COMPUTATIONAL FLUID DYNAMICS STUDY ON TWO-PHASE CO_2 DISPERSION IN A NEUTRAL ATMOSPHERE

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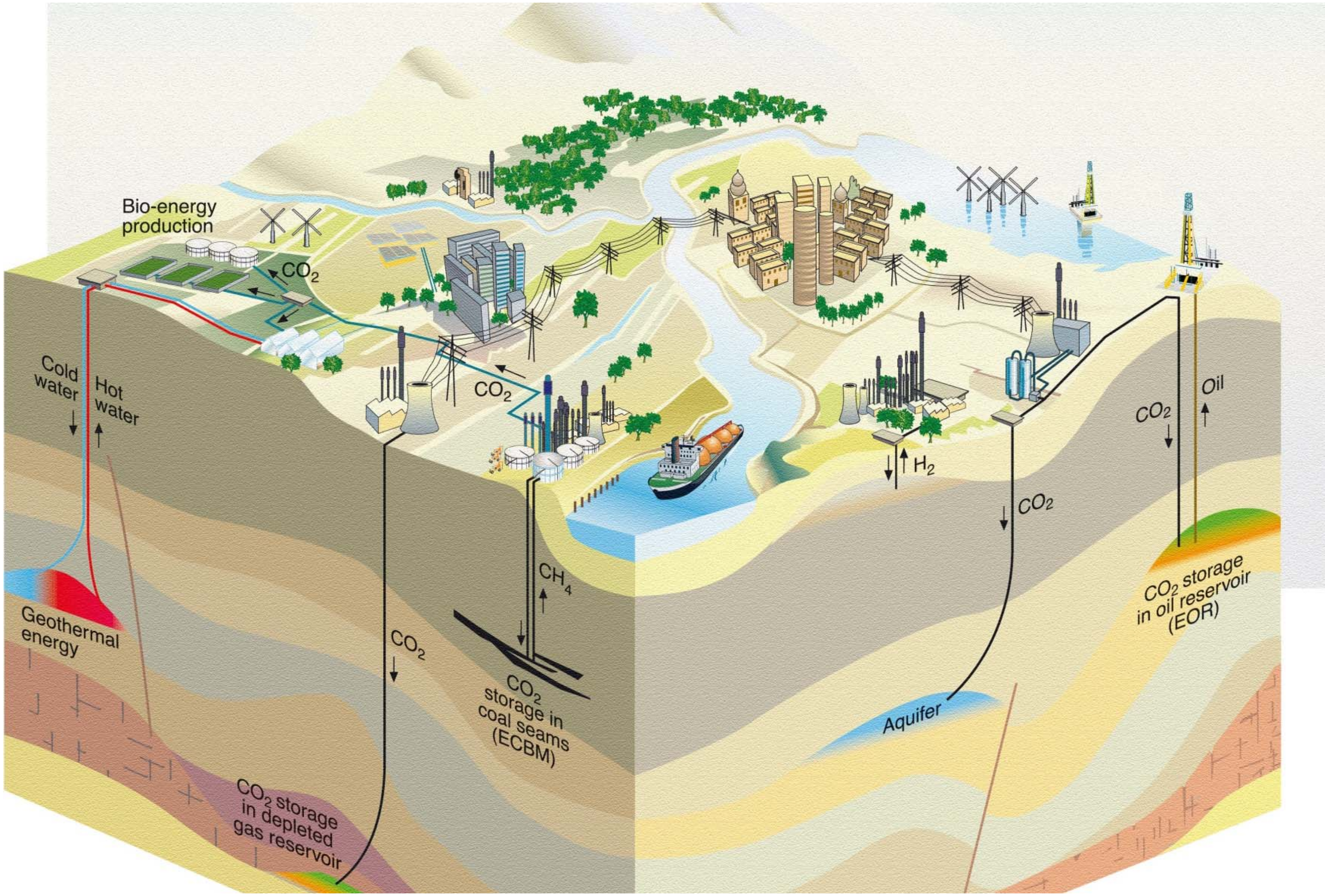
CCS – Carbon Capture and Storage



Toxicity properties of CO_2

Exposure time (min)	1% lethality (vol% CO_2)	50% lethality (vol% CO_2)
1	11	15
10	8	11
30	7	9
60	6	8

