molecular weight (kg/kmol)	Specific gravity (cf. ambient air)
LNG	~ -162ºC	18.5	1.7
LPG	~ -42°C to -1°C	44 – 58	2 – 2.2
Refrigerant	e.g50°C	e.g. 30	1.4

#### Dense gases – why so special?

• Density gradients in a flow can have significant impact on the turbulence in the flow:



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Cowan & Britter (1994)

#### Stable stratification – energy sink term

• Energy budget (with boundary layer approximation):



 $\mathcal{B} = q\overline{\rho v}/\rho_0$  is the buoyancy consumption term  $\frac{1}{2}\overline{q^2} = \frac{1}{2}\overline{u_i^2}$  is the turbulent kinetic energy

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#### Stable stratification – energy sink term

• Energy budget (with boundary layer approximation):

TKE
$$\frac{\partial_{\frac{1}{2}}\overline{q^{2}}}{\partial t}$$
= $\mathcal{P}$  $\mathcal{B}$  $\mathcal{E}$  $\mathcal{A}$  $\frac{\partial}{\partial y} \left( \frac{1}{2} \overline{q^{2} v} + \frac{\overline{pv}}{\rho_{0}} \right)$ Horizontal  
Re stress $\frac{\partial_{\frac{1}{2}}\overline{u^{2}}}{\partial t}$ = $\mathcal{P}$  $+$  $\Psi_{11}$  $\mathcal{E}_{11}$  $\mathcal{A}_{1}$  $\frac{\partial_{\frac{1}{2}}\overline{u^{2} v}}{\partial y}$ Vertical  
Re stress $\frac{\partial_{\frac{1}{2}}\overline{v^{2}}}{\partial t}$ = $-\mathcal{B}$  $+$  $\Psi_{22}$  $\mathcal{E}_{22}$  $\mathcal{A}_{2}$  $\frac{\partial}{\partial y} \left( \frac{\overline{v^{3}}}{2} + \frac{\overline{pv}}{\rho_{0}} \right)$ 

$$\mathcal{P} = -\overline{uv}\partial\overline{U}/\partial y$$
 is the production term  
 $\mathcal{B} = g\overline{\rho v}/\rho_0$  is the buoyancy consumption term  
 $\frac{1}{2}\overline{q^2} = \frac{1}{2}\overline{u_i^2}$  is the turbulent kinetic energy

• Anisotropy increases with stability :  $\sqrt[n]{-uv} / k (\sim C_{\mu}^{\frac{1}{2}})$ 

#### Research in dense gas dispersion

- Is prodigious and long-established!
- For example (to name just a few):
  - Britter (1974), McQuaid (1976)
  - Maplin Sands and Burro full-scale trials (1980)
  - Wheatley & Webber review (1985)
  - Britter McQuaid workbook, HSE (1988)
  - König-Langlo & Schatzmann wind tunnel tests (1990)
  - Cleaver review paper (2007)
  - Ivings et al (2007) HSE report



#### What does "validation" mean?

- Press article from one of the Commercial CFD code vendors:
  - Code X has been "validated" against 33 dense gas experiments
  - Scenarios that can be modelled using X include ... dispersion from LNG spills
- This code is based on a simple linear-EVM k-epsilon turbulence closure model.
- Validated?
- Really?

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#### Simple test case

- Ljuboja and Rodi (1980)
  - 2D jet spreading along a wall lab tests
  - Isothermal (constant density) case:
    - similarity arguments can prove: b ~ X
  - Increasing stability:
    - reduced turbulence levels
    - reduced entrainment
    - reduced spreading rate





#### Can CFD reproduce this?

- Start with isothermal case
  - actually fairly challenging
  - presence of wall damps vertical turbulence
  - linear growth well captured, though
  - results broadly acceptable

Closure scheme	Spread rate cf. expts	
Std k-ε	+22%	
Non-lin. k-ε	+15%	
RSM	+15%	
V2F	+3%	
k-ω SST	-5%	



#### Can CFD reproduce this?

- How about stably stratified cases?
- All available closure models in commercial CFD codes: unabashed linear jet growth.
- Significant under-prediction of hazards from this scenario.
- None can reproduce the "stabilising" effect of the stratification.



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### Why is CFD struggling here?

- Standard turbulence closure models are missing the key physics
- ... the stabilising effect of the dense gas.
- Closure model needs to:
  - Allow for anisotropy
  - Reduce vertical diffusivity
  - Dampen turbulence production rate
- These features are not present in standard isotropic gradient diffusion eddy viscosity models.

### Why is CFD struggling here?

- Solutions:
  - Algebraic stress model is a cheap way forward:
    - eddy viscosity model with constants (C<sub>μ</sub>, σ<sub>t</sub> etc) that change with stability e.g. Ljuboja & Rodi (1980)
  - Full Reynolds stress model (6 stresses + 3 scalar fluxes)
- Also, but impractical:
  - LES (but not DES ... unless based on above ASM)



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#### Conclusions

- Standard CFD closure models cannot reproduce the stabilising effect of density gradients.
- These will provide non-conservative predictions of gas concentration in the mid to far-field.
- For correct prediction:
  - an advanced closure model must be used,
  - that accounts for turbulence anisotropy
  - and the dampening effect of stability.
- None of the commercial codes currently provide this.
- Despite this, some codes are "validated" for these flows what does this mean?