Large Eddy Simulation

combustion of ultra-low methane

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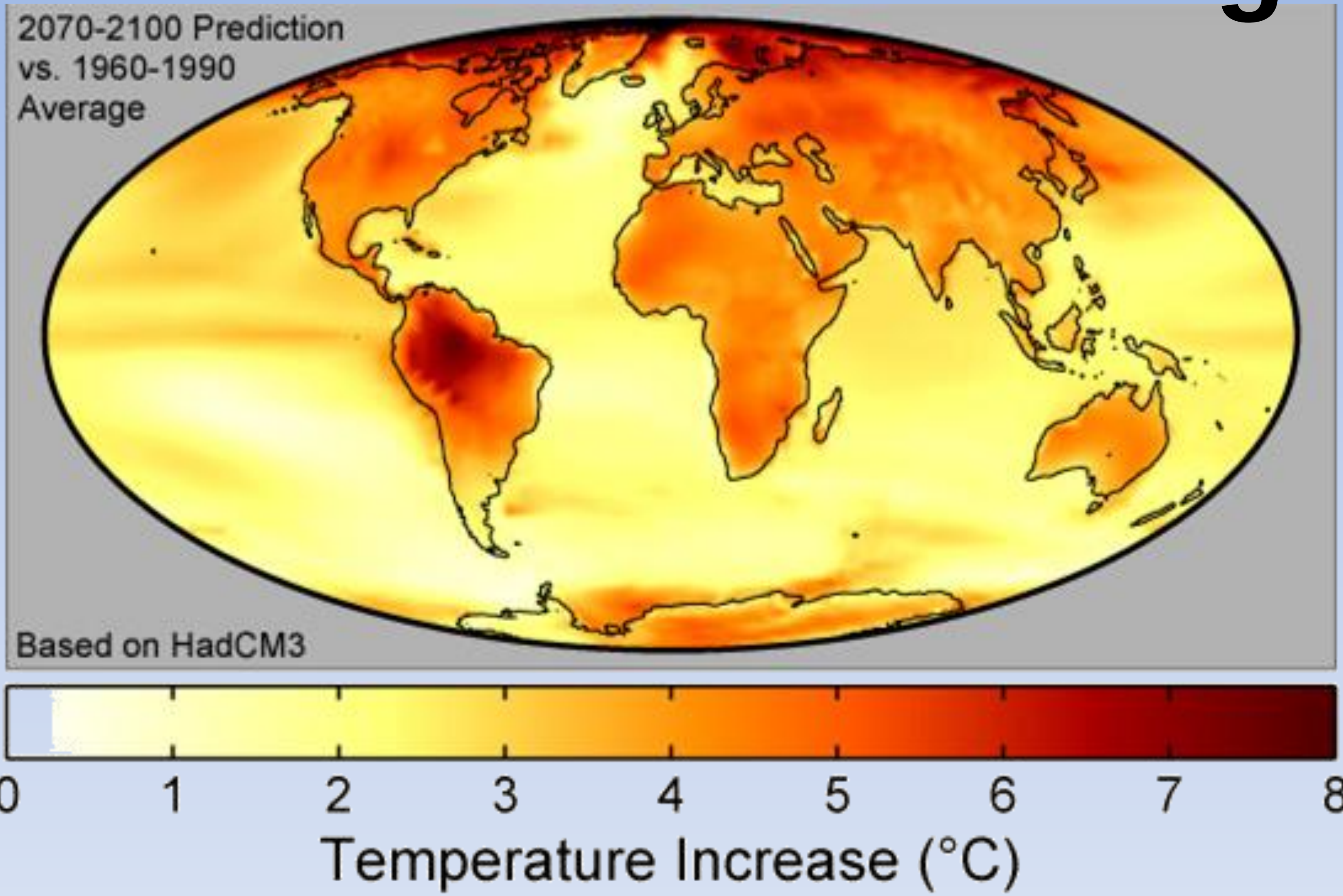
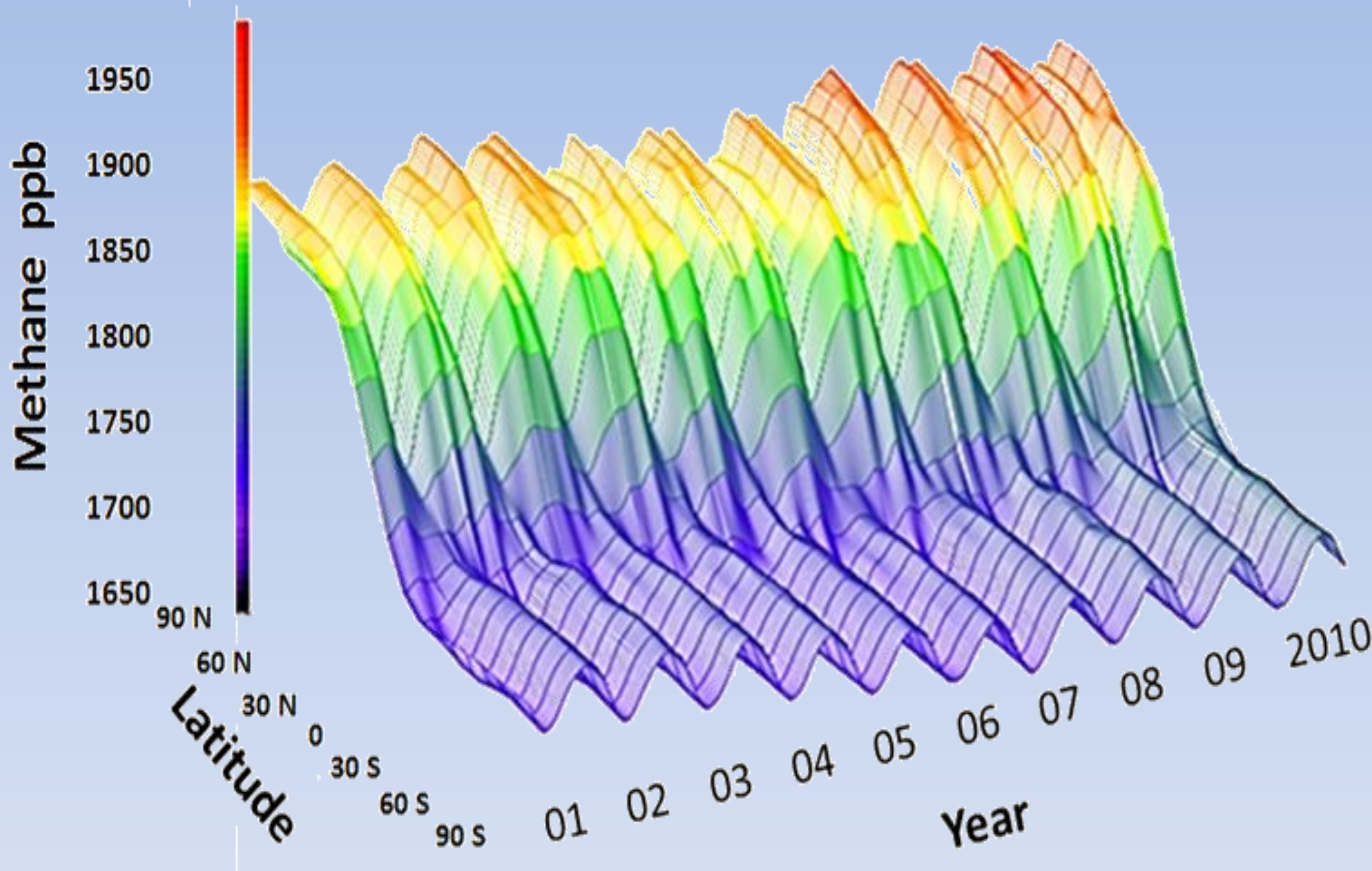
Implications of Methane

- **A global GHG**
- **Potential for Arctic Feedback loop**
- **Sources**
- **Distribution**
- **Significance**

Global Climate Change



More Methane in the Arctic



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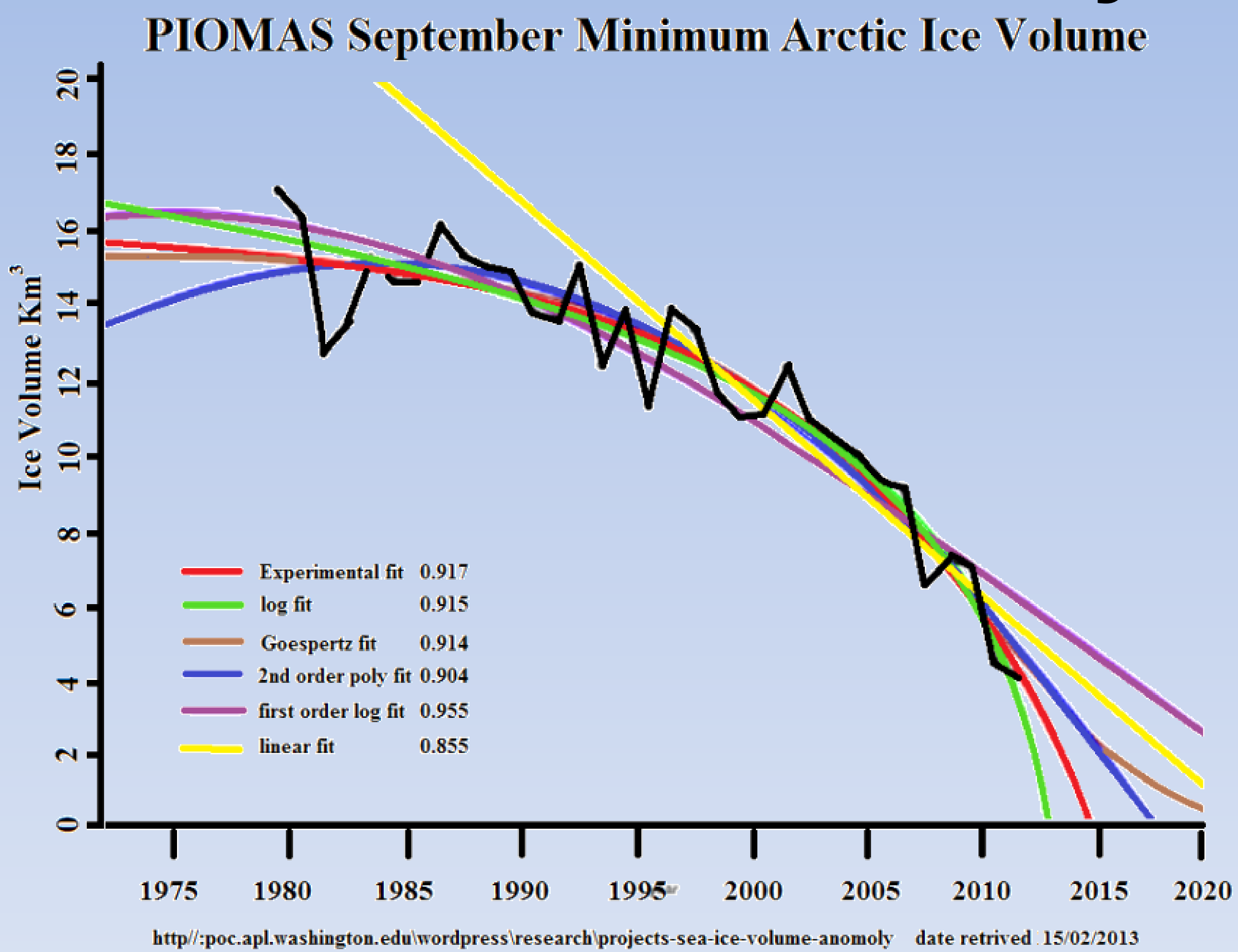
PIOMAS Measured Arctic ice volumes Projections - ice free Arctic by 2035 ?



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Permafrost Methane Flame

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Ventilation Air Methane - high volume low concentration methane source.

Capturing methane from VAM is challenging, routinely escapes to atmosphere.

Mitigating VAM has the benefits of providing an energy source and reducing the atmospheric Greenhouse Gas (GHG) burden.

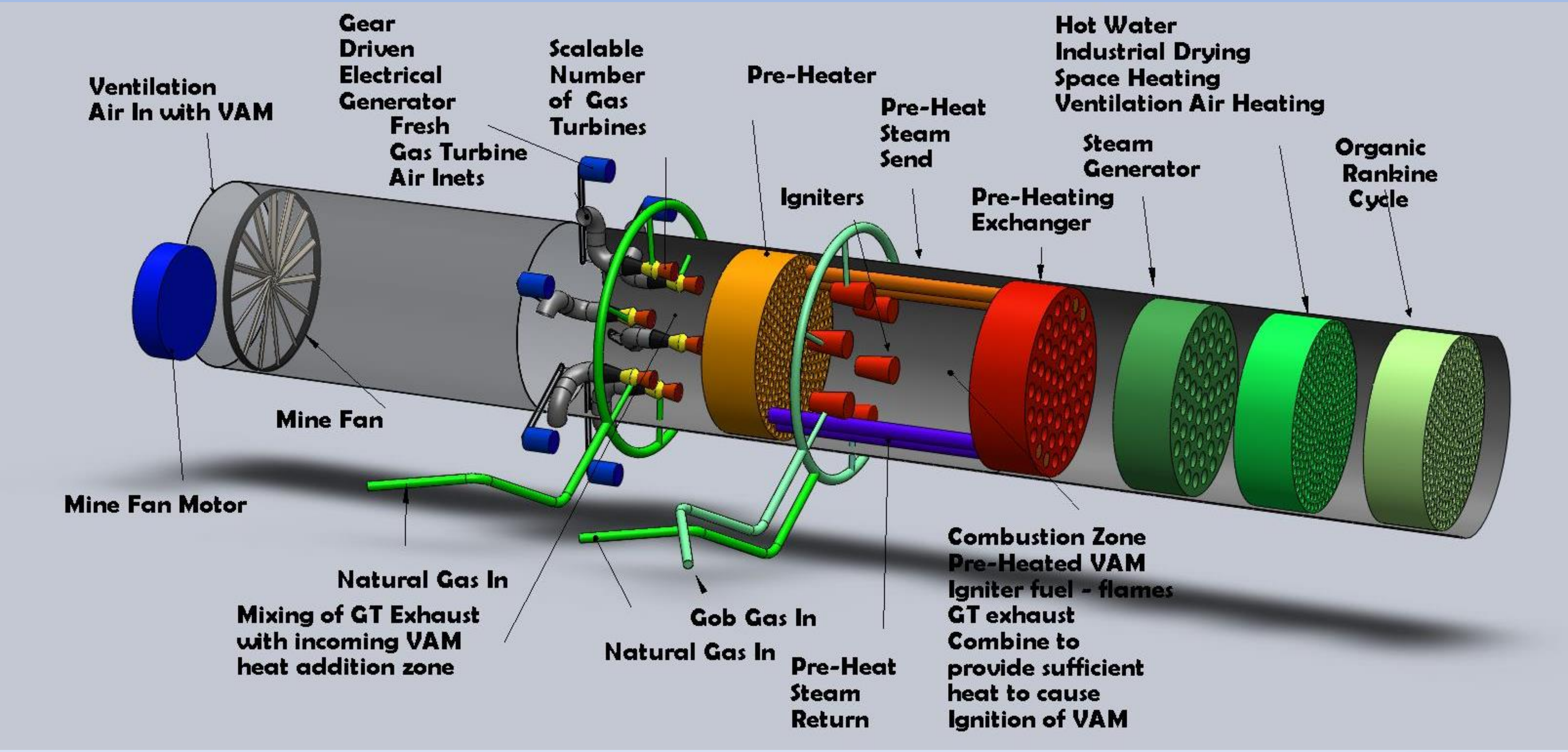
Methane is often quoted as having 17–23 times the GWP of carbon dioxide on a 100-year time horizon. BUT the GWP varies over the atmospheric residency time.

The GWP is 56 over the first 20 yrs., 21 over 100 yrs. and 6.5 over 500 yrs.

Any reduction in atmospheric methane would be beneficial.

A 100 m^3/s flow, 0.1–1% VAM - 3.8–38 MW of exploitable thermal power.

The VamTurBurner©



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Analytically
The Balanced First Order Combustion Equation

$$CH_4 + 2(O_2 + aN_2) \rightarrow CO_2 + 2H_2O + 2aN_2$$

$$Y_{CH_4} = \frac{1}{1+\frac{S}{\phi}\left(1+\frac{aW_{N_2}}{W_{O_2}}\right)} = 5.5\%$$

This means that for methane in air the perfect stoichiometric ratio exists when a mixture contains 5.5% CH_4 in air, or it is at the best methane concentration in air for ignition, the slightest spark would ignite the mixture.