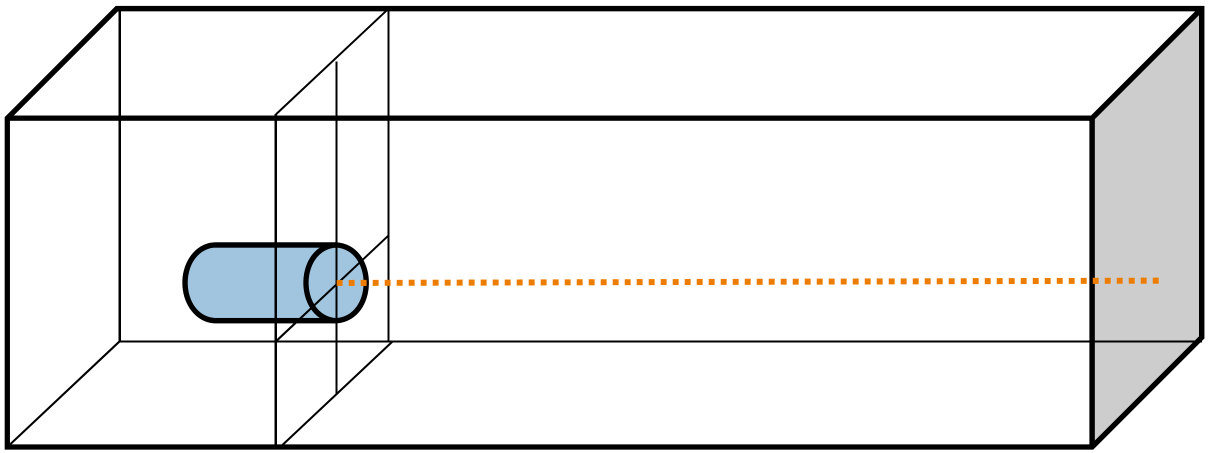
Source: S. Connolly and L. Cusco, Hazards from high pressure carbon dioxide release during carbon dioxide sequestration processes, Proc. Int. Symp. Loss Prevention and Safety Promotion in the Process Industry, Edinburgh, 22-24 May 2007

CFD in atmospheric conditions

- Pre-requisite: correctly describe Atmospheric Boundary Layer (ABL) behaviour over domain:
  - Velocity
  - Turbulence
  - Temperature & pressure (non-neutral ABL)

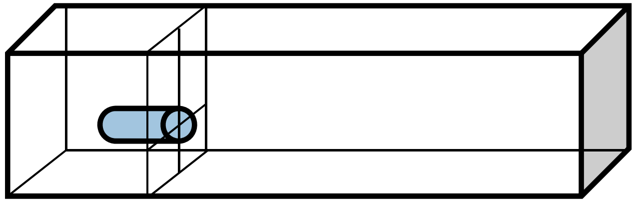
- Recommendations from COST 732 (neutral ABL,RANS)
  - Computational grid
  - Domain extent and blockage
  - Boundary conditions

Case Description



Test-case: small scale release
Comparison-case: large scale release

Test case



Domain size:	300x100x50 m^3
Source location:	1 m height
Initial pressure:	100 bar
Initial temperature:	15 °C
Source mass flow rate:	33 kg/s
Source diameter:	5 cm
Source temperature:	293 – 195 K
Source solid fraction:	0 – 50 mass%

Fluent v12.1

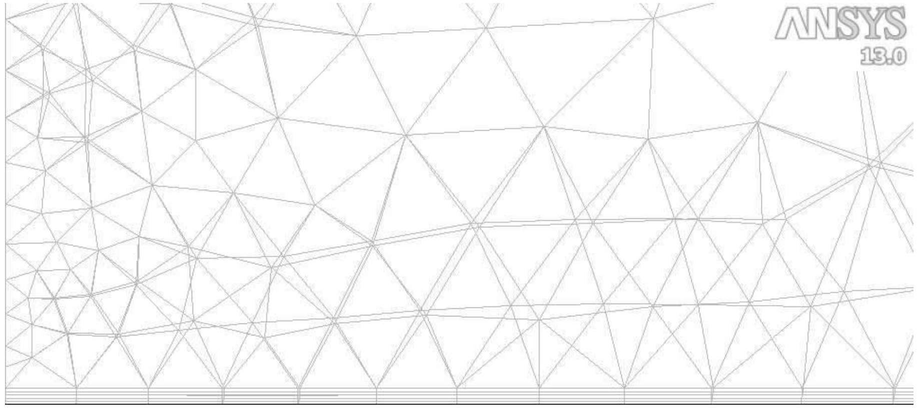
2-phase model:
Discrete Phase Model

Turbulence model: standard kε

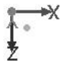
Cell sizes:	3 cm^3 - 120 m^3
Number of cells:	135 000

Boundary conditions:

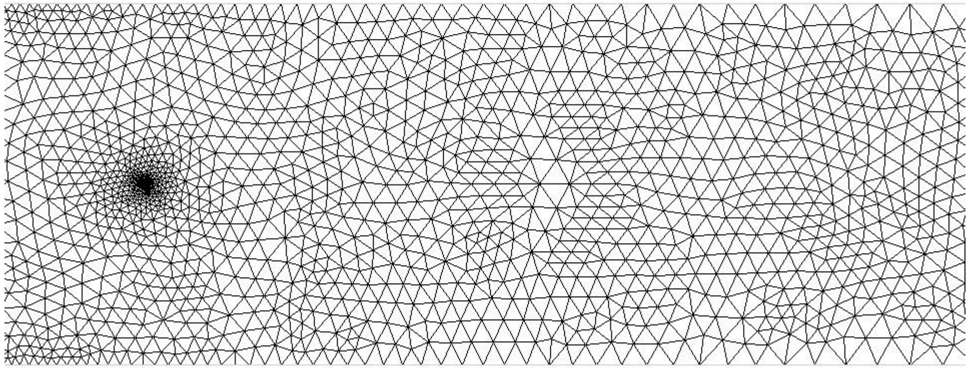
- Sides: symmetry planes
- Top: wall
- Inflow: velocity inlet
- Outflow: pressure outlet
- Bottom: wall with wall functions



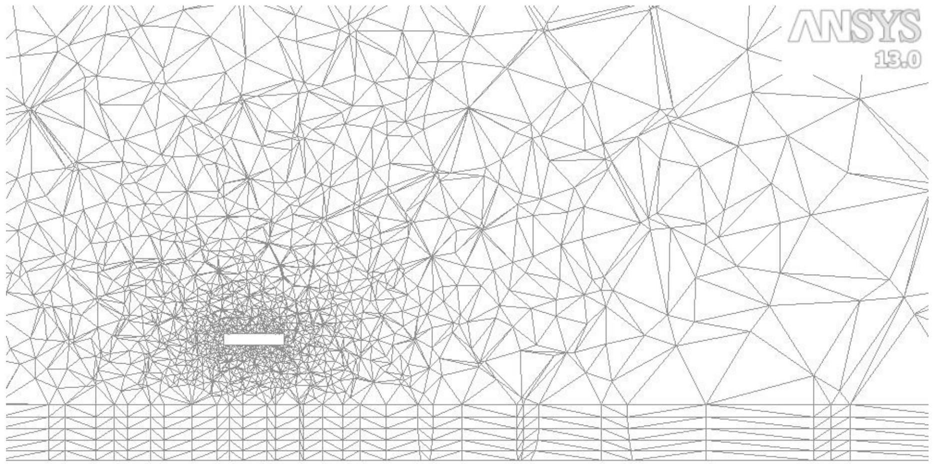
Mesh

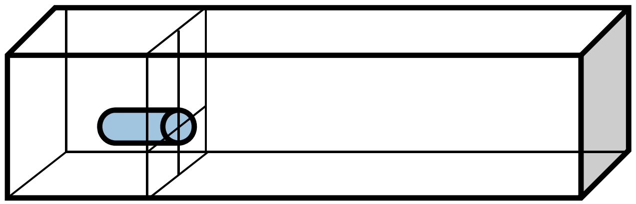


Bottom mesh



Mesh – side view






Variations in test case

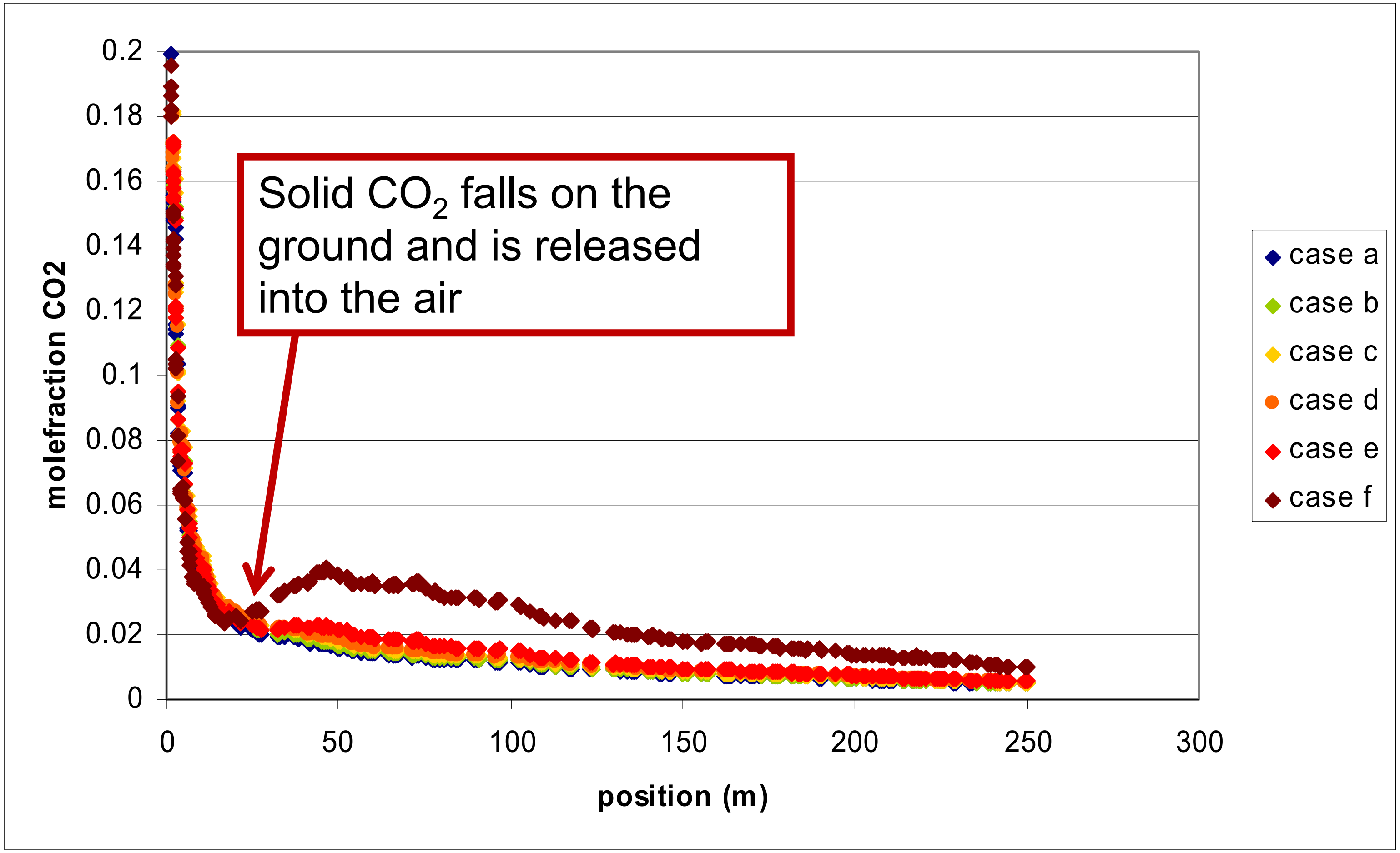
Several fraction of solid are used:

	Type of release	T (K)	%mass of solid
A	Gas	293	-
B	Gas	250	-
C	Gas	195	-
D	Gas + solid	195	1
E	Gas + solid	195	10
F	Gas + solid	195	50

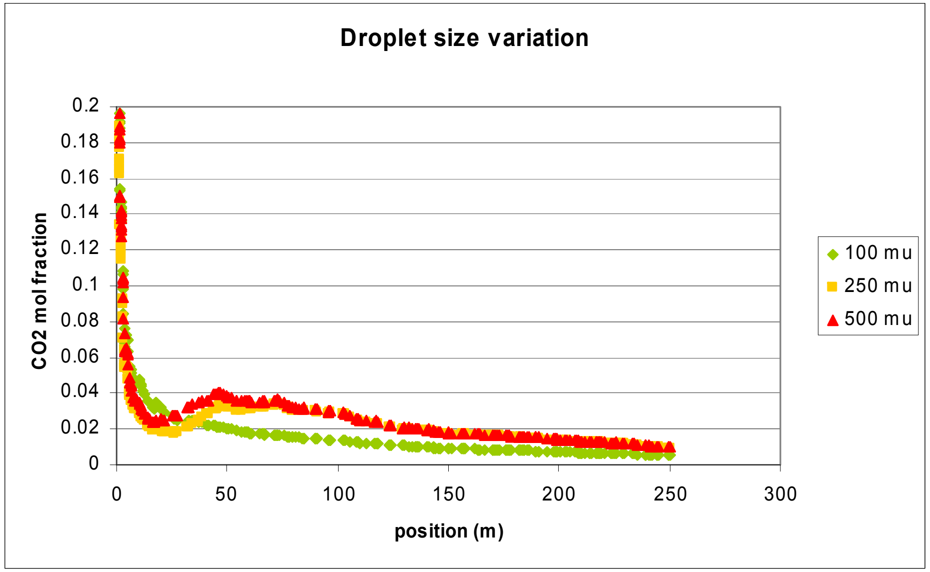
With case F sensitivity studies are performed on the presence of solid particles:

wall boundary conditions
particle size
gravity

CO_2 mole fraction for cases a-f

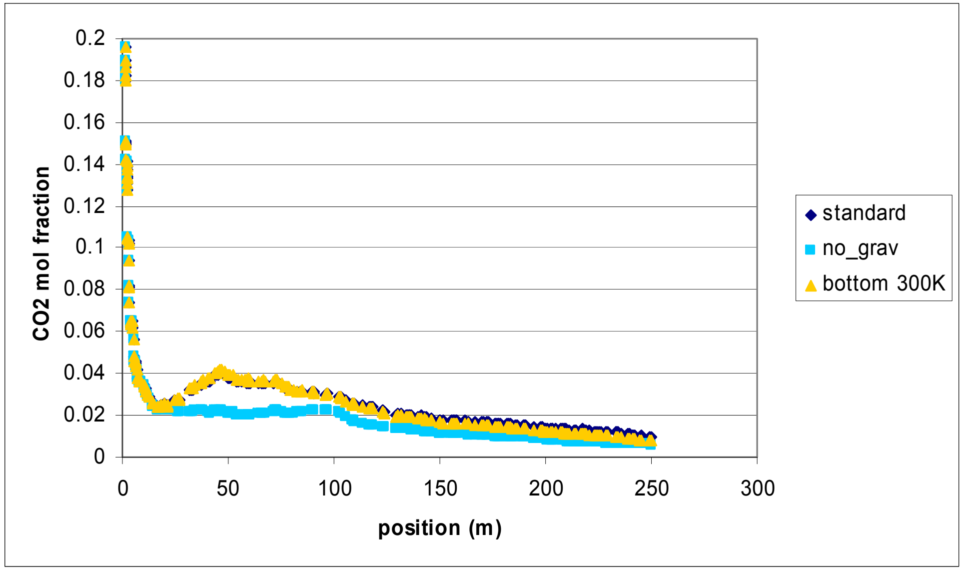


Variations for sensitivity analysis

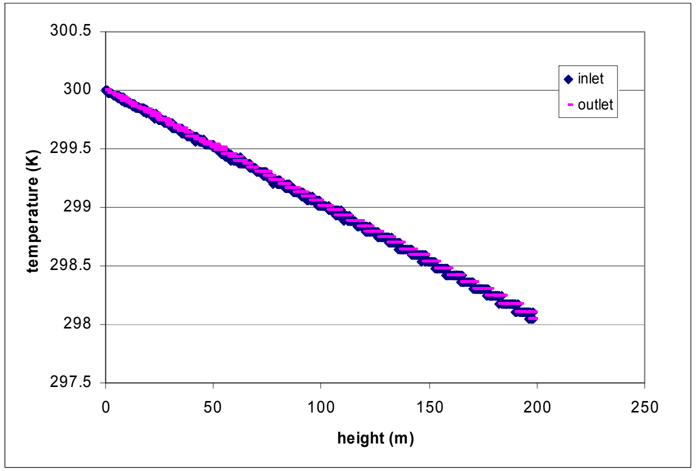


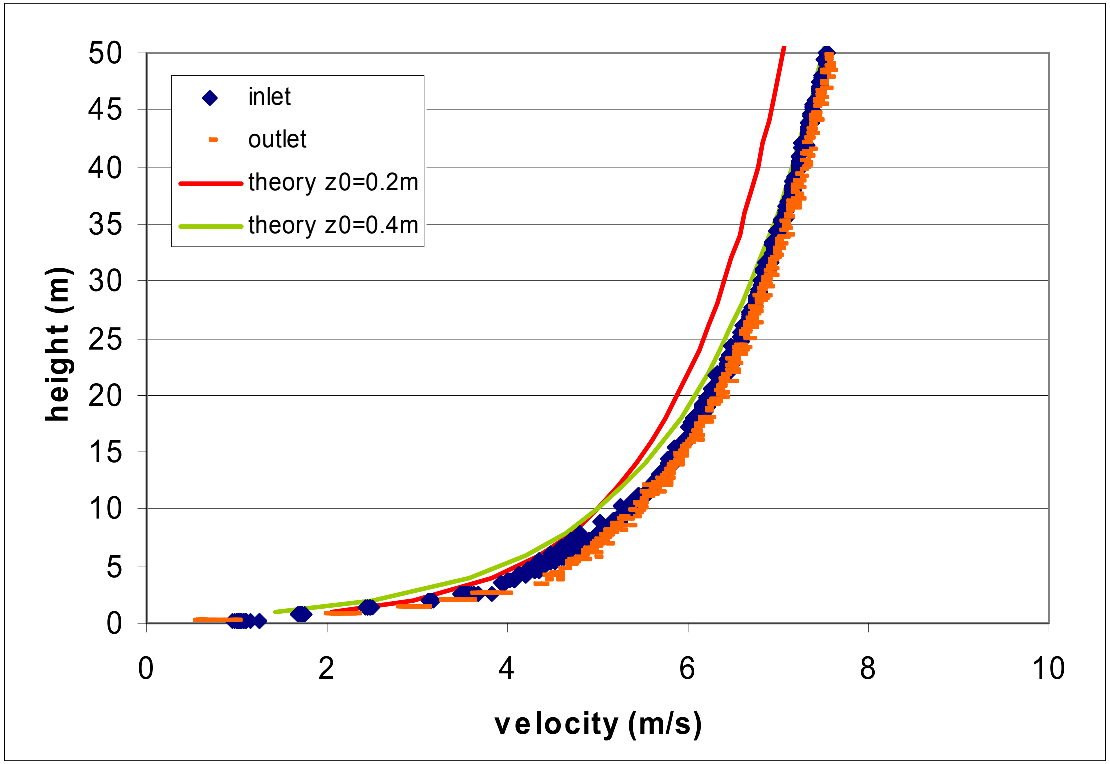
100 µm droplets do not rain out

Without gravity no rain out



Atmospheric Boundary layer: D5

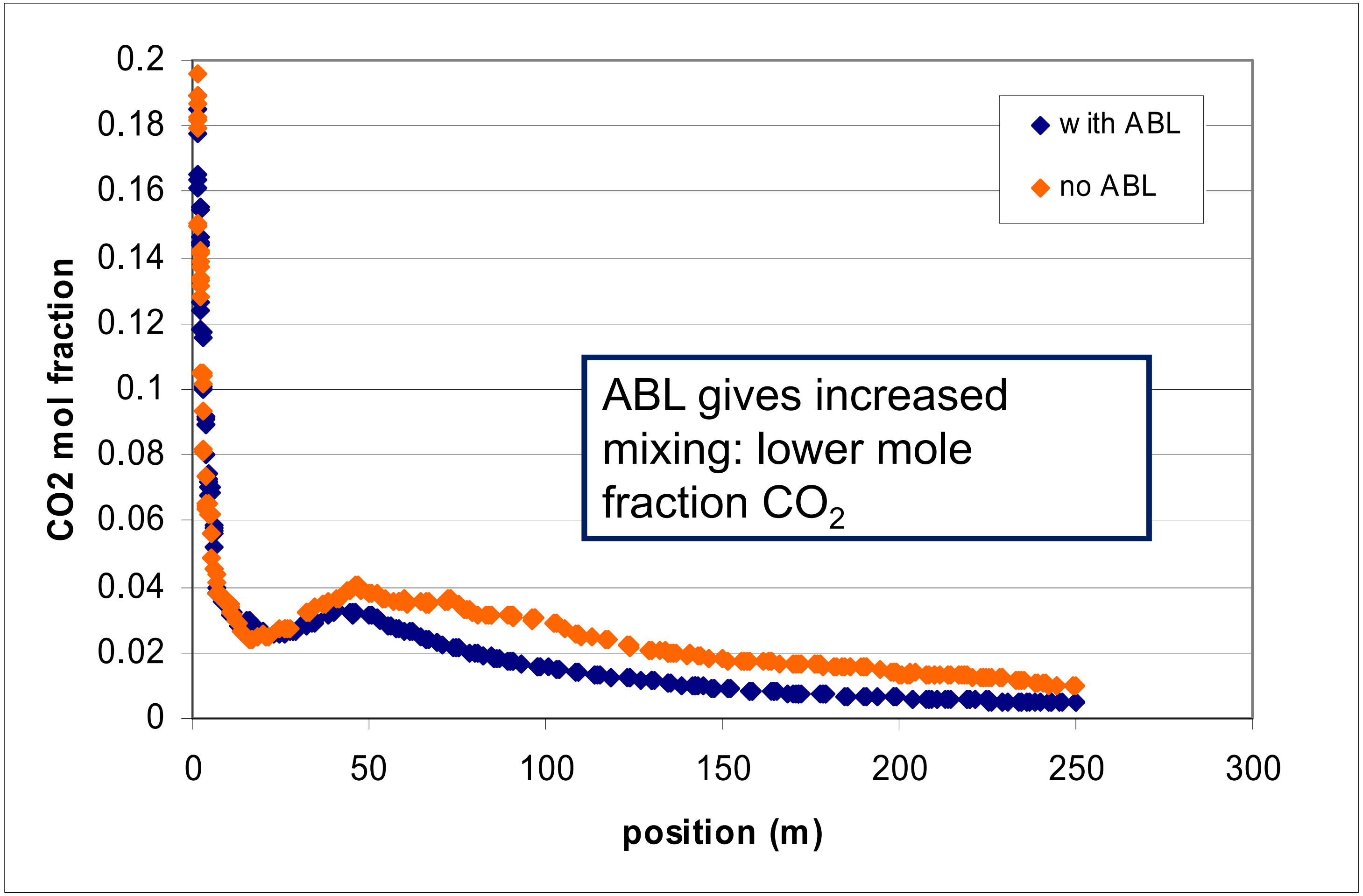




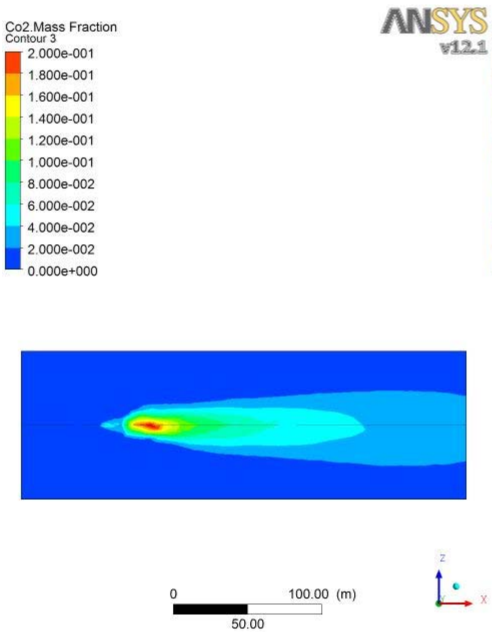
- 2D ABL periodic conditions
- 3D ABL: 2D result at inlet

- Inlet = outlet velocity and temperature profile in 3D
- 2D profile 10% off from theoretical profile, increase mass flow will resolve this

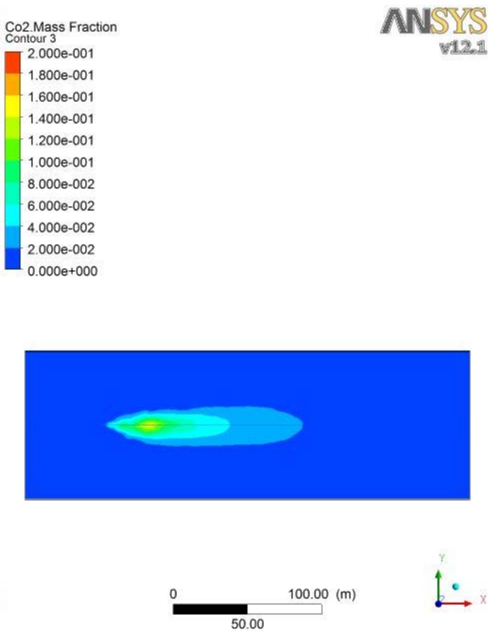
Effect of ABL-modelling on concentration



Top view of CO_2 mass fraction contours

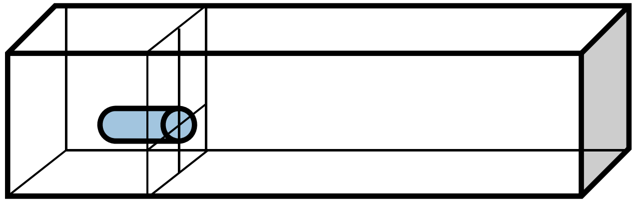


Uniform inlet velocity



D5 ABL

Comparison case



Domain size:	800 x 400 x 200 m^3
Source location:	5 m height
Initial pressure:	150 bar
Initial temperature:	20 °C
Source mass flow rate:	5628 kg/s
Source diameter:	298 cm
Source temperature:	195 K
Source solid fraction:	0 and 64.4 mass%

Fluent v12.1

2-phase model:
Discrete Phase Model

Turbulence model: standard kε

Cell sizes:	3 10^{-3} – 5 10^3 m^3
Number of cells:	175 000

Source: T.A. Hill, J.E. Fackrell, M.R. Dubal, S.M. Stiff, Understanding the consequences of CO_2 leakage downstream of the powerplant, Energy Procedia (2010)

Boundary conditions:

- Sides: symmetry planes
- Top: velocity inlet
- Inflow: velocity inlet
- Outflow: pressure outlet
- Bottom: wall with wall functions

Resulting volume%

	Fluent vapour	Fluent 150 µm
200 m	8.9 %	10.4 %
300 m	6.6 %	7.1 %
400 m	5.2 %	5.3 %

- Including particles increases effect distances

Resulting volume%

	Fluent vapour	Fluent 150 µm	CFX vapour	CFX 50 -150 µm
200 m	8.9 %	10.4 %	15.5 %	18.6 %
300 m	6.6 %	7.1 %	11.0 %	12.1 %
400 m	5.2 %	5.3 %	8.2 %	8.1 %

- Including particles increases effect distances (Fluent and CFX)
- No experimental data available for validation

Source Phast and CFX data: T.A. Hill, J.E. Fackrell, M.R. Dubal, S.M. Stiff, Understanding the consequences of CO_2 leakage downstream of the powerplant, Energy Procedia (2010)

Resulting volume%

	Fluent vapour	Fluent 150 μm	CFX vapour	CFX 50 -150 μm	Phast
200 m	8.9 %	10.4 %	15.5 %	18.6 %	11.3 %
300 m	6.6 %	7.1 %	11.0 %	12.1 %	8.1 %
400 m	5.2 %	5.3 %	8.2 %	8.1 %	6.4 %

- Including particles increases effect distances (Fluent and CFX)
- No experimental data available for validation
- CFX over estimates with respect to Phast, Fluent underestimates with respect to Phast

Source Phast and CFX data: T.A. Hill, J.E. Fackrell, M.R. Dubal, S.M. Stiff, Understanding the consequences of CO_2 leakage downstream of the powerplant, Energy Procedia (2010)

Differences in CFD calculations

- Particle size (single value or distribution)
- Description ABL
- Level of turbulence in jet

Conclusions

- Method is shown to perform CFD on dispersion of evaporating particles in atmospheric conditions
- Only verification with integral model and other CFD model is done: good comparisson
- Continue development of CFD for atmospheric dispersion