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Numerical Approach for flue gas CO2 capture in a supersonic nozzle

by Erwin George, Agathe Jarry , Mailys Pale and Samuel Saysset

Copenhagen

International Gas union Research Conference 2014

International Gas Union Research Conference

IGRC COPENHAGEN 2014

September 17-19

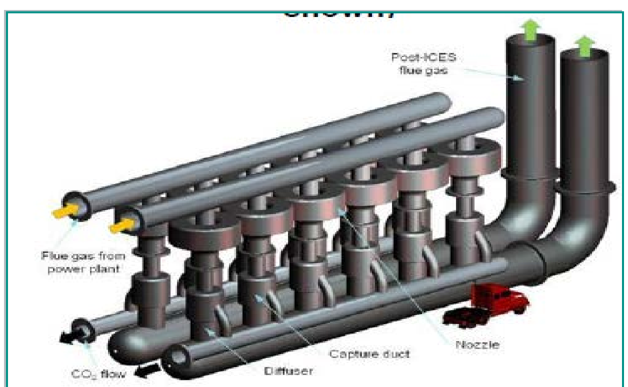
Gas Innovations Inspiring Clean Energy

Goal of this study :

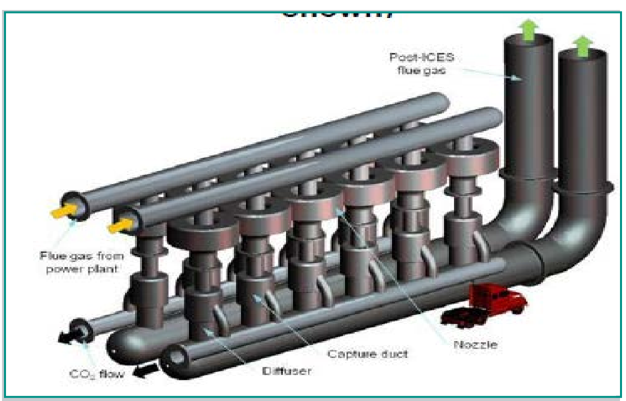
CRIGEN is involved in CO2 Capture technologies. Two particularly promising technical options using flue gas compression followed by expansion have been identified :

- **Fluidized Bed : A proportion of CO2 is first frozen in a FB, and the remainder during flue gas expansion in a turbine.**
- **Supersonic Expansion : CO2 is frozen and captured as flue gases are thoroughly cooled in an expansion nozzle operating at supersonic regime.**

⇒ Solution evaluated here



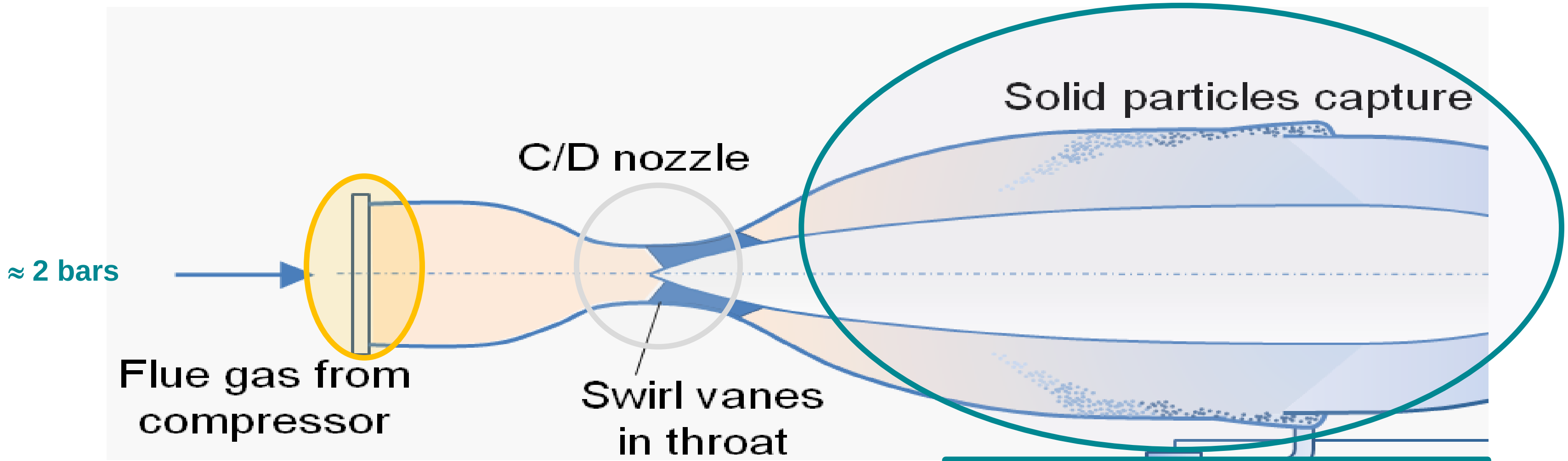
OUTLINE



- Context
- Technology concept, available information
- Goal of the study
- 1D numerical approach
- 2D approach based on 1D results
- 3D (CFD) modeling
- Conclusions and Prospects

NB : This study relies on data provided by ATK and ACEnT under confidentiality agreement with GDF SUEZ