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Model for Calculating the Adiabatic Flame Temperature for Methane Combustion

$$T_2 = T_0 + \frac{\sum_1^k v'_k C^m_{p,k}(T_1 - T_0) + Q^m}{\sum_1^k v''_k C^m_{p,k}} \quad where\ Q^m = \sum_1^k (v'_k - v''_k)\Delta H^{0,m}_{f,k} = \sum_1^k v_k \Delta H^{0,m}_{f,k}$$

$$T_2 = T_0 + \frac{\left(C^m_p(CH_4) + 2C^m_p(O_2) + 2aC^m_p(N_2)\right)(T_1 - T_0) + Q^m}{\left(C^m_p(H_2O) + C^m_p(CO_2) + 2aC^m_p(N_2)\right)}$$

Species		H_2O	O_2	CH_4	CO_2	N_2	
T_1 = 300 K	$C_p^m(T_1)$	33.4304	29.0551	35.5404	37.1869	28.8400	J/mole K
T_2 = 1788.077 K	$C_p^m(T_F)$	49.5266	37.3498	75.3891	59.5397	35.6658	J/mole K

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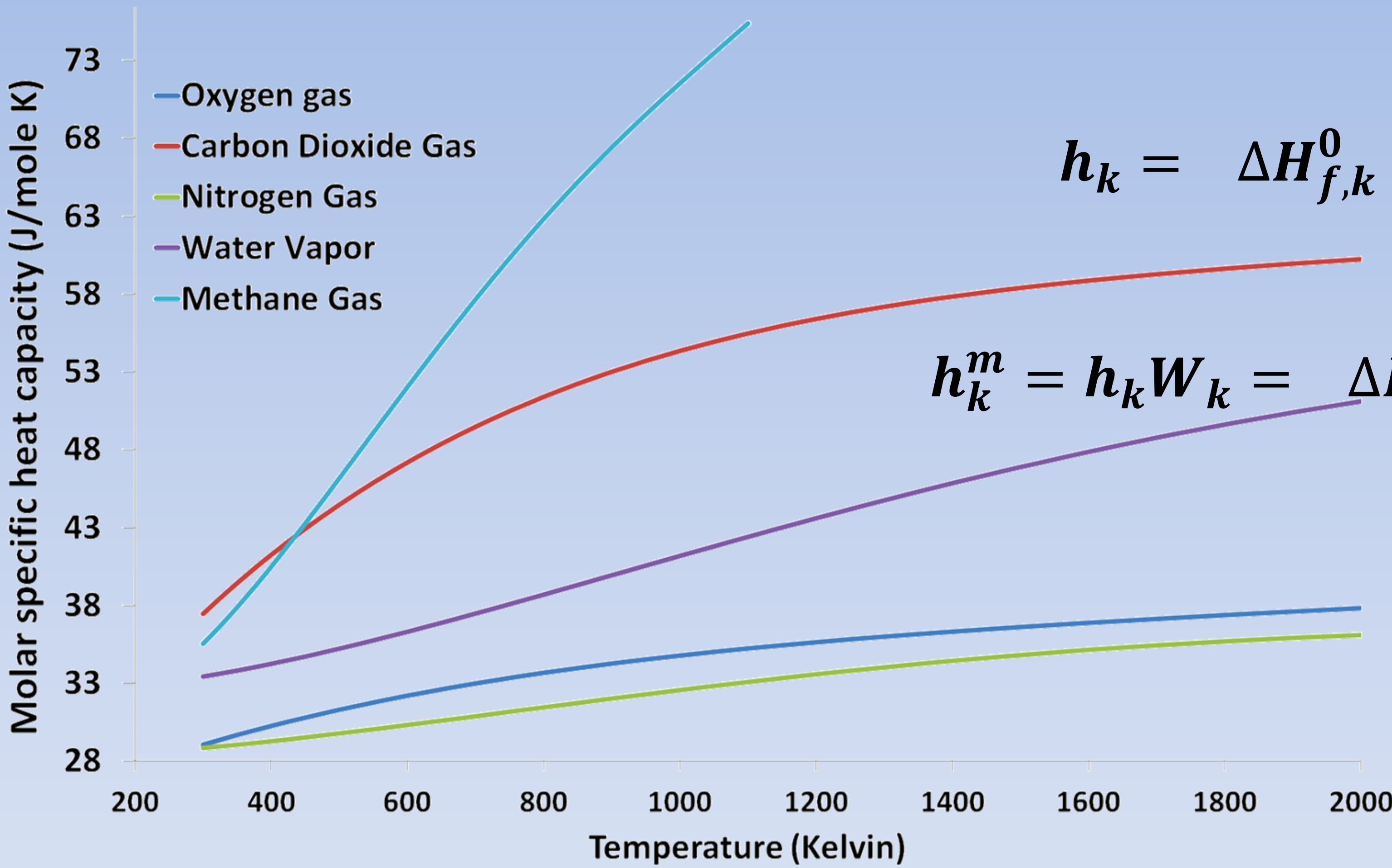
Specific Heat Capacities

used for regression equations



$$h_k = \Delta H^0_{f,k} + \int_{T^0}^{T} C_{pk}\, dT$$

$$h_k^m = h_k W_k = \Delta H^0_{f,k} W_k + \int_{T^0}^{T} C_{pk} W_k\, dT$$

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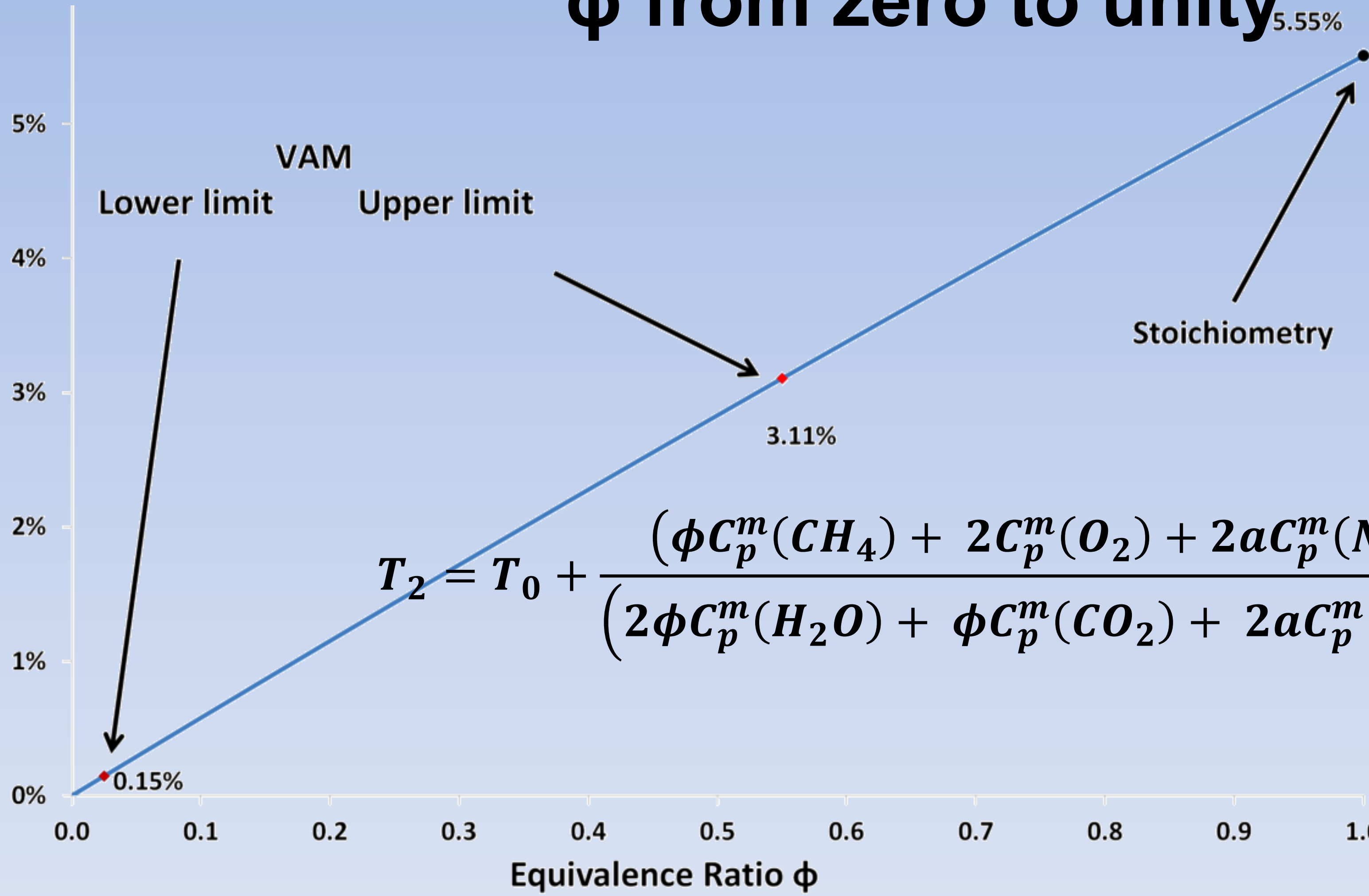
The zone of potential VAM available to the VamTurBurner© expressed as the equivalence ratio for ϕ from zero to unity



$$T_2 = T_0 + \frac{\left(\phi C_p^m(CH_4) + 2C_p^m(O_2) + 2aC_p^m(N_2)\right)(T_1 - T_0) + \phi Q^m}{\left(2\phi C_p^m(H_2O) + \phi C_p^m(CO_2) + 2aC_p^m(N_2) + 2(1-\phi)C_p^m(O_2)\right)}$$

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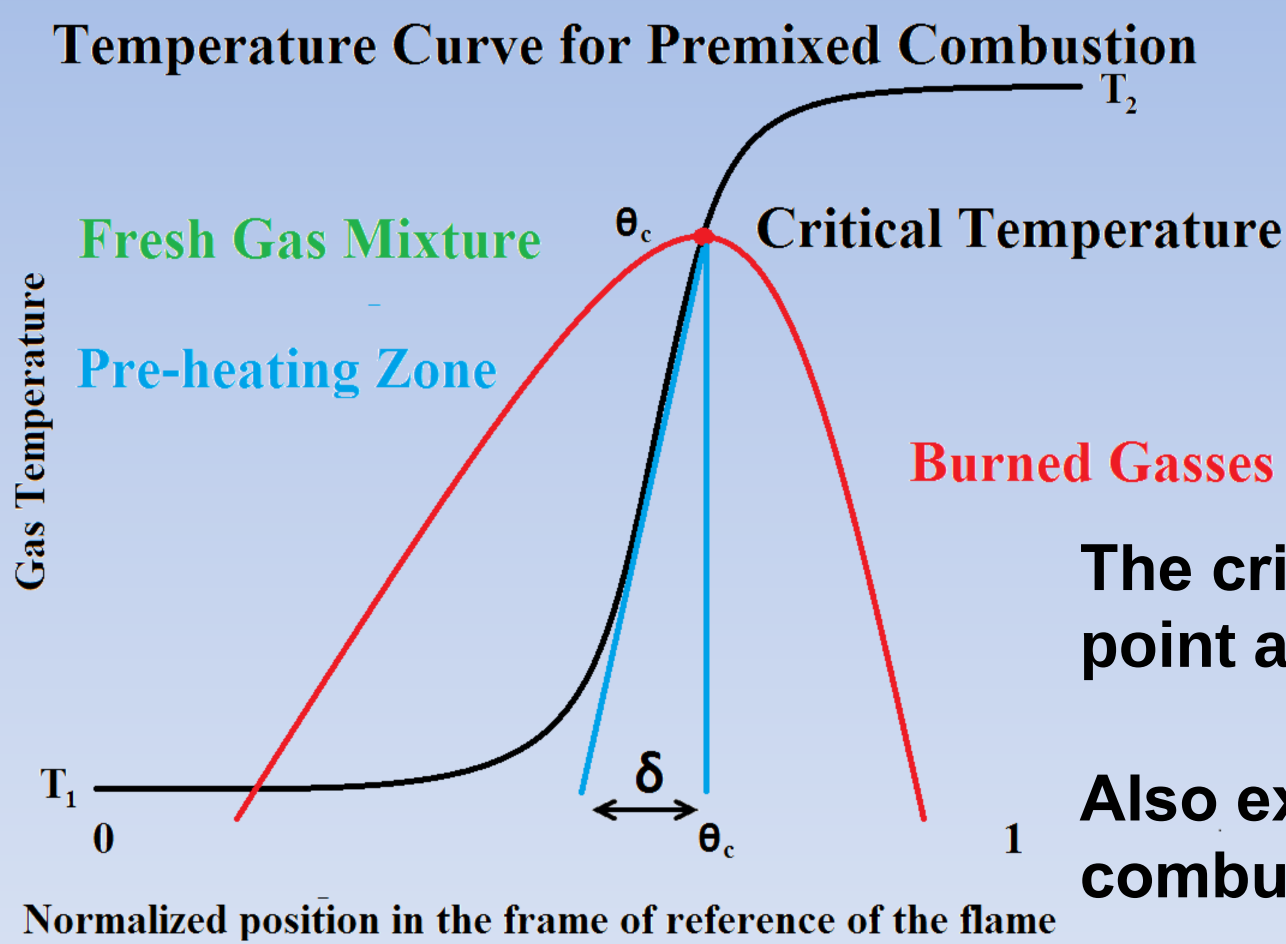
Premixed Combustion

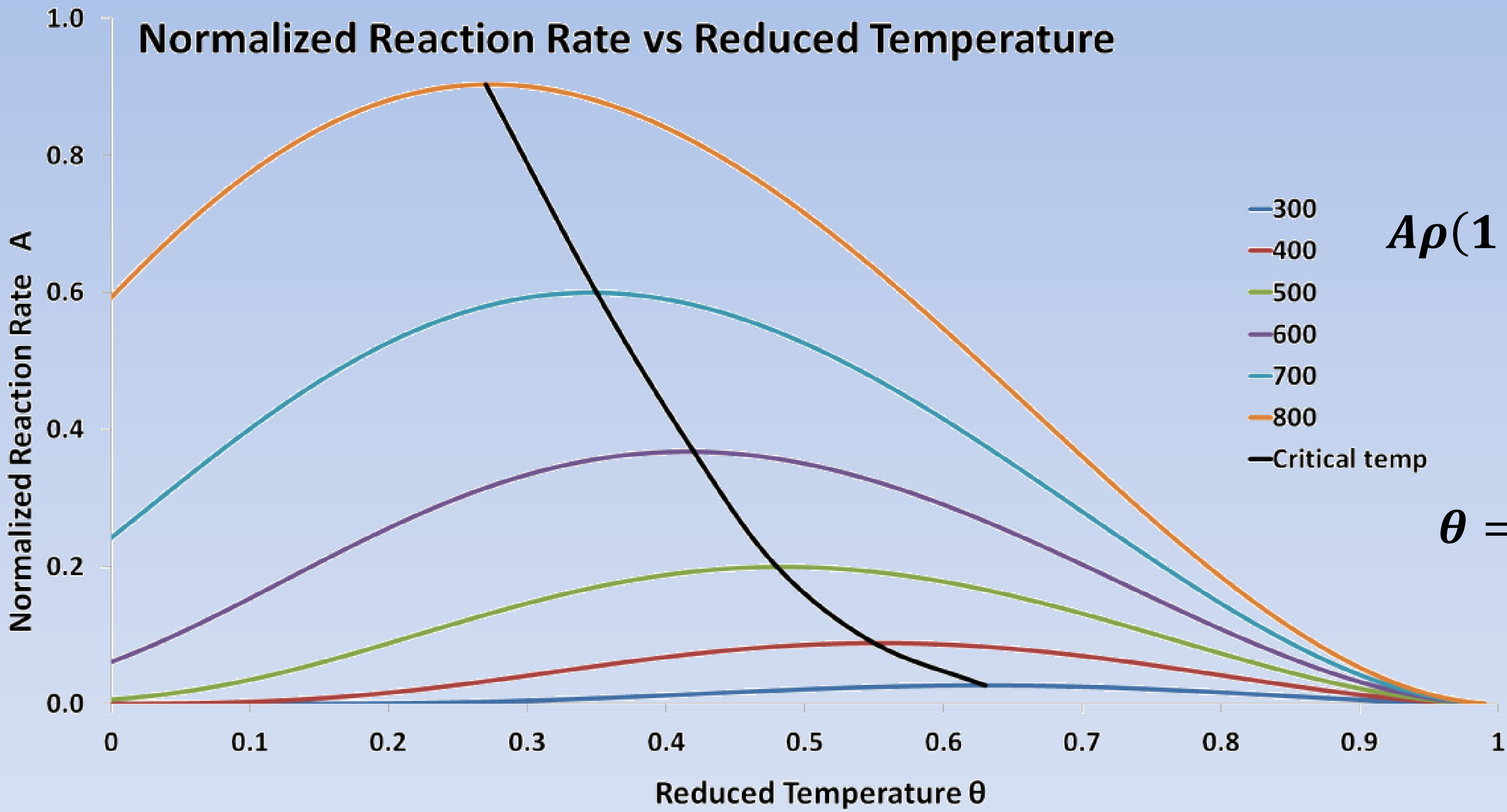


The critical temperature θ_c is the point at which combustion starts.

Also explains "spontaneous combustion"

The normalized reaction rate versus the reduced temperature for a methane VAM flow entering the pre-heating zone.

Combustion occurs when the temperature reaches θ_c the critical temperature.



$$A\rho(1-\theta)e^{\left(-\frac{\beta}{\alpha}\right)}\frac{\mathbf{e}^{\left(-\beta\frac{1-\theta}{1-\alpha(1-\theta)}\right)}}{1+\alpha\frac{\theta}{1-\theta}}$$

$$\theta = {(T-T_1)}/{(T_2-T_1)}$$

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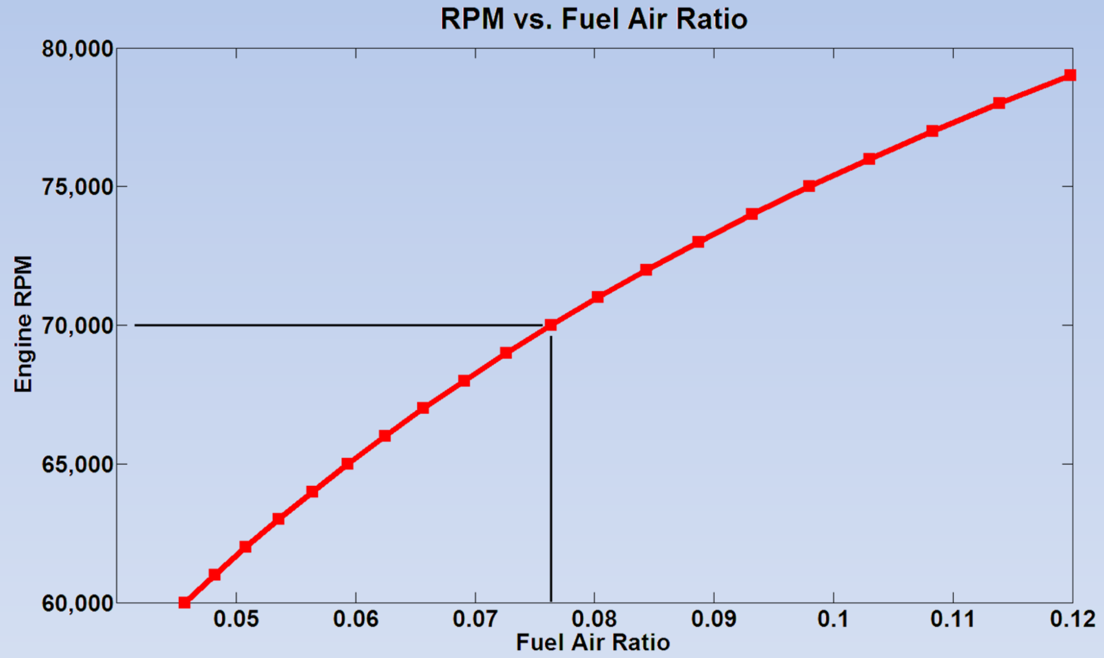
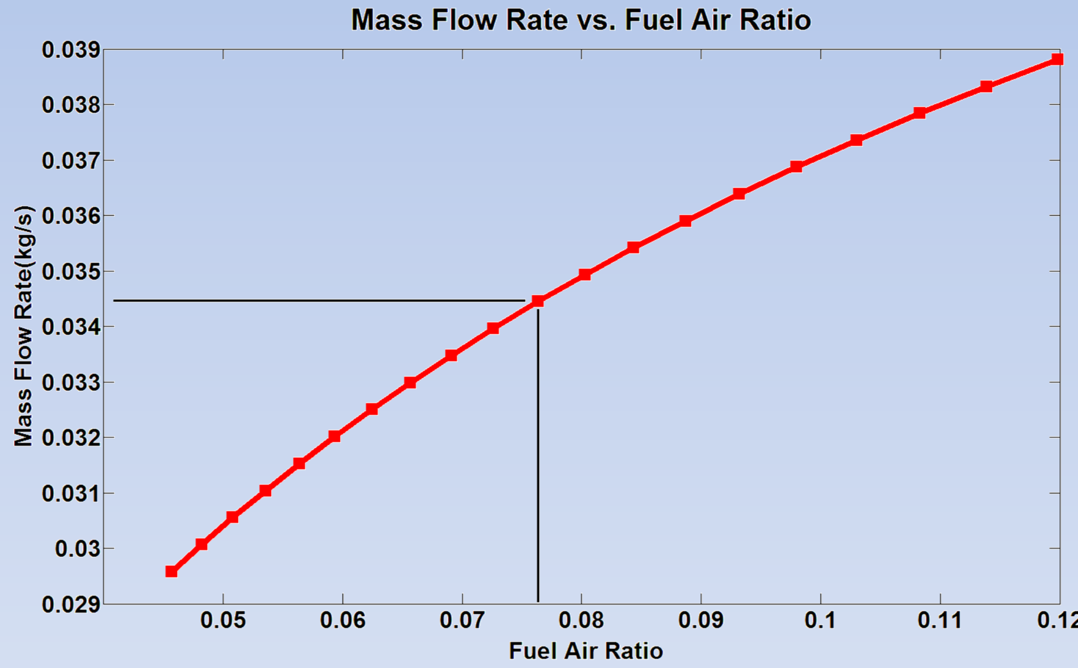
MATLAB program for VamTurBurner© design

$$\frac{A}{A^*} = \frac{(\gamma+1)}{2}^{\frac{-(\gamma+1)}{2(\gamma-1)}} \frac{\left(1 + M^2\left(\frac{\gamma-1}{2}\right)\right)^{\frac{\gamma+1}{2(\gamma-1)}}}{M}$$





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Large eddy simulation (LES)

Large eddy simulation (LES) is a technique used in the computational fluid dynamics modeling of turbulence. It was initially suggested by Smagorinsky in 1963, while studying the simulation and the study of the dynamics of the atmosphere's general circulation, the same year as Lorentz discovered the chaotic behaviour of atmospheric turbulence. Deardorff expanded the concept by studying the details pertaining specifically to LES. Deardorff advanced and developed the concepts of sub-grid scale effects simulated with eddy coefficients proportional to the local velocity deformation (Deardorff, 1970). LES is a mathematical technique useful for solving problems in combustion dynamics, but is also applicable to other fields of computational physics.

LES puts controls or limits on the Navier–Stokes equations in order to select the appropriate range of length scales for the solution, this is a critical element in the computation because the goal is a reduction of computational cost, which allows for larger scale and more simulations. A simplified version of the Navier-Stokes equations, shown below, is essentially an expression of Newton's second law of motion for a fluid, for a detailed derivation the reader is referred to Batchelor, 1967.

$$F_{gravity} + F_{pressure} + F_{viscous} = ma$$

The key point is that a large eddy simulation is fundamentally a low-pass filtering operation not dissimilar to a frequency filter used to split the treble and bass on an audio speaker system. A low pass filter reduces the computational extent by avoiding the computations pertaining to the small scale eddies or the high frequencies.

To establish a sensible cut-off point, assumptions regarding the cascade of energy from the larger scale eddies in the flow to the next smaller scale is required.

It is expected that this energy transfer is achieved without a loss of kinetic energy to viscous forces.

This is equivalent to stating that the energy dissipation is due solely to the inertial term, which is nonlinear in the Navier-Stokes equations or the energy dissipation $\epsilon = \nu k_o^3 |\nabla u(x,t)|^2$ is constant over the spatial and temporal existence of the flow

The second somewhat obvious, but equally important assumption is that the amount of energy flowing from the larger scale to the smaller scale is consistent with the conservation of energy; thus, the amount of energy flowing from the larger scale equals the amount of energy arriving at the smaller scale.

The LES governing equations for multi-species reacting compressible flows are presented in (Mira-Martinez, Cluff and Jiang, 2013), which are comprised of

- The continuity equation or conservation of mass
- Conservation equations
  - Momentum
  - energy
- The species equations

The filtered stress tensor $\overline{\tau_{ij}}$ is obtained neglecting the effect of the unresolved field and is given by:

$$\overline{\tau_{ij}} = \overline{\bar{\mu}\left\{\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i} - \frac{2\partial\tilde{u}_k}{3\partial x_k}\delta_{ij}\right\}}$$

$$\bar{q}_j = -\overline{\bar{K}\frac{\partial \widetilde{T}_i}{\partial x_j}} + \bar{\rho}\sum_{m=1}^{N}\widetilde{h_m}\,\overline{\bar{D}_m\frac{\partial \widetilde{Y_m}}{\partial x_j}}$$

Where $\overline{K}$, $\widetilde{T}$, $\bar{D}_m$ *and* $\tilde{h}_m$ are the filtered thermal conductivity, temperature, diffusion coefficient and enthalpy of species $\boldsymbol{m}$ respectively. The thermal conductivity is obtained by using a constant Prandtl number, set to 0.7, for each species contained in the flow field $= \frac{\mu c_p}{Pr}$.

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The four step mechanism for species chemical kinetics

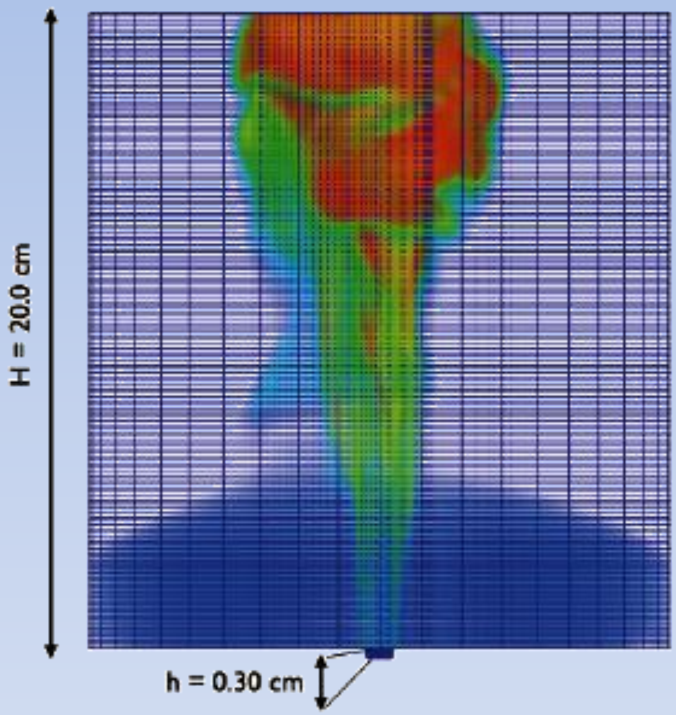
$$C_nH_{2n} + {}^{n}/_{2}\,O_2 \rightleftharpoons nCO + (n+1)H_2 \quad \longrightarrow \quad CH_4 + {}^{1}/_{2}\,O_2 \rightleftharpoons CO + 2H_2$$

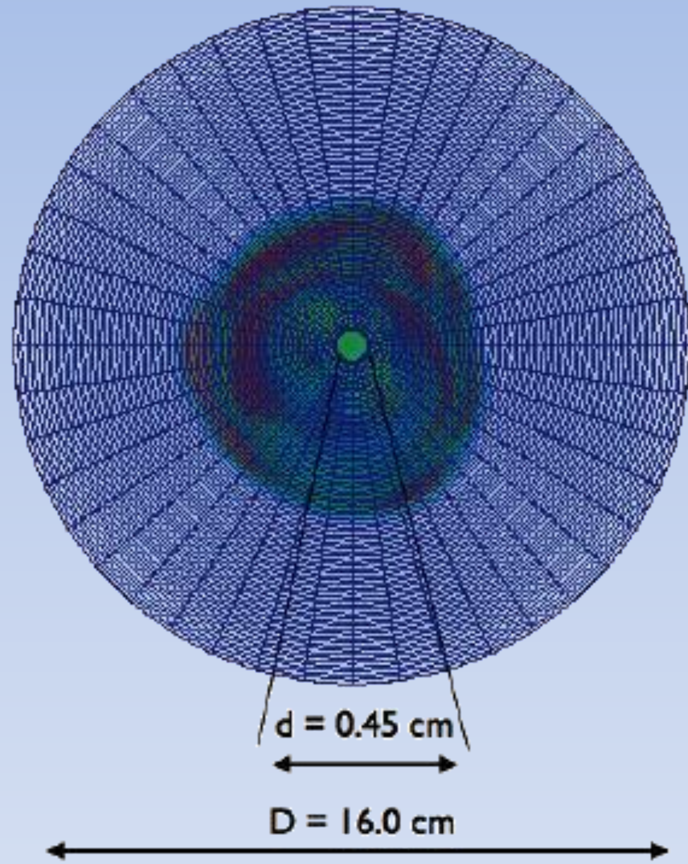
$$C_nH_{2n} + nH_2O \rightleftharpoons nCO + (2n+1)H_2 \quad \longrightarrow \quad CH_4 + H_2O \rightleftharpoons CO + 3H_2$$

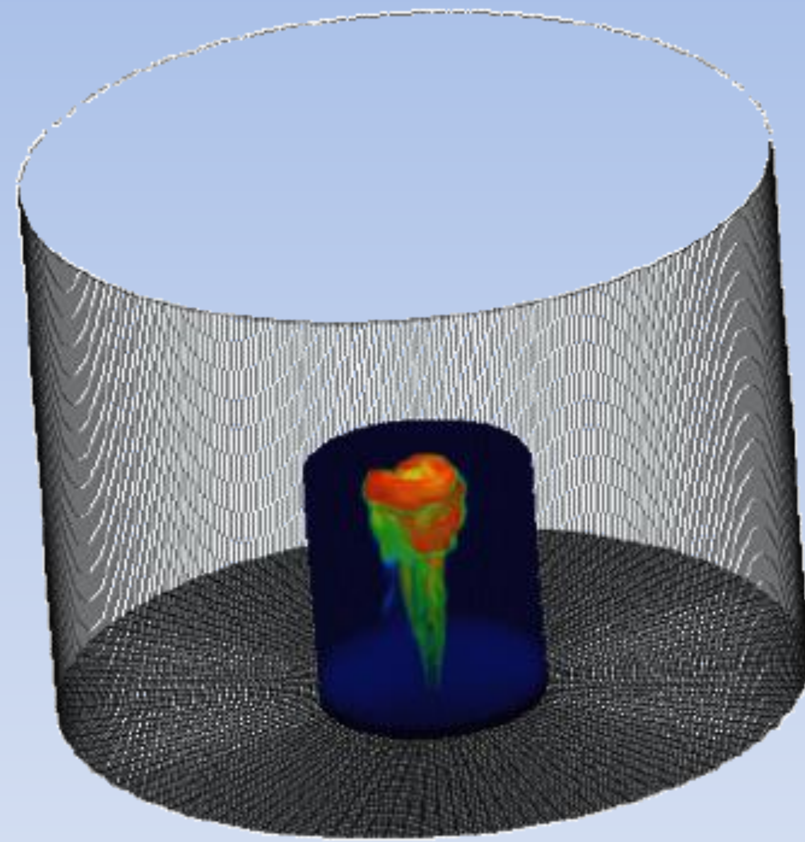
$$H_2 + {}^{1}/_{2}\,O_2 \rightleftharpoons H_2O$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

Description of the computational domain and embedded domain in a realistic configuration







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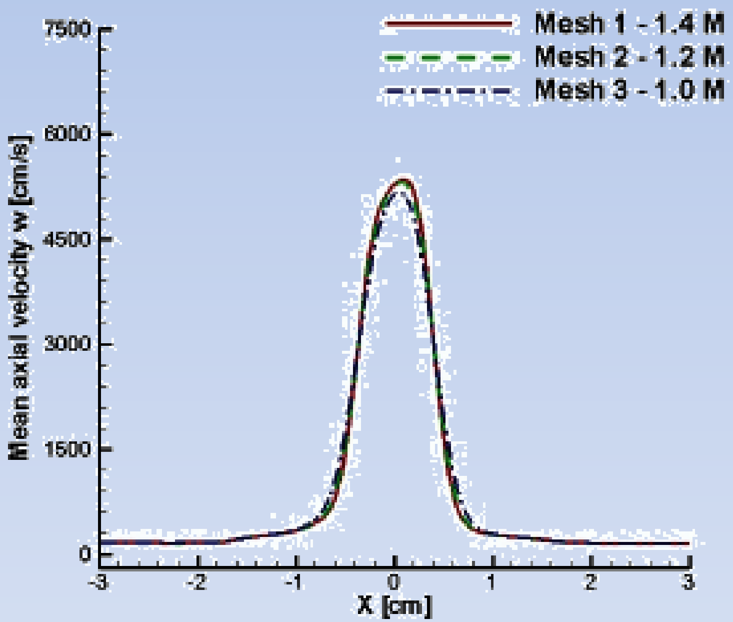
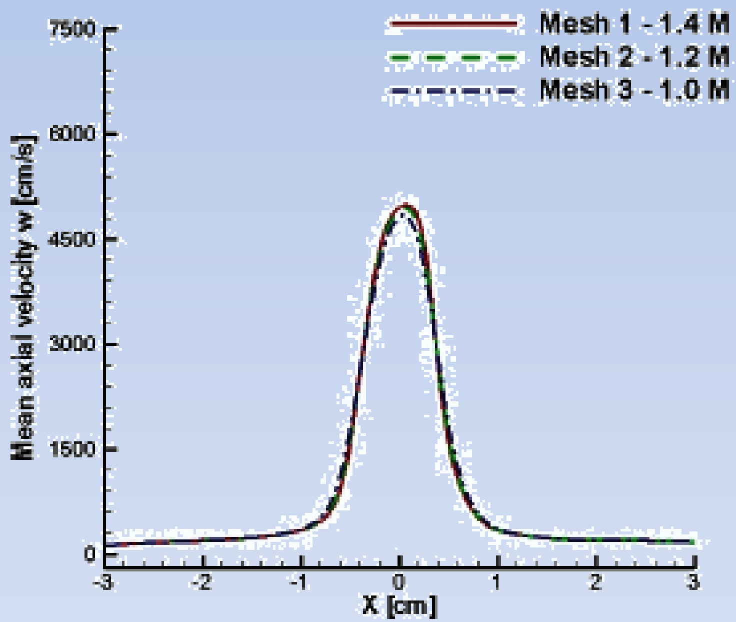
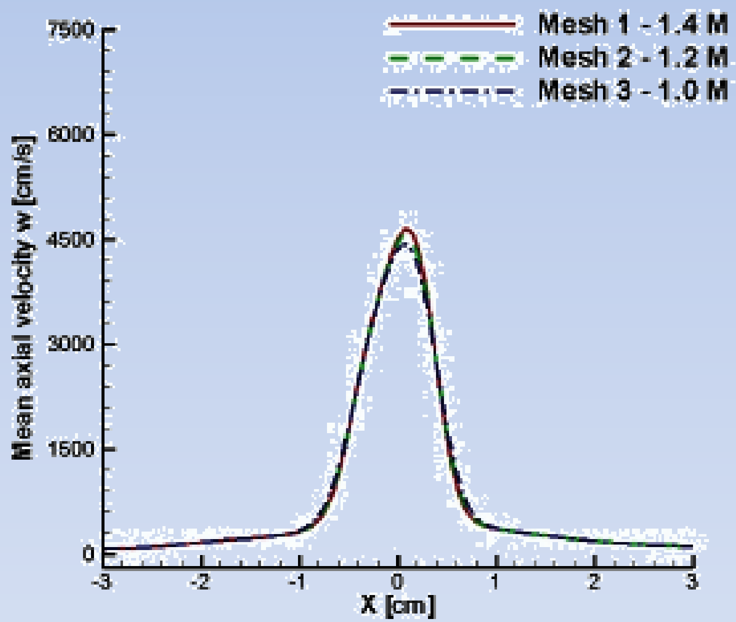
Mesh analysis







Large Scale Eddy

Simulation

Results

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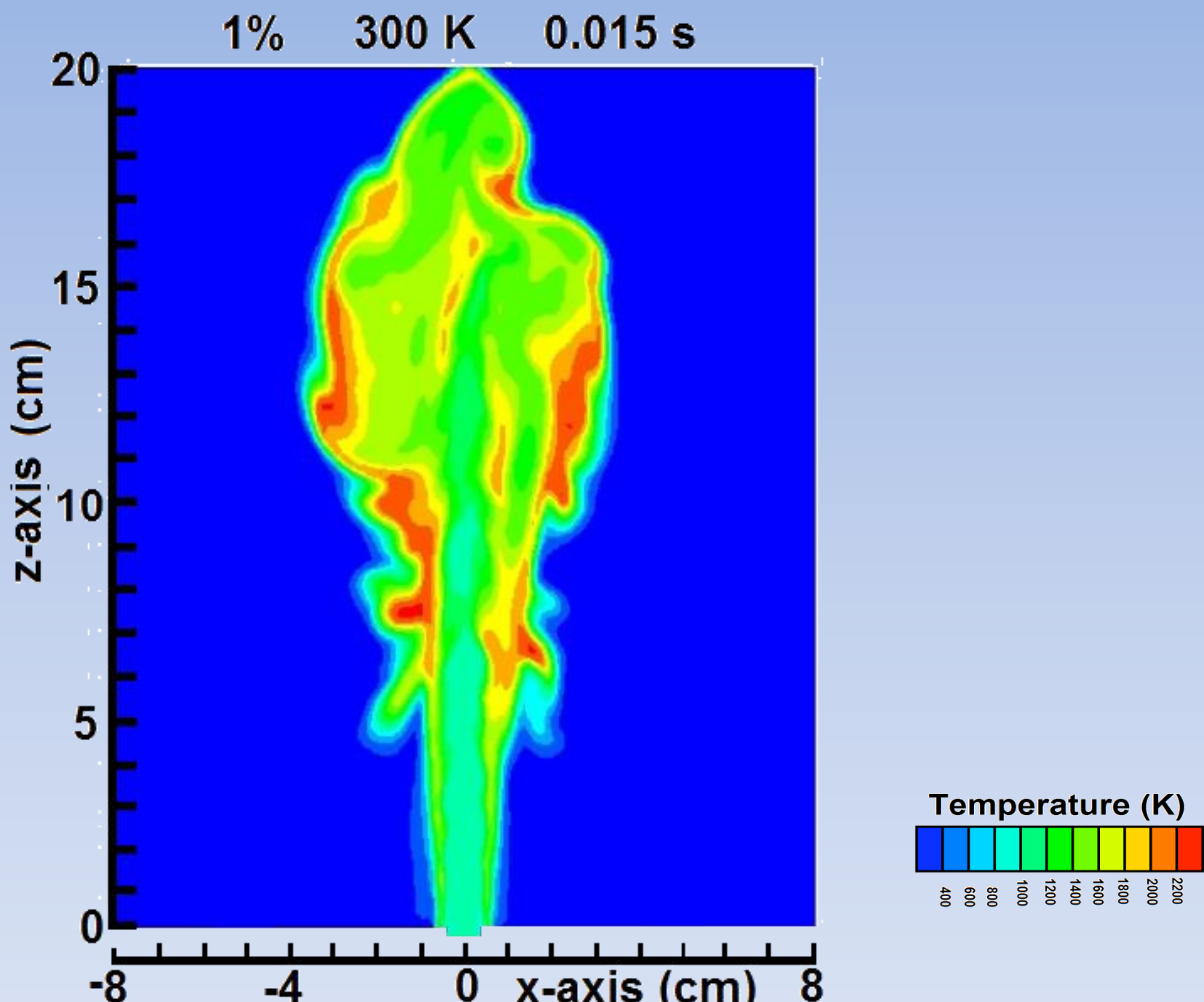

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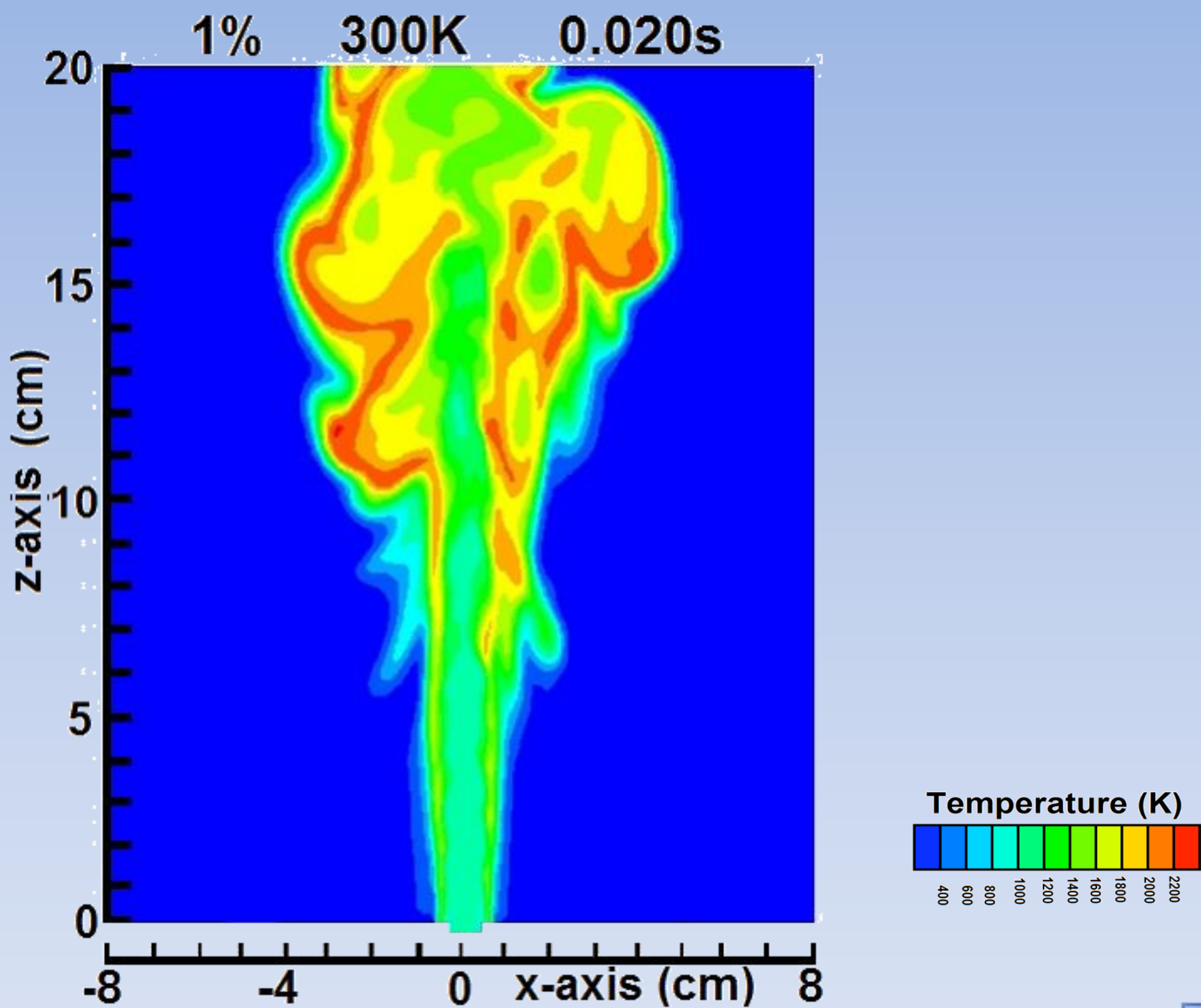

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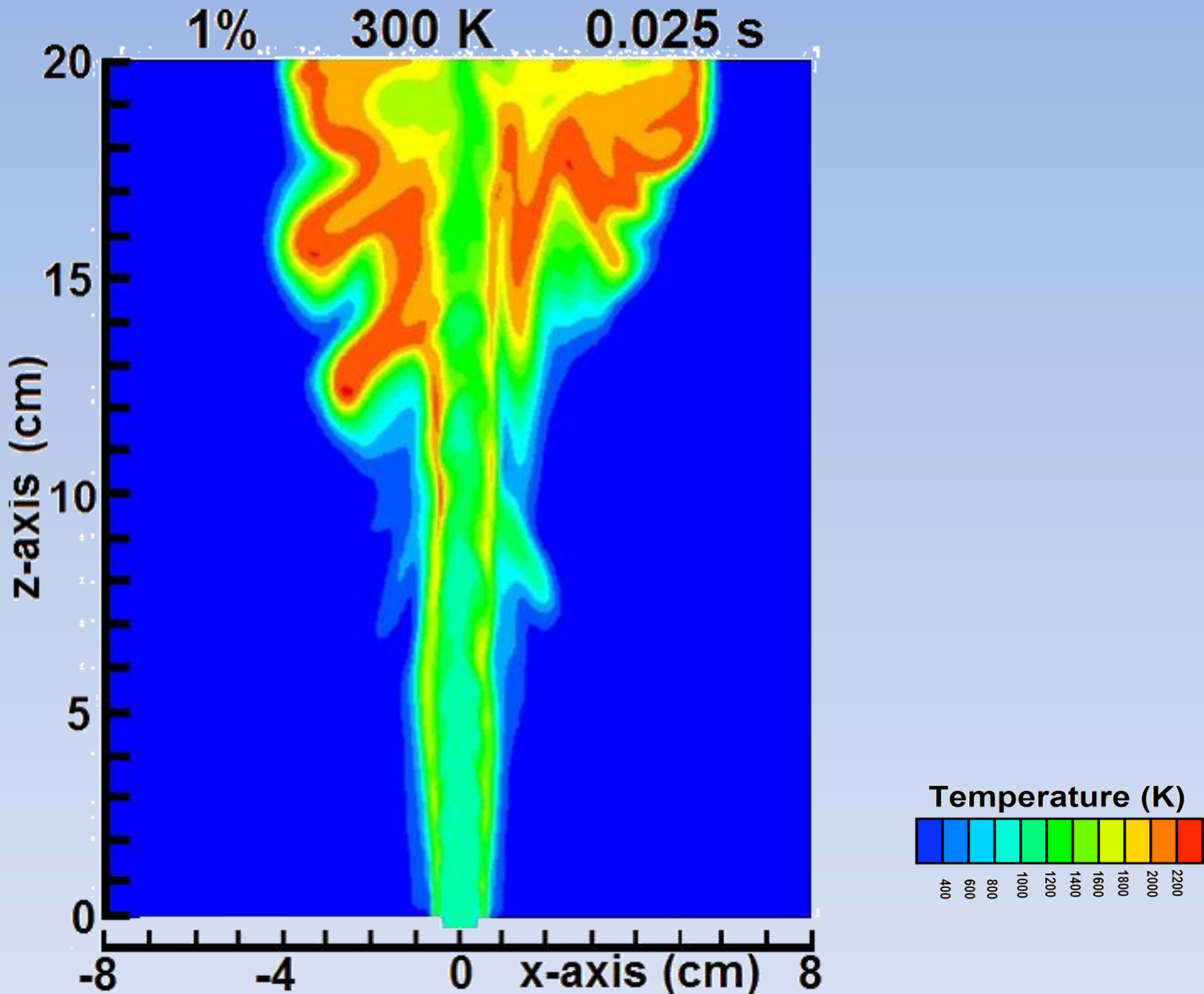

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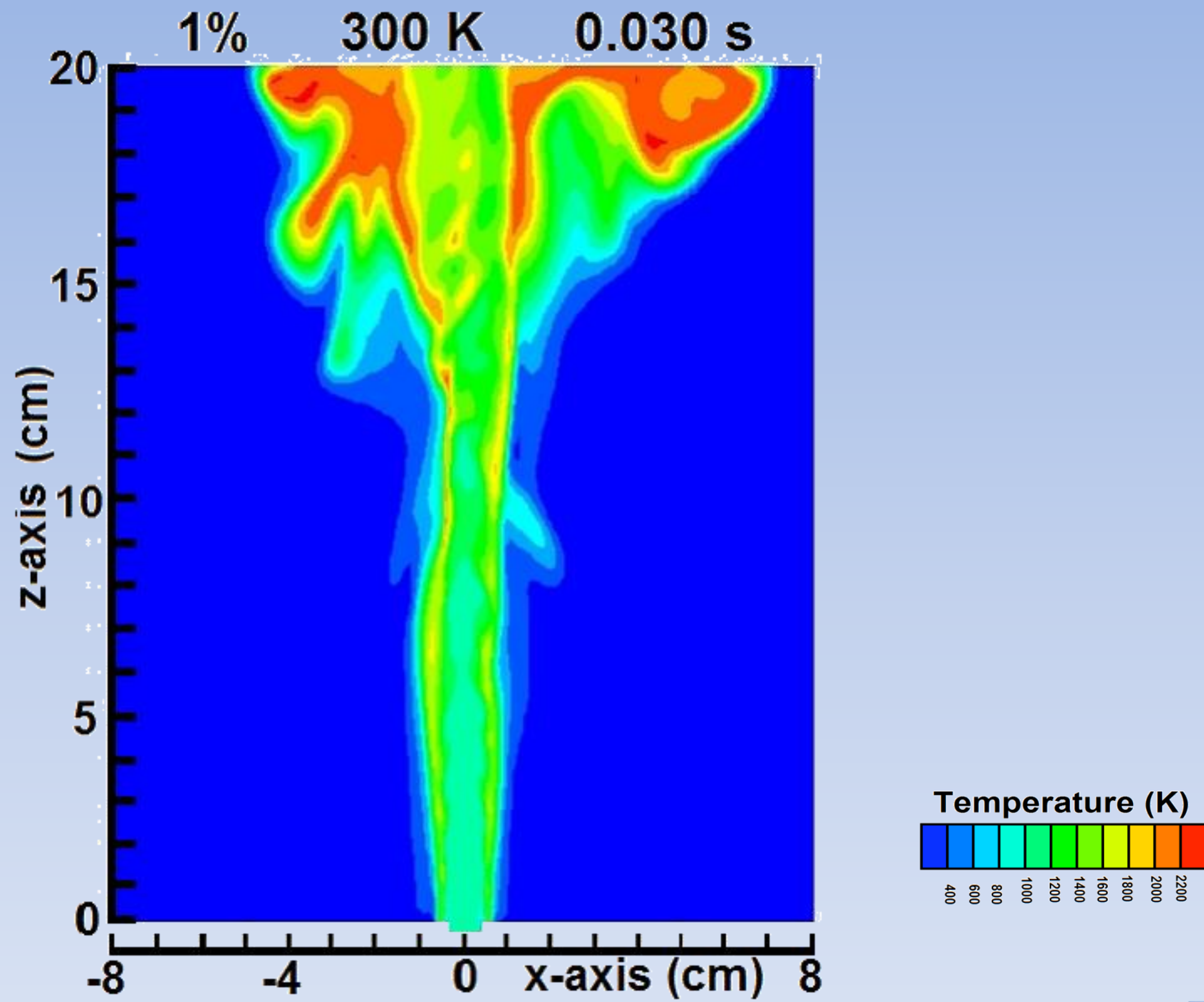

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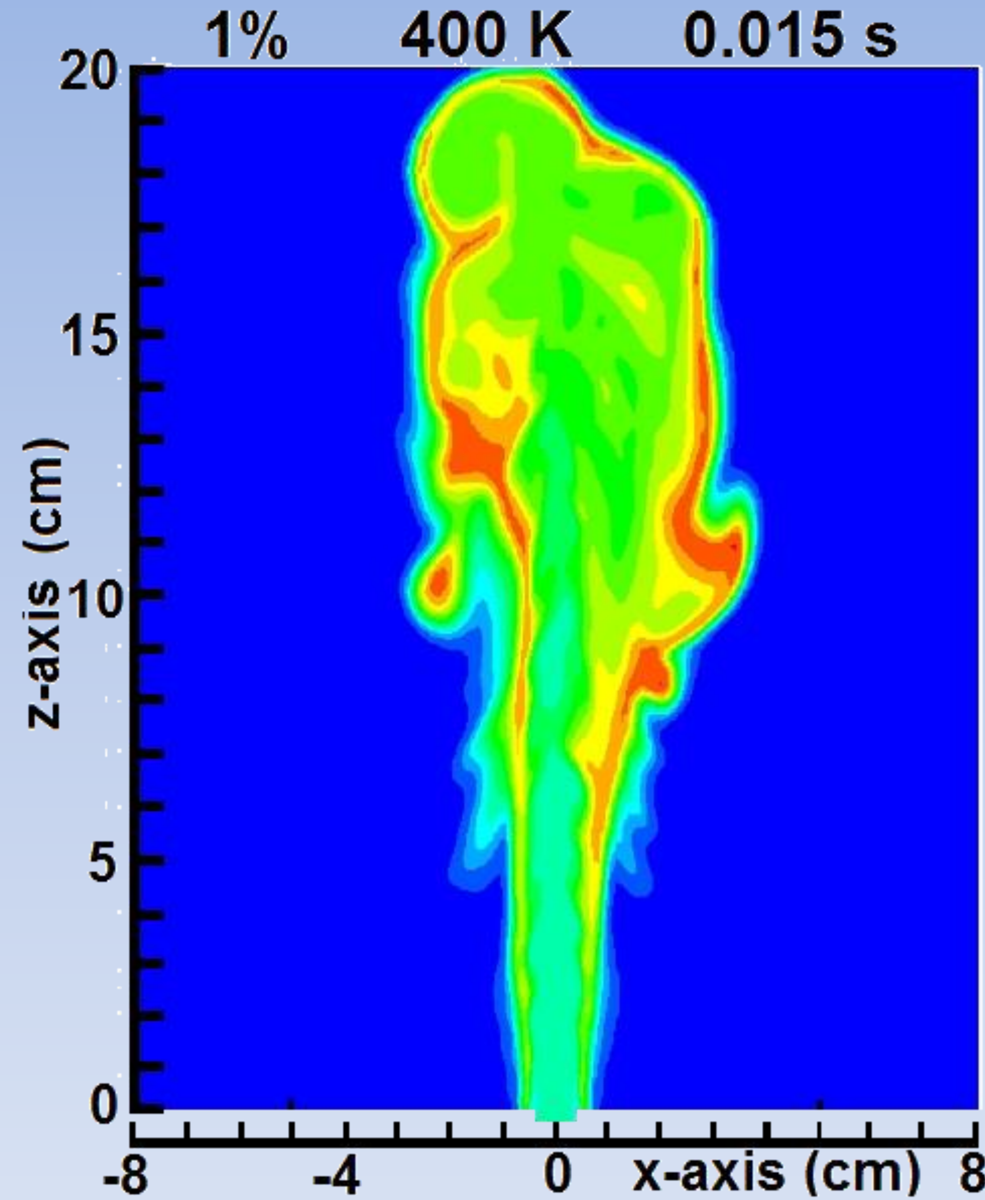

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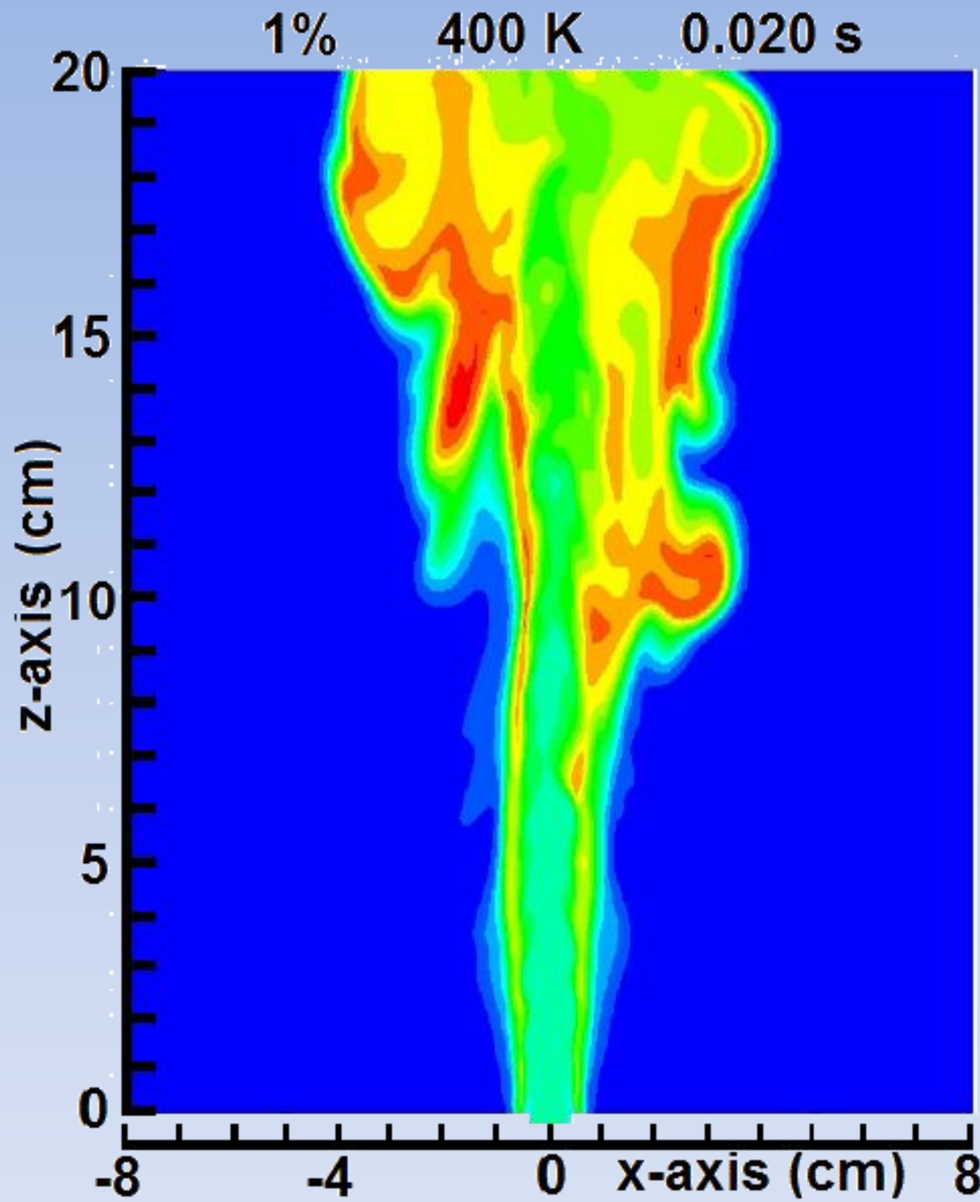

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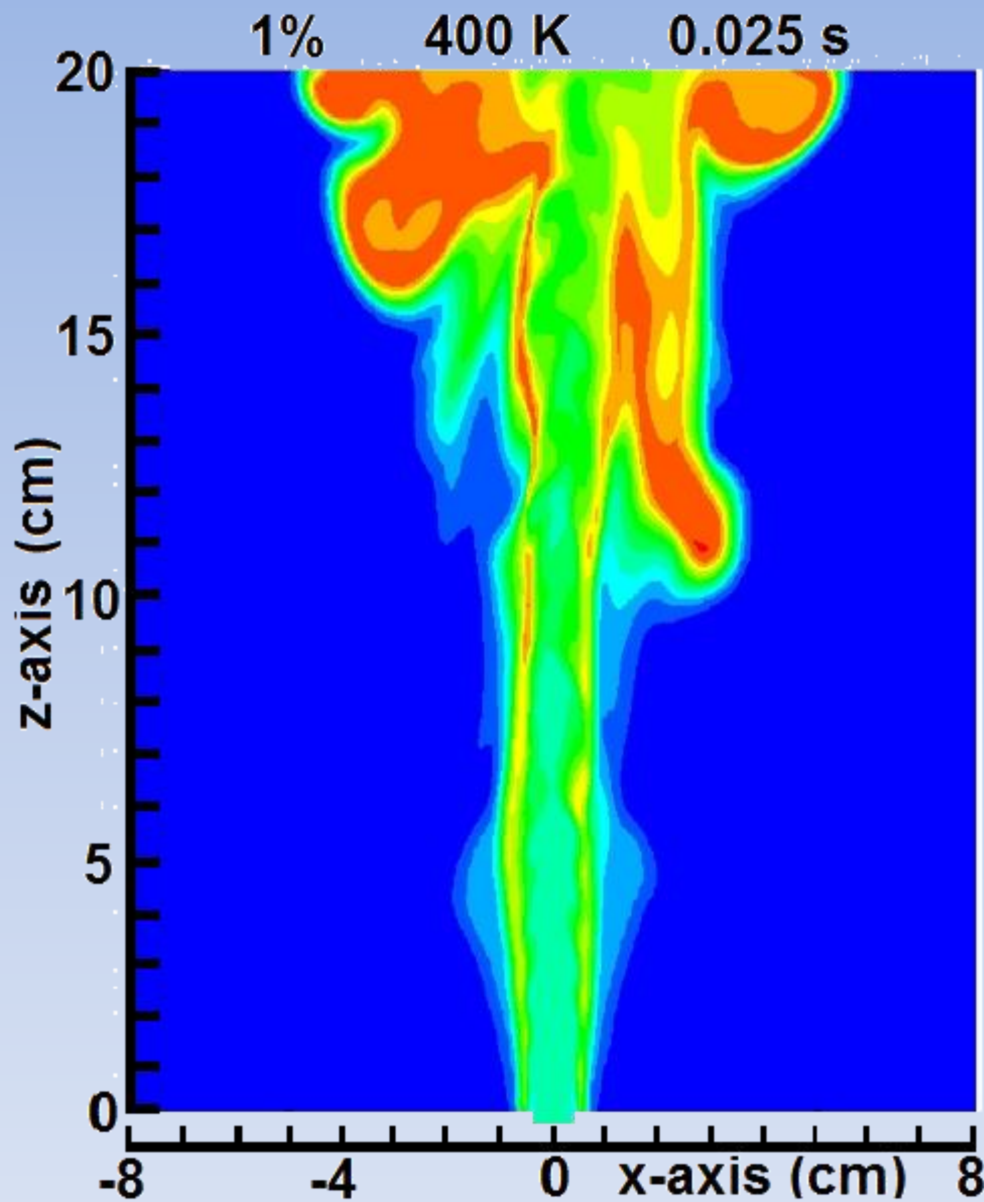

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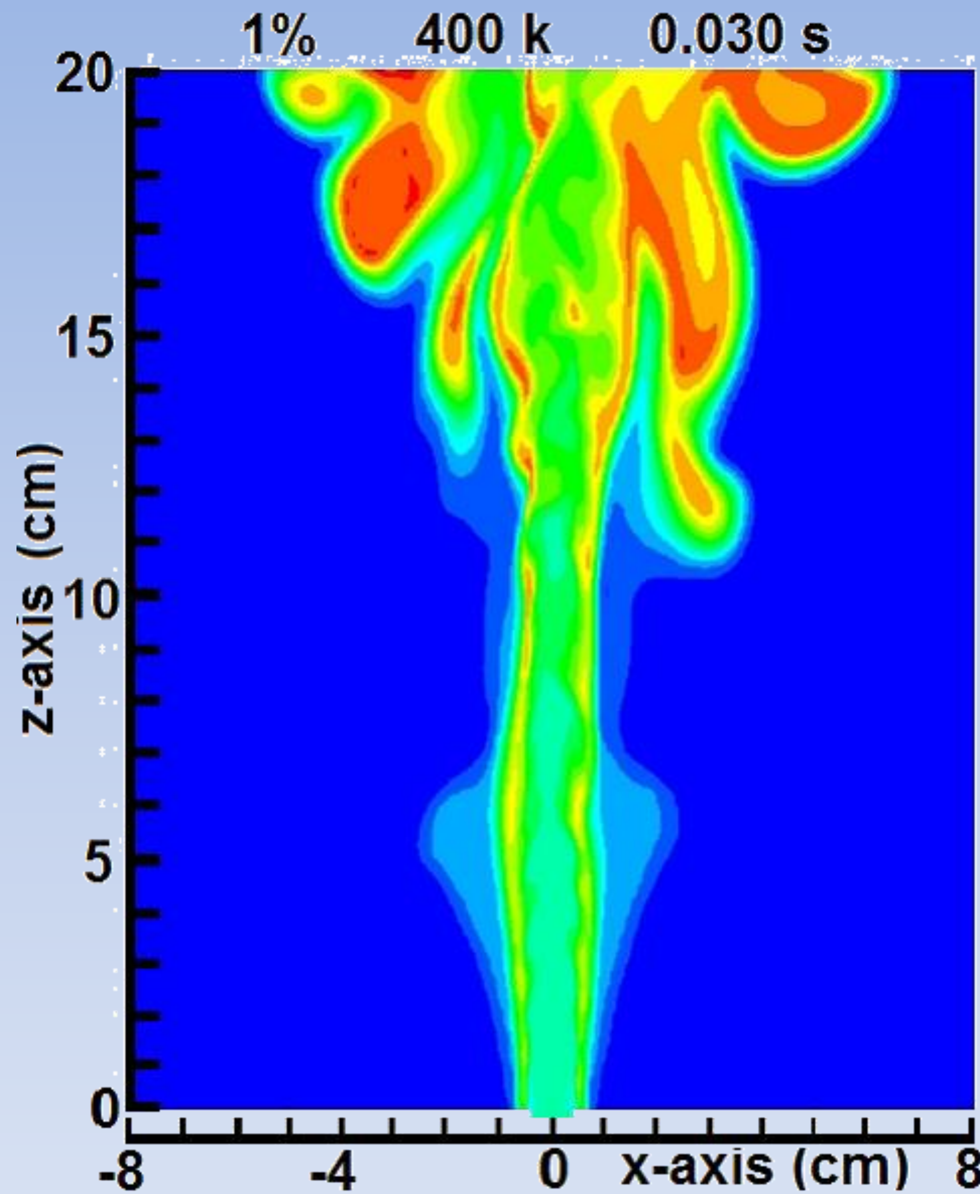

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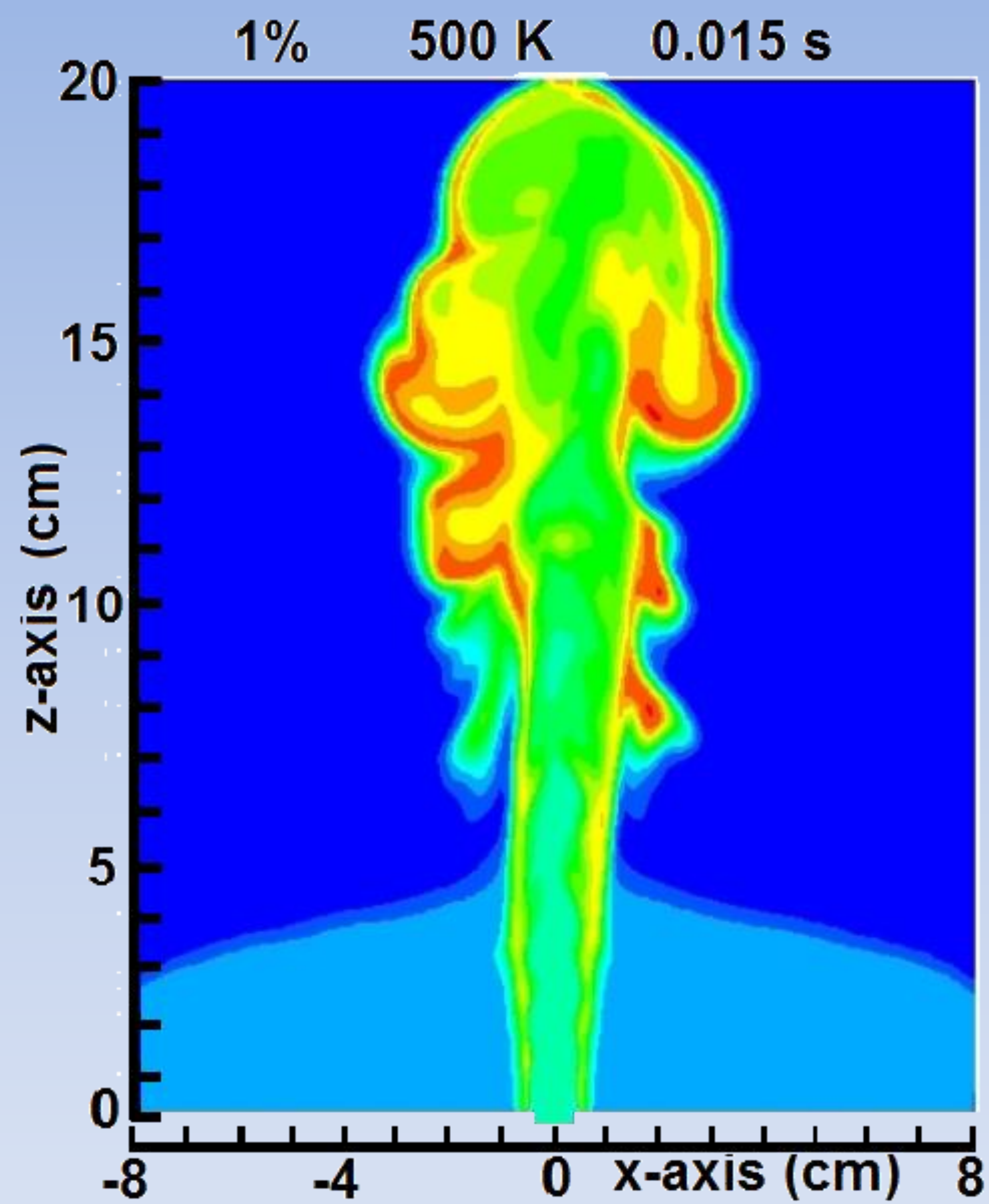

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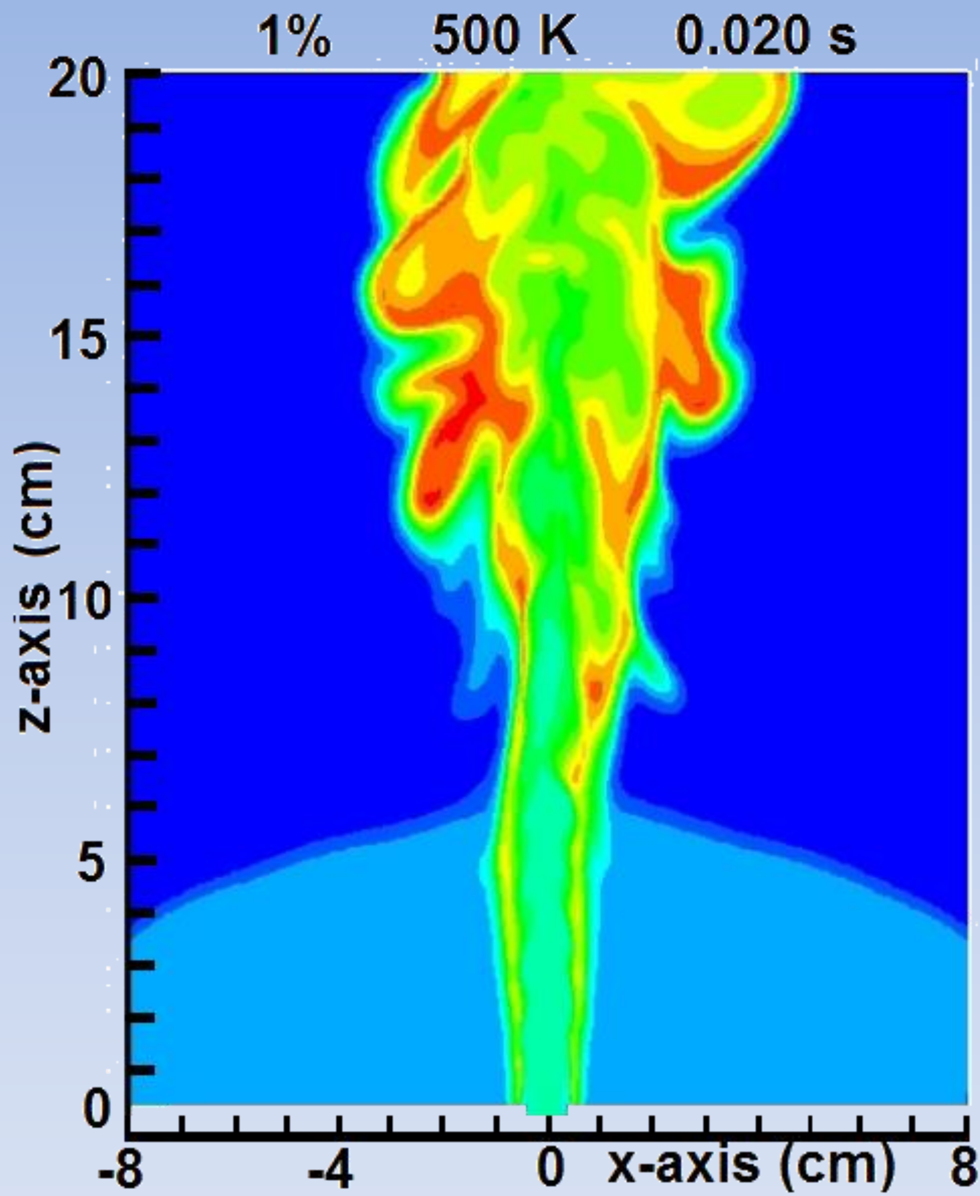

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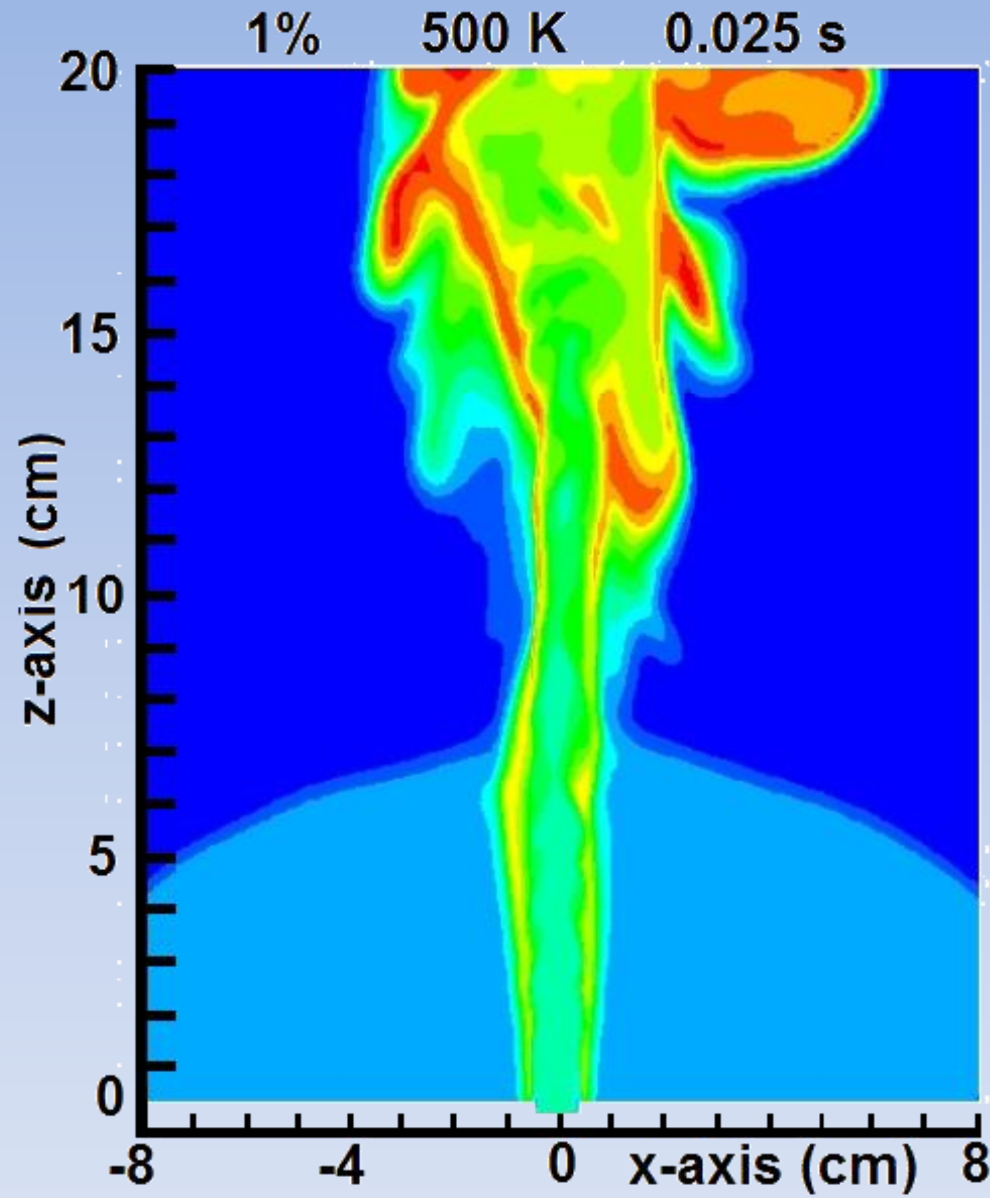

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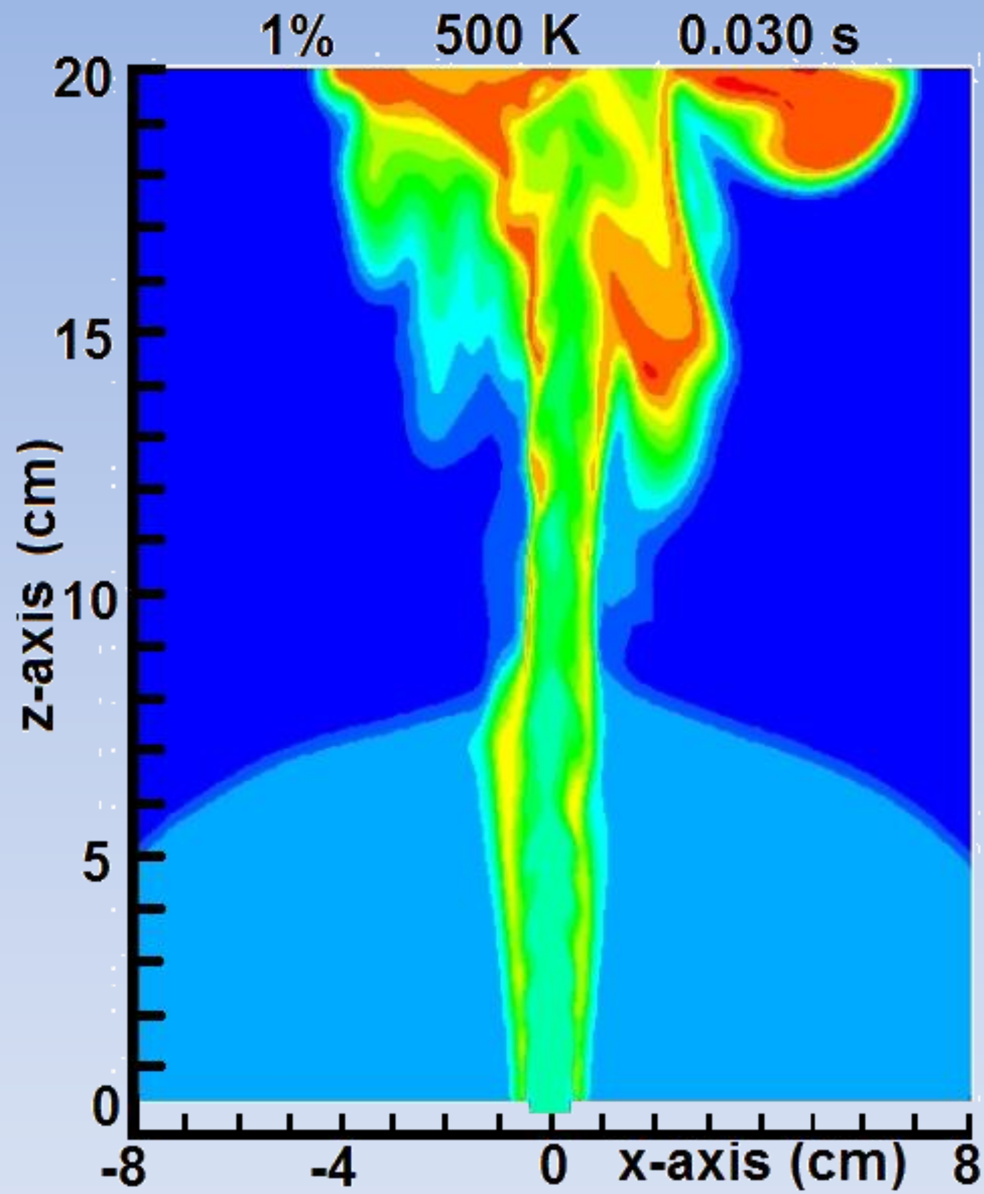

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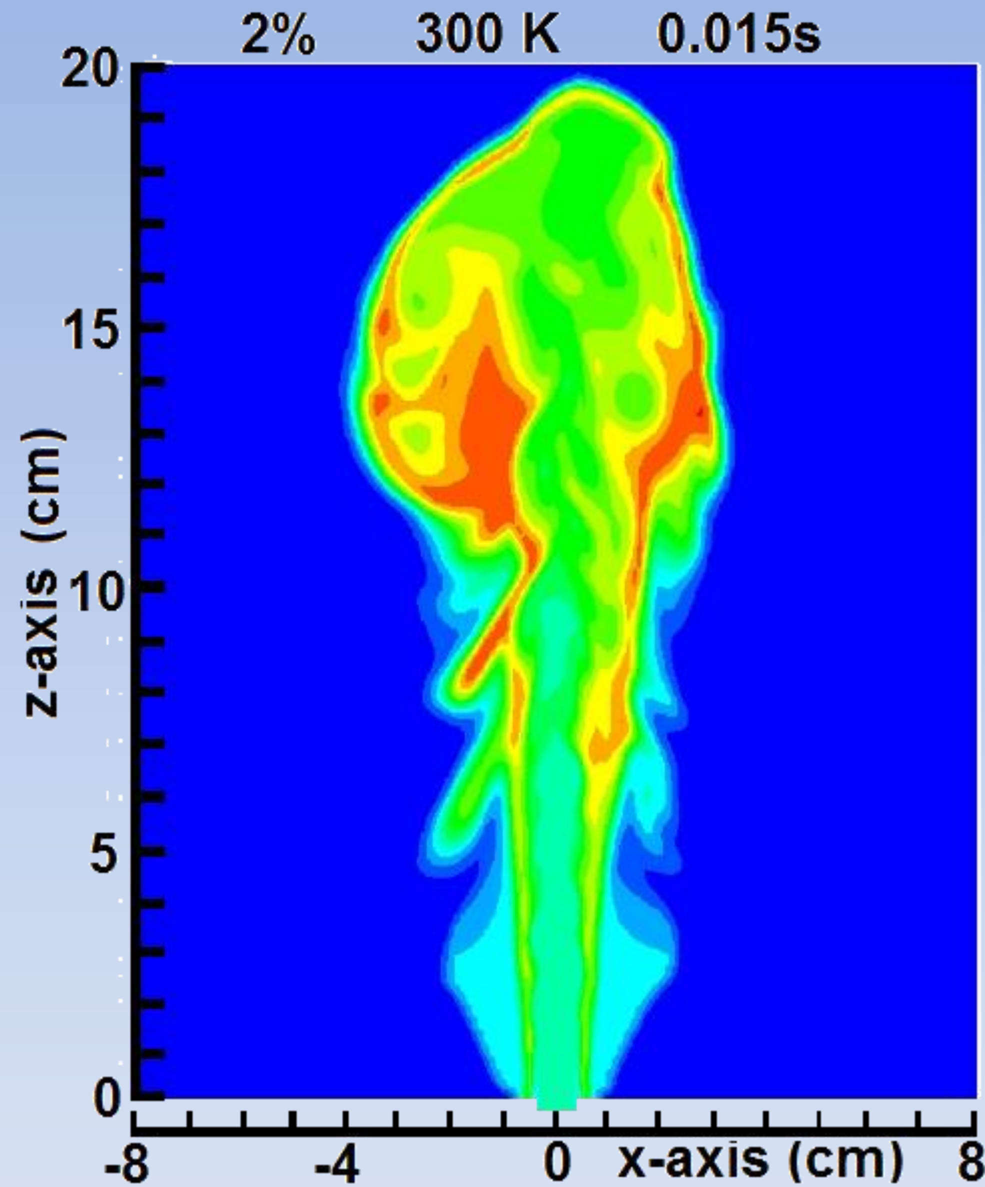

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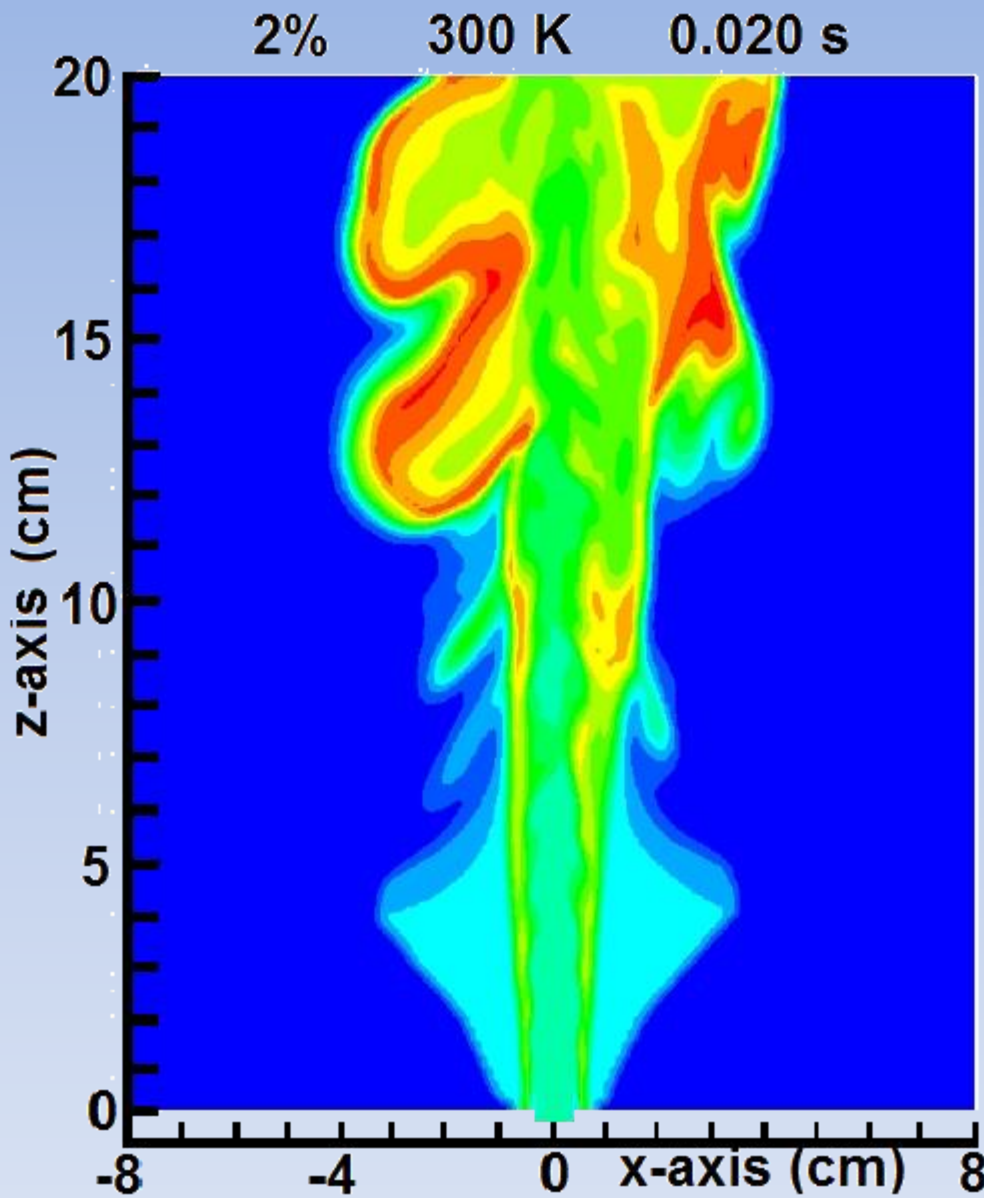
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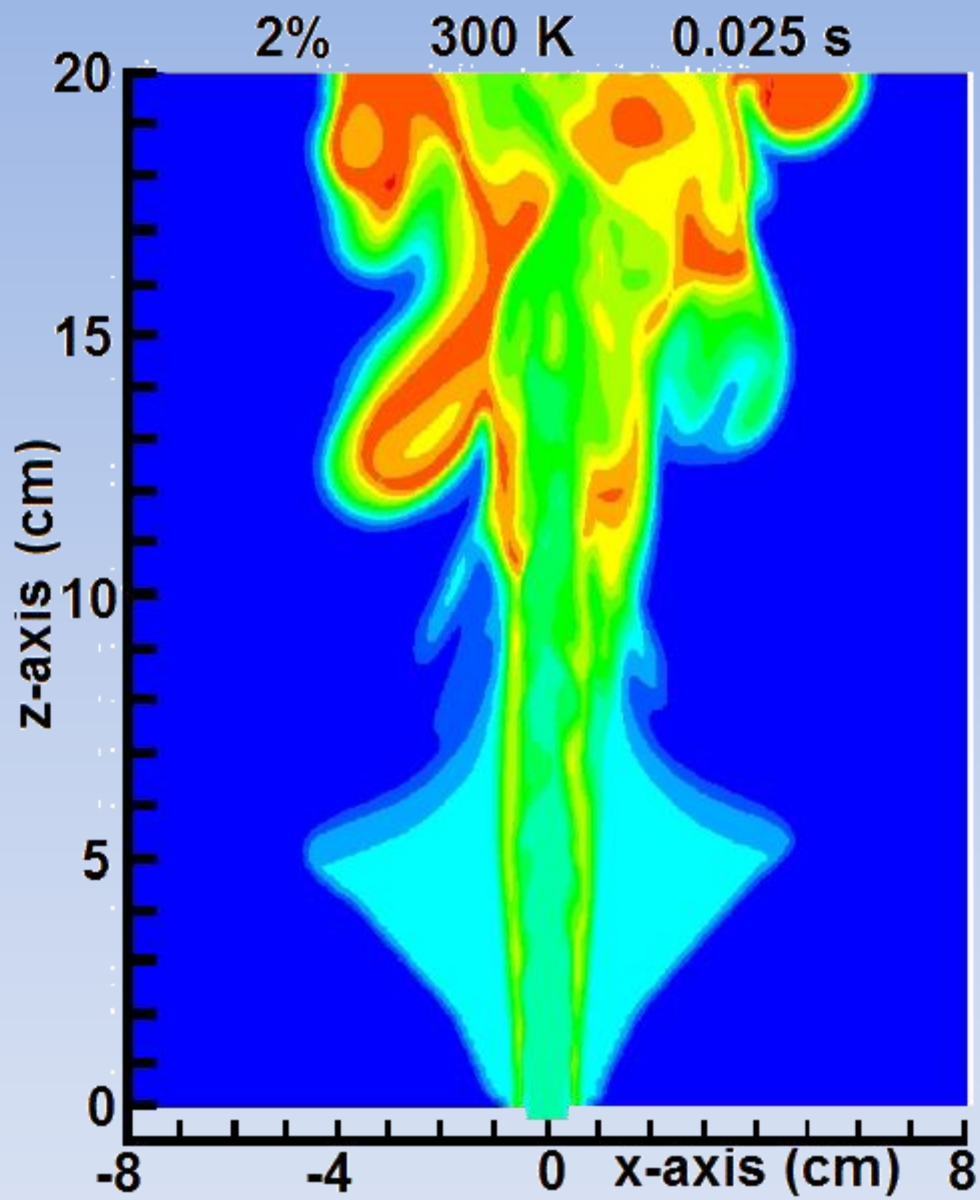

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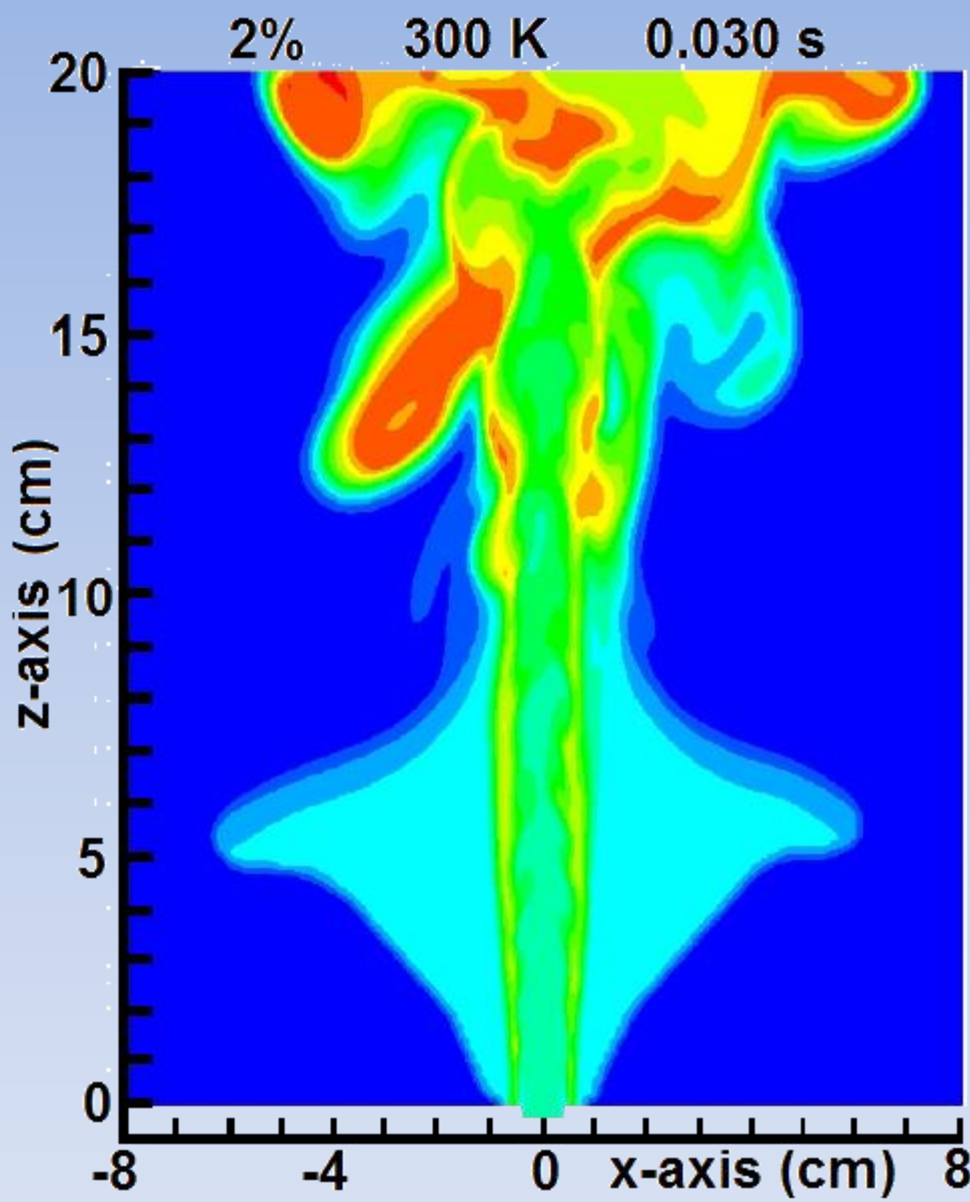

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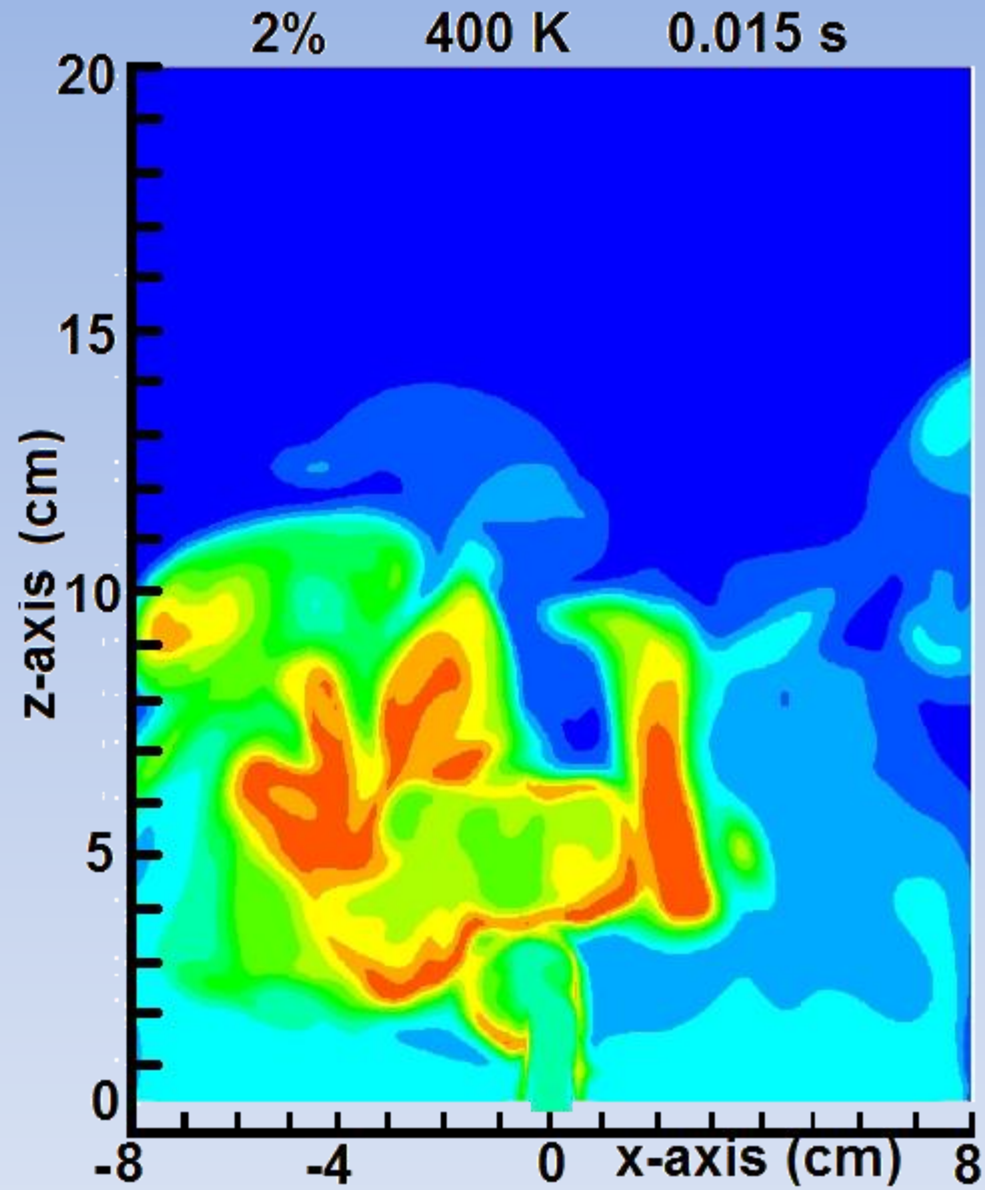

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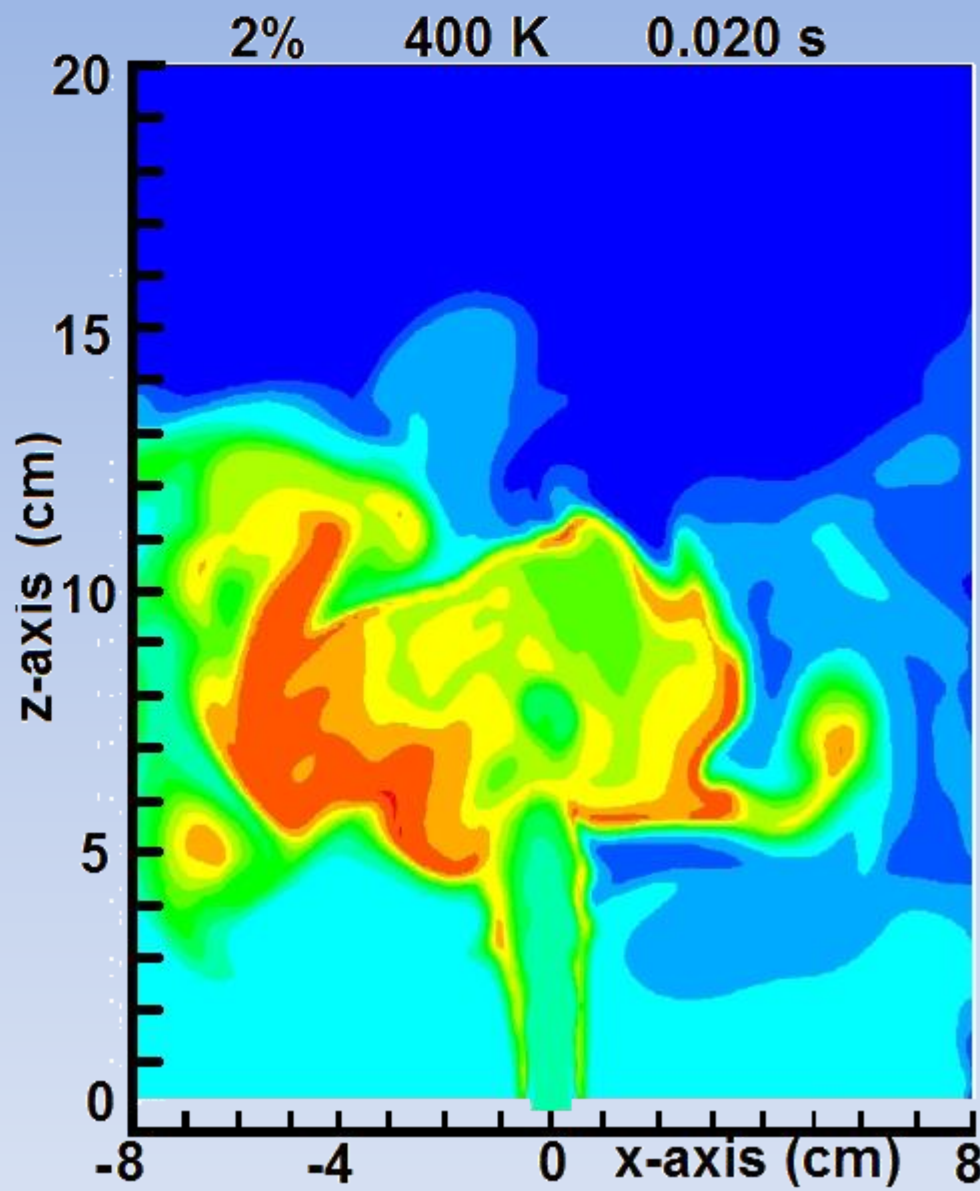

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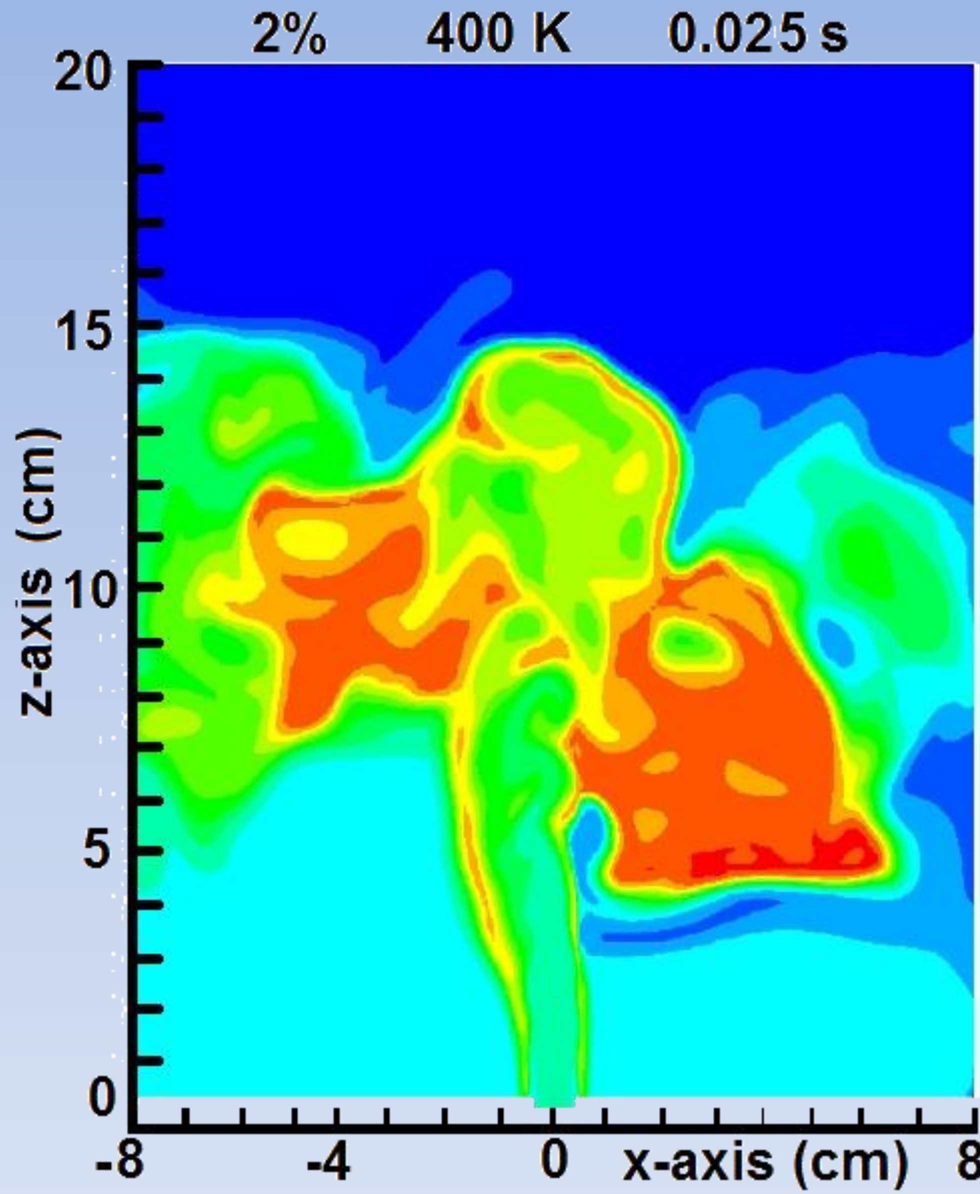

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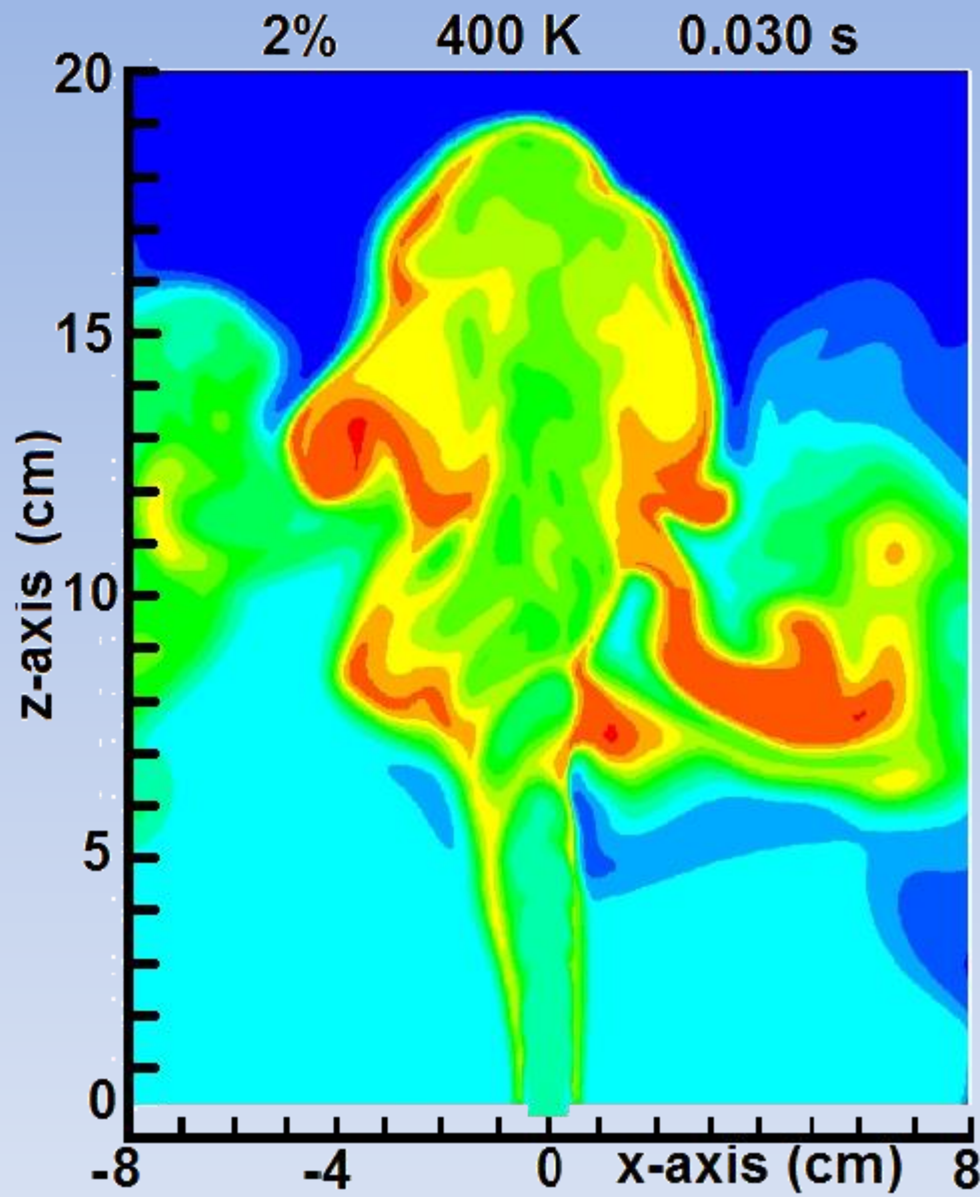

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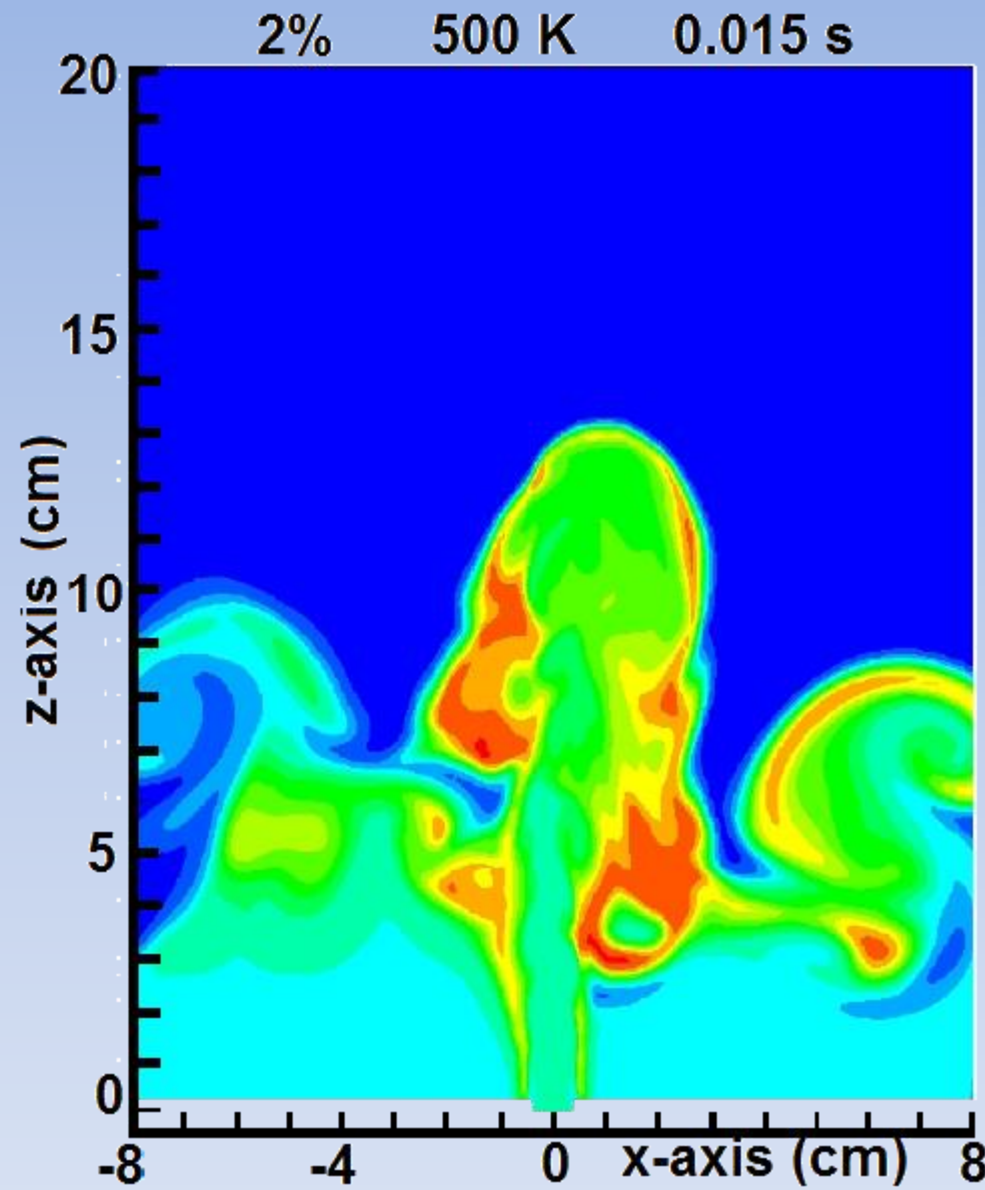

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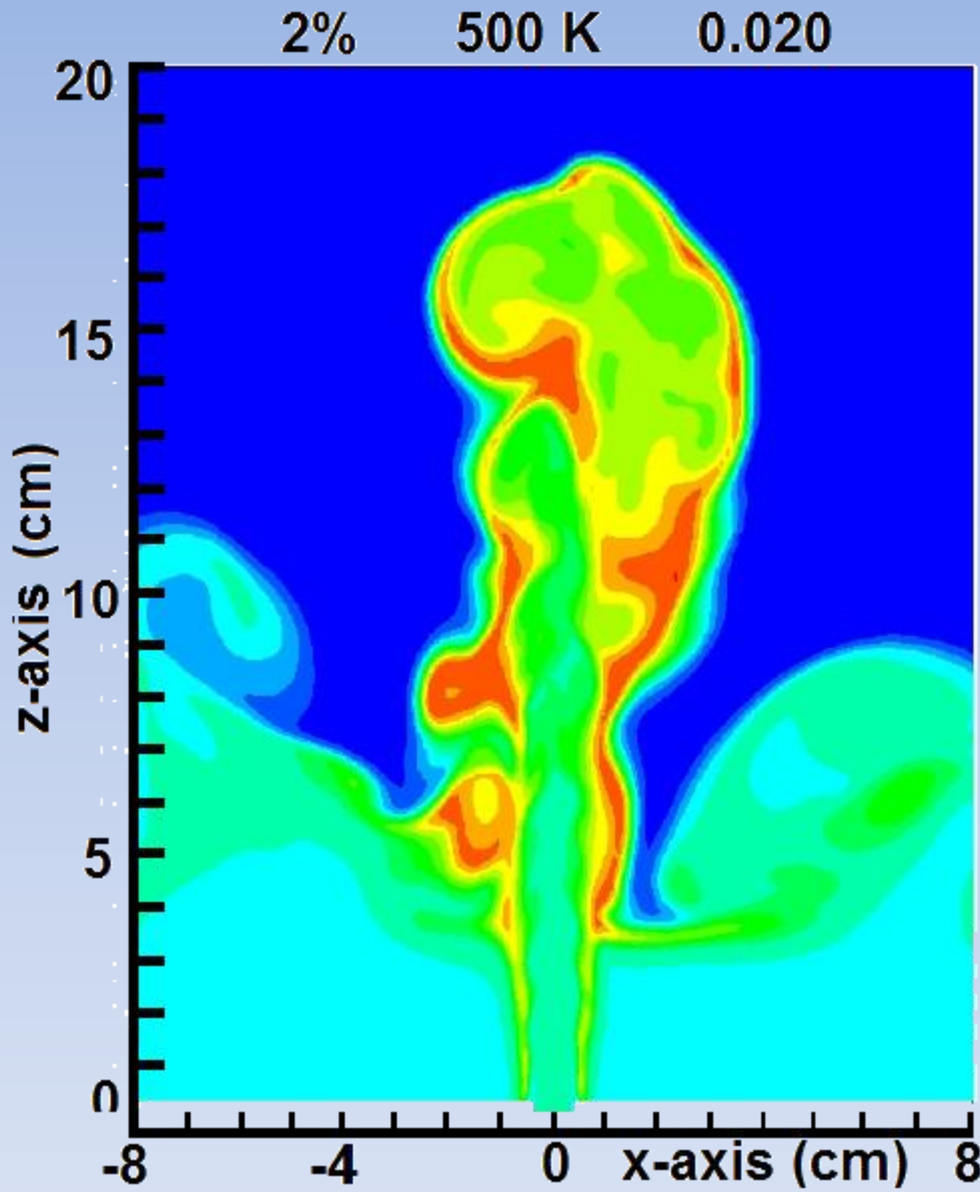

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