Technology concept



Convergent ; **Mach < 1**
Subsonic regime

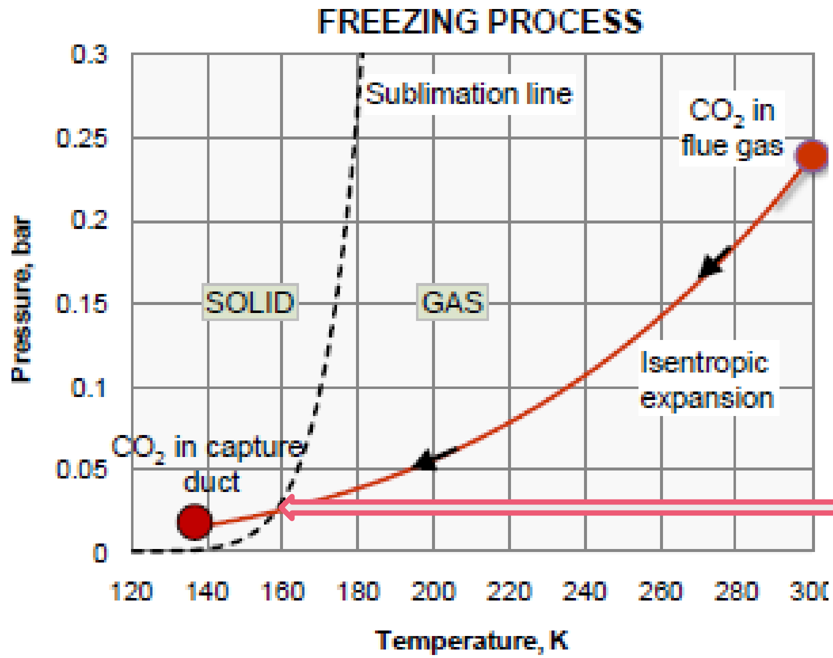
Throat ; **Mach = 1**
Transitional regime +
« shock waves »

Divergent ; **Mach →3-5**
- Rapid isentropic expansion
- CO_2 freezing starts
- CO_2 solid particles to capture

According to ATK and ACEnT,

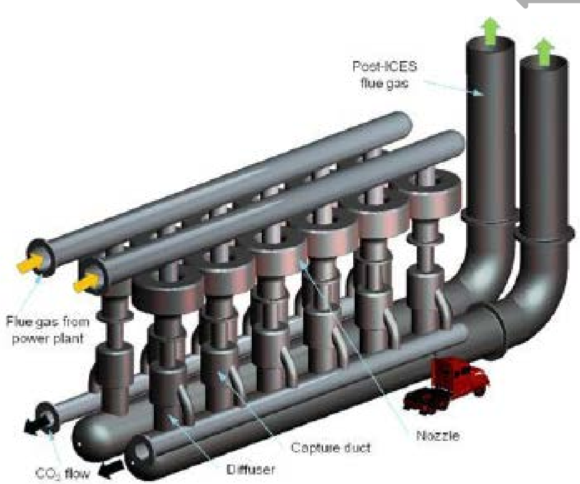
- Freezing starts at **-113°C ~ 0.2 bar (P_{tot})**
- Targeted nozzle conditions at the divergent outlet : **~-138°C ~ 0.07 bar (P_{tot})**
- CO_2 solid particle density is 10 times higher than the gas one : swirling stream would favor their recovery (centrifugal effect)

Concept of the Technology : Feasibility



Antisublimation starts

Stream direction



- Industrial Scale Concept – data from ATK and ACEnT

→**1.5 m supersonic nozzle diameter (C-D nozzle)**
- ✓**~ 45 MW_e**

→**Supersonic nozzle length would be below 5 m.**
- ✓**Moderate footprint of the facility**

→ **About 12 nozzles for a conventional coal power plant**

Goal of the study : does at it work as stated ?

→ To answer this question :

- **Check CO_2 frosting feasibility**
  - Does the system reach (P,T) conditions for which CO_2 would desublimate ?
  - How much CO_2 would desublimate ?
- **Check nozzle sizing provided by ATK and ACEnT**
- **Check the impact of shock waves on the nozzle performance**
  - How do shock waves induced by supersonic flow impact (P,T) conditions ?
    - → Are conditions for desublimation still reached ?
    - → Are there areas where CO_2 particles could sublimate again ?
  - Would CO_2 particles move to wall regions due to supersonic stream and shock waves interactions?
- **Check the impact of desublimation phenomenon on the nozzle performance**
  - How would the latent heat released by CO_2 desublimation impact on (P,T) conditions in the nozzle ?
  - How would the change in mass rate impact on (P,T) conditions in the nozzle ?

Modeling approach to answer these questions

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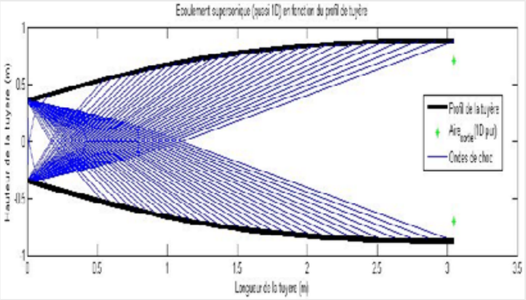
Level of accuracy

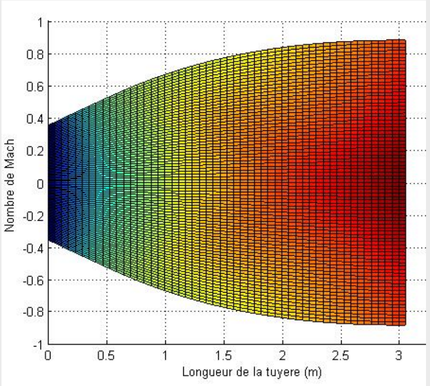
FUNDAMENTAL

APPLIED

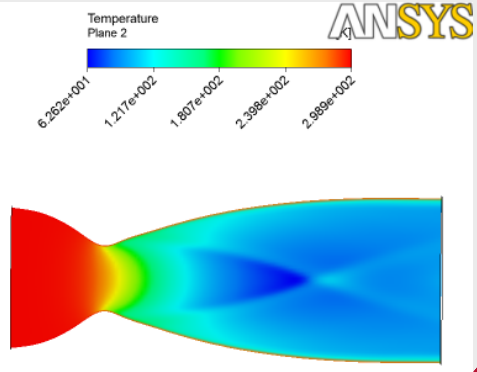
1D



2D



3D



Fundamental approach and feasibility

- Nozzle shape
- Rough sizing
- Sensitivity study on main operating parameters
- P,T, M profile → frosting ?

Identification of fluid heterogeneity

- Impact of shock waves
- Corrected (P,T,M) profile

→ Still frosting ?

One step towards full characterization

- Full 3D Euler-Euler approach
- Steady / unsteady phenomena

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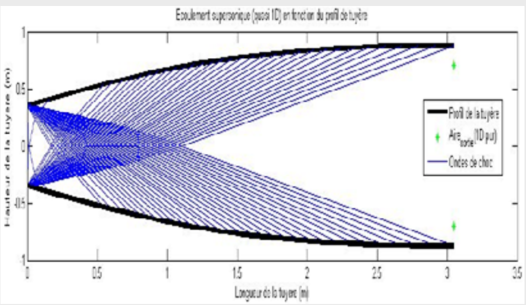
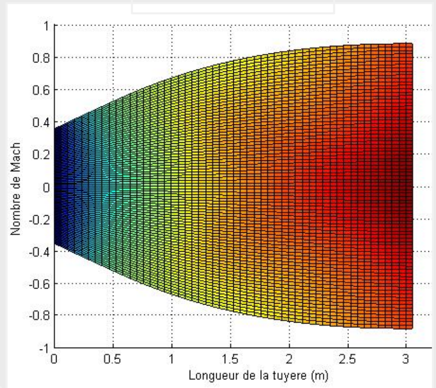
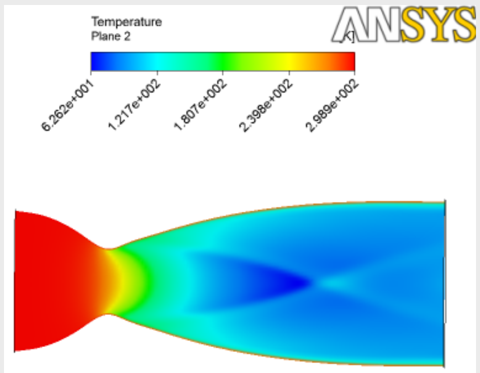


2D



3D



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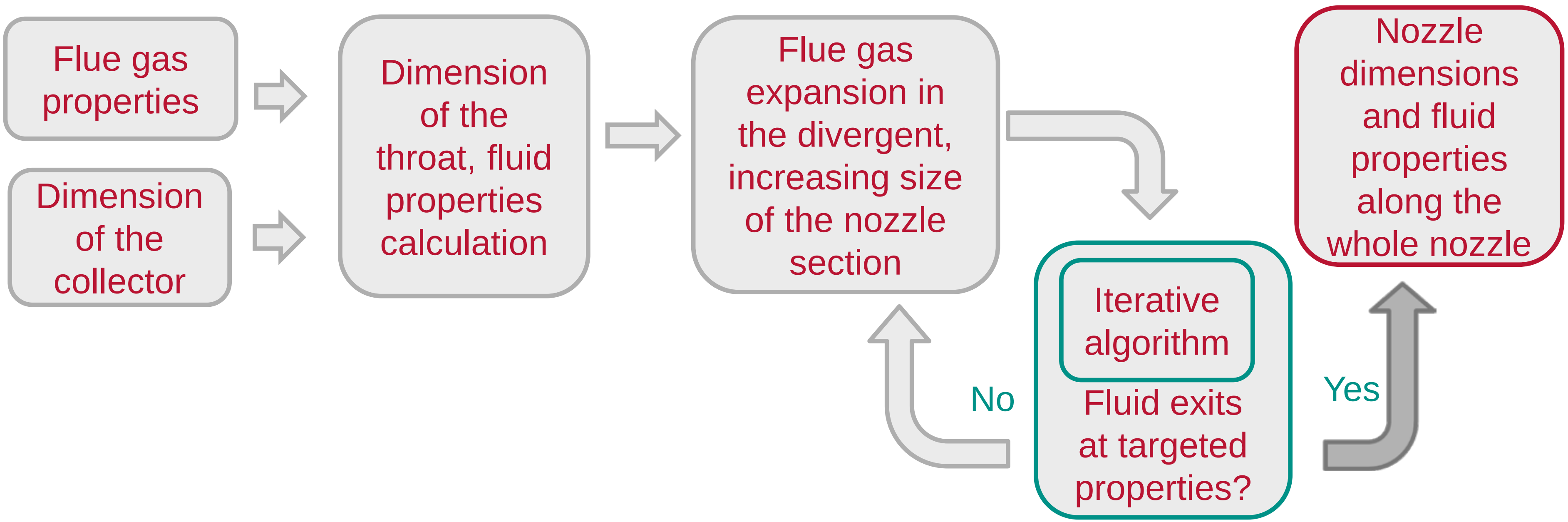
1D Numerical Approach : methodology

- **Matlab® program written at CRIGEN**
  - Estimates the maximum flue gas mass flow that could be treated
  - Calculates the nozzle dimensions with targeted exit properties (P, T)
  - Calculates the flow properties in the supersonic nozzle
  - Models shock waves starting from the throat : nozzle shape corrected within 1D approach

- **Methodology**



1D Numerical Approach : Hypothesis and Conditions

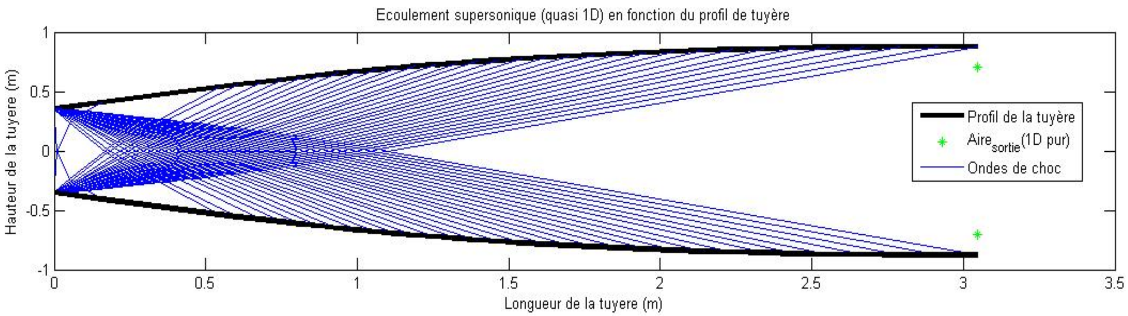
- **1D axis-symetrical computations**
- **Isentropic Compressible Flow with area change**
  - Andersen works for 1D and pseudo 2D (correction with shock waves locations)
- **Normal shock waves in the duct**
- **Flue gas (85%N_2 - 15%CO_2) treated as a perfect ideal gas**

- **Boundary conditions for flue gas at the inlet :**
  - Mass flow rate : 80 kg/s (~45MW_{eNet})
  - Temperature : 26°C
  - Pressure : 2 bar_{abs}
  - Diameter of collecting duct (before convergent) : 1.5 m

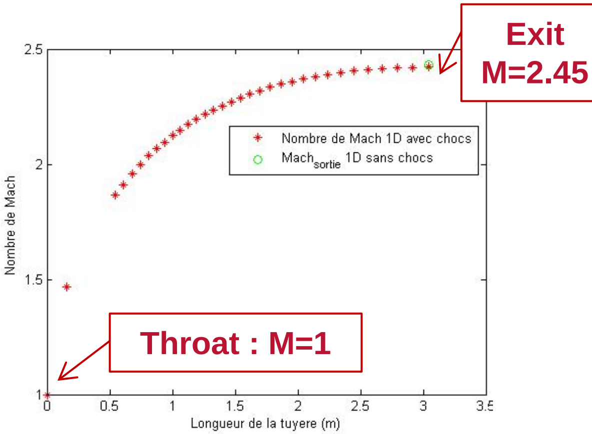
- **Boundary pressure condition for flue gas at the exit**
  - Pressure : 0.07 bar_{abs}

1D Numerical Approach : Results

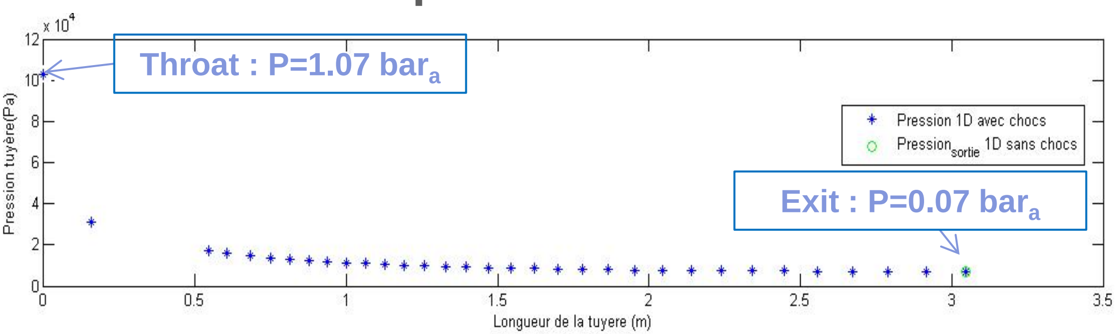
Shape of the nozzle and shock waves



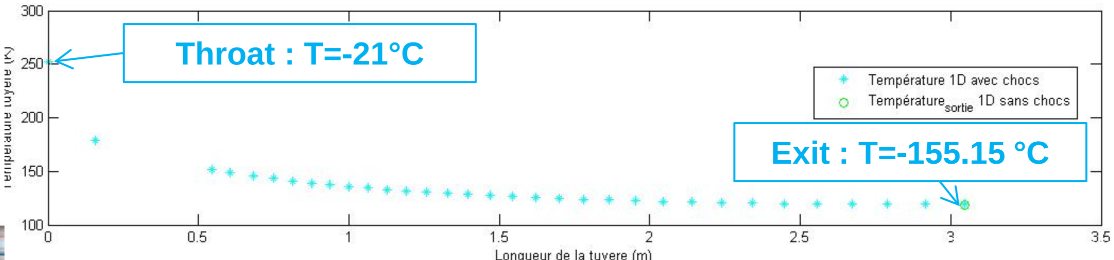
Mach Number



Pressure profile



Temperature profile

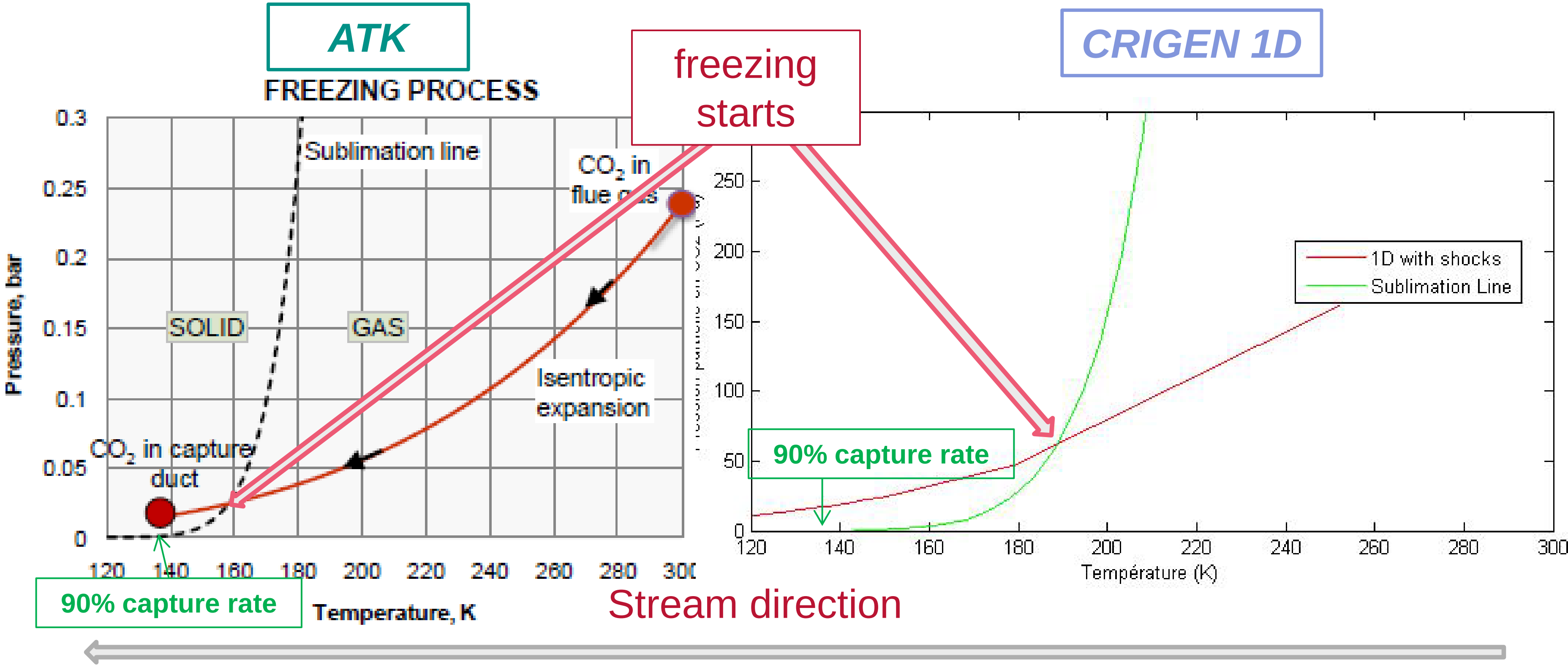


Computed dimensions in good agreement with targeted values for :

- nozzle dimensions,
- pressure level at the exit,
- temperature level for freezing feasibility

⇨ **Accurate location?**

1D Numerical Approach : CO_2 freezing?



- The feasibility seems achievable in CRIGEN's computed nozzle shape
- The location of the freezing starting point is about 7 cm after the sonic throat

  →good agreement with freezing measurement on ATK's lab-scale test facility

Modeling approach to answer these questions

Level of accuracy

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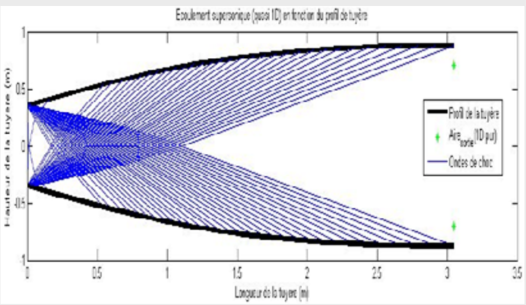
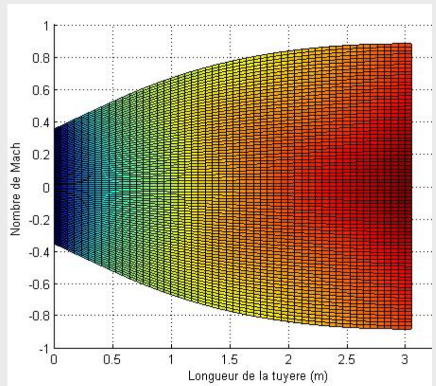
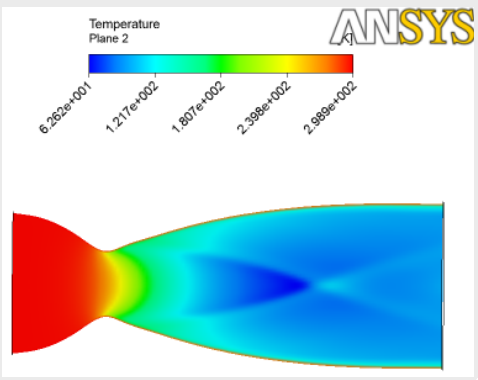


2D



3D



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→ Still frosting ?

One step towards full characterization

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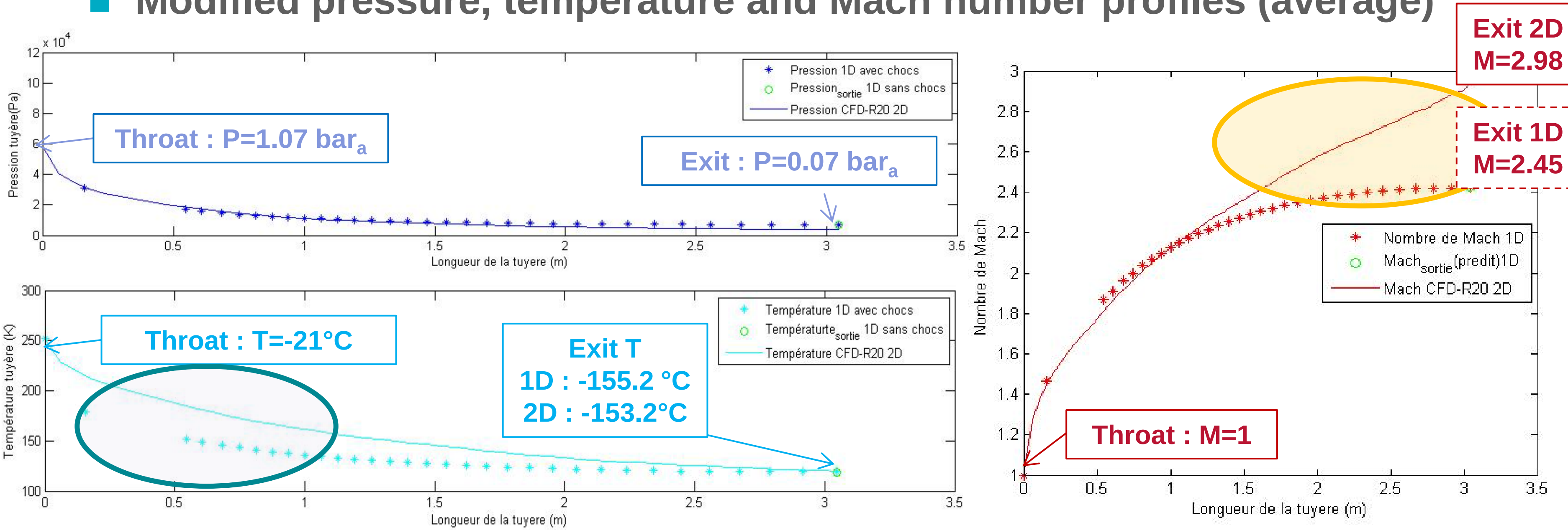
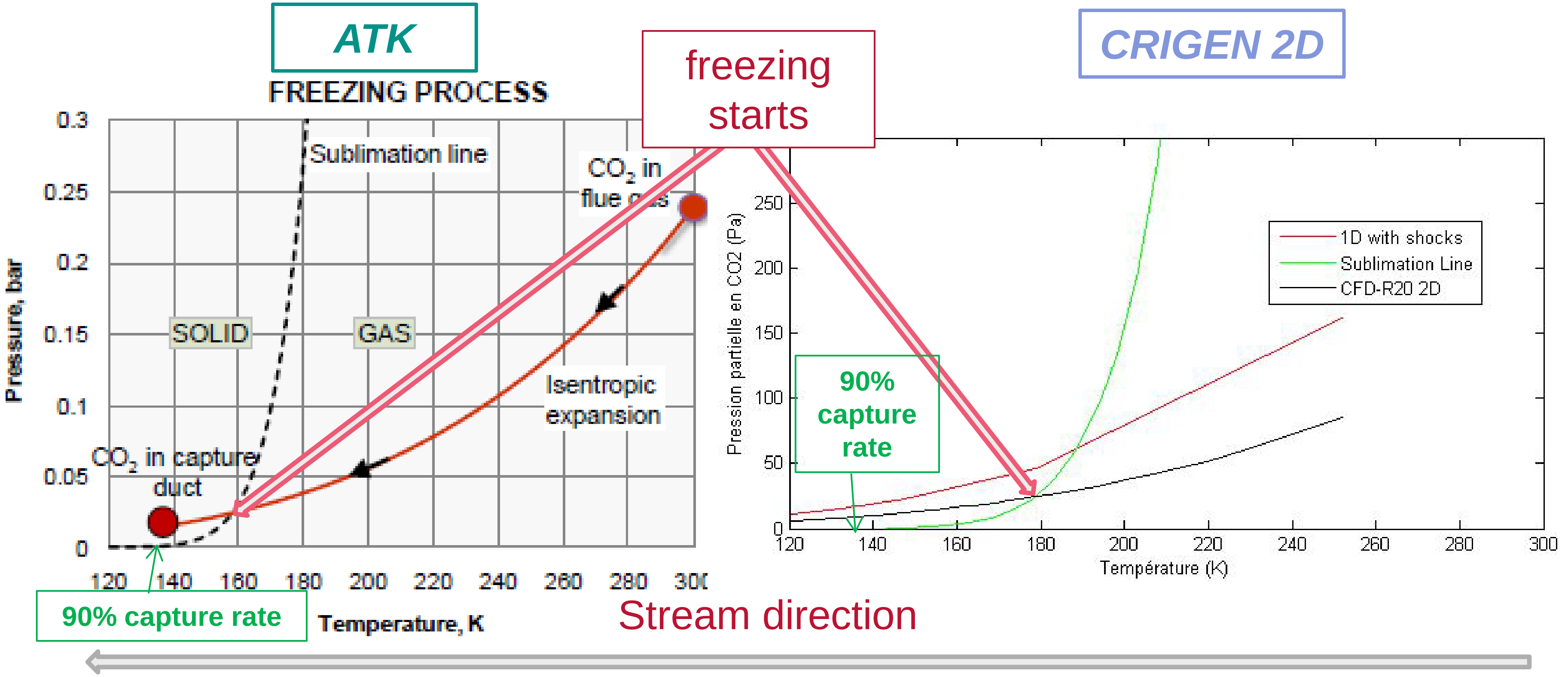
2D Matlab® Approach : Principle and 1D Corrections

- **A 2D mesh is computed based on contour simulated in 1D**
- **Gas parameter values are corrected in the radial direction**
  - Fluid heterogeneity, shock waves impact on Mach, temperature and pressure
  - Correction of 1D calculations by taking those phenomenon into account
- **Modified pressure, temperature and Mach number profiles (average)**



- Reduced impact of 2D approach on Pressure (shock waves considered in 1D too)
- Great impact on Mach number and Temperature (not considered in 1D)

2D Numerical Approach : CO_2 freezing?

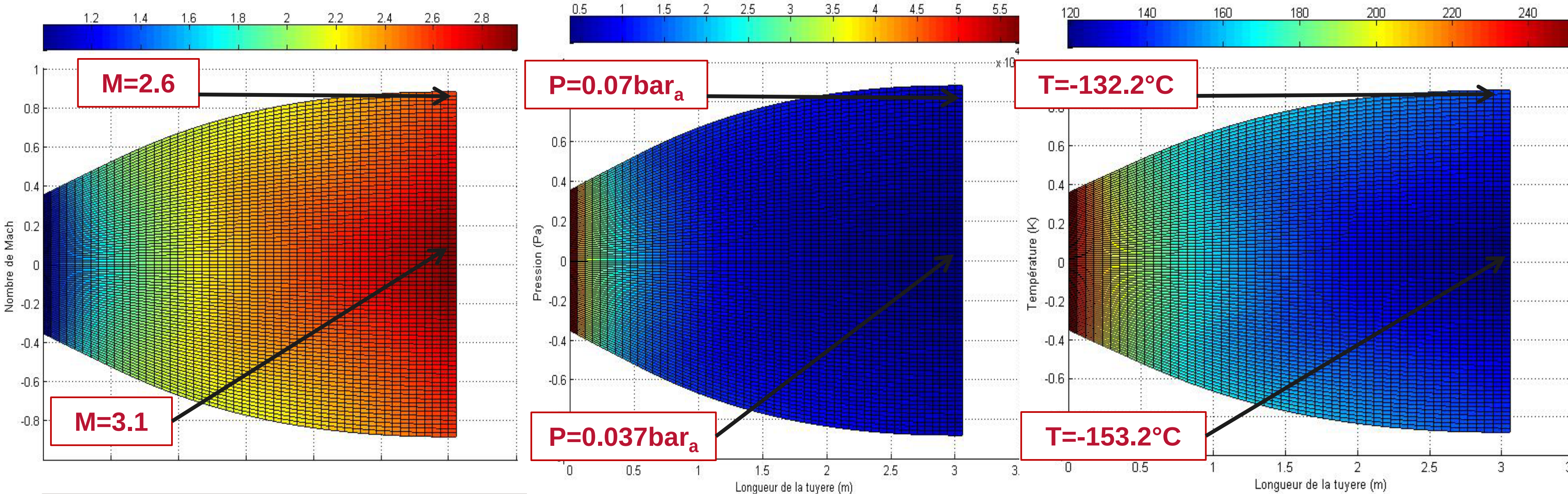


- **The feasibility seems achievable in CRIGEN's computed nozzle shape**

→**Freezing would be slightly delayed (starts at about 15 cm)**

2D Matlab® Approach : Heterogeneous Fields

- **Mach number**
- **Pressure**
- **Temperature**



- **Considering 2D aspects is important due to shock waves interactions with fluid**
- **Powerful 1D/2D Matlab® tool to:**
  - investigate operating conditions of the nozzle depending of gas composition and mass flow rate,
  - improve the understanding of phenomena occurring in the nozzle
- **Nevertheless, a 3D approach could be interesting to model some aspects more accurately**

Modelling approach to answer these questions

Level of accuracy

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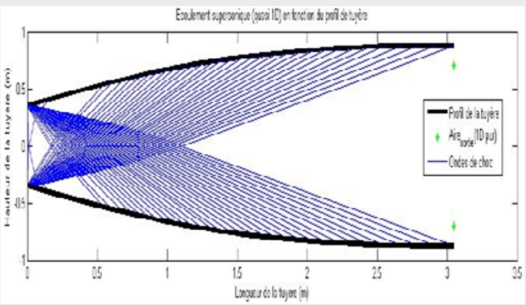
APPLIED

1D



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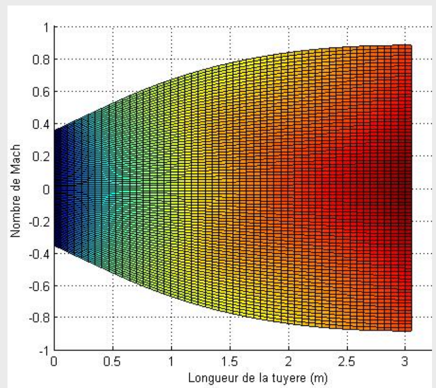
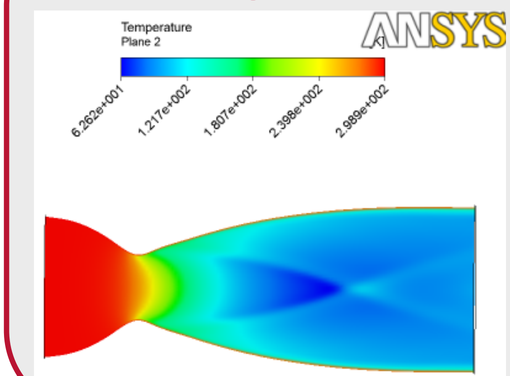


3D



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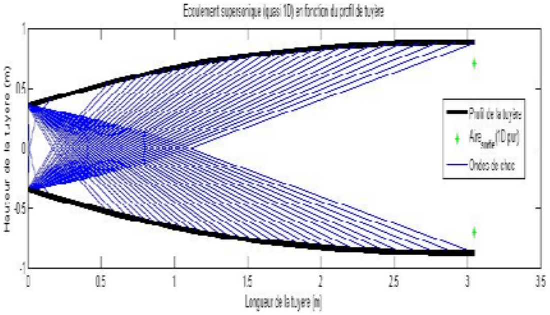
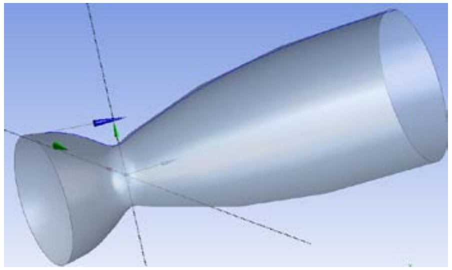
3D CFD simulations of the nozzle

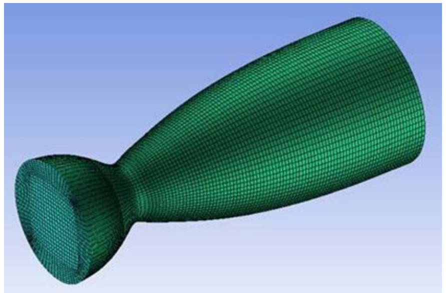
- **ANSYS-Fluent® V14.0 is used**
- **Nozzle shape is obtained from CRIGEN Matlab® tool**



Matlab



CAO geometry



1 million cells structured mesh

- **Fluid has exactly the same properties as in 1D/2D approach**
- **Importance of shock waves in the nozzle (3D effects)**

3D CFD simulations : Preliminary Steady State Results

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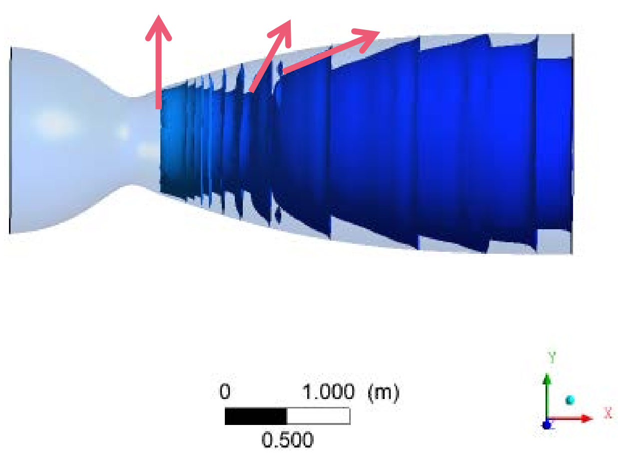
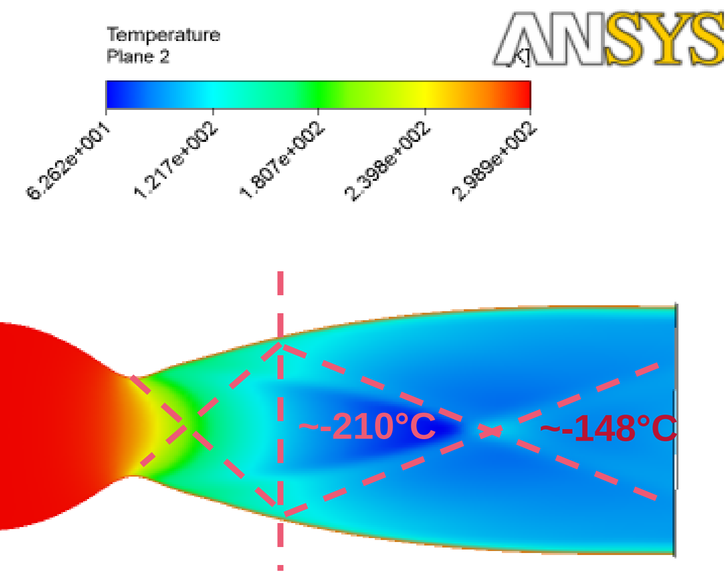
- 3D CFD simulations give the same trends as the 1D computation for shock waves …



- But here normal shock waves transform into oblique waves.



- Predicted heterogeneity on pressure and temperature fields is higher using CFD (3D effects, and shock waves reflections)

Final comparison : 1D, 2D, 3D computed values vs. ATK and ACEnT's provided data at the exit of the nozzle

	ATK	CRIGEN (1D)	CRIGEN (2D)	CFD (3D)
Diameter	IN : ~1.5 m Throat: ~1/3 of inlet diameter (*)	In : 1.5 m Throat : 0.709 m Out : 1.76 m	In : 1.5 m Throat : 0.709 m Out : 1.76 m	In : 1.5 m Throat : 0.709 m Out : 1.76 m
L	< 5 m (*)	3.05 m	3.05 m	3.05 m
Freezing point P T M	Close to the throat 0.2bar$_a$ -114°C ~ 2	7 cm after 0.4 bar$_a$ -85°C 1,46	15 cm afte 0.3 bar$_a$ -95°C 1,48	14 cm after 0.26 bar$_a$ -106°C 1,91
Exit T M	~ 0.07 bar$_a$? 3-5	~ 0.07 bar$_a$(fixed) -155,15°C 2.45	~ 0.037-0.07 bar$_a$ (calculated) -153,15°C 2.99	~ 0.017-0.078 bar$_a$ (calculated) -170,3°C 3.55

- **Flow properties are coherent.**
- **Void zone in the Mach cone has a greater impact on temperature levels than with the Matlab® tool.**

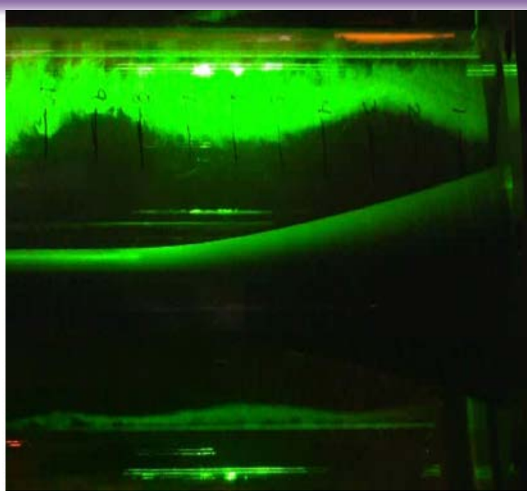
Conclusions and Prospects

- **CRIGEN has developed flexible 1D, 2D tool to investigate flue gas expansion in a supersonic nozzle**
  - → **Computed values for nozzle dimensions are consistent with those announced by developers** 1.5 m ø * 3-4m L
  - → **Desublimation seems to be achievable as announced by developers**

- **3D CFD computations**
  - → **Show more precisely flue gas heterogeneity behavior in the nozzle**
  - → **Yet confirm desublimation conditions are achievable in the nozzle**

- **Outcoming studies : taking into account more phenomena**
  - → **Impact of desublimation on performance : released latent heat and decreasing fluid flow - CFD**
  - → **Particles behavior in the nozzle (and particles impact on flow properties) – CFD**
  - → **New nozzle shapes (for iso-section) - CFD**
  - → **Unsteady simulations for start-up / shut-downs - CFD**

- **Supersonic expansion is a powerful process that can be adapted to many separation applications**
  - → **CRIGEN tools created to characterize ICES system can be adapted to other gas separation conditions.**



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Any question ?

Copenhagen

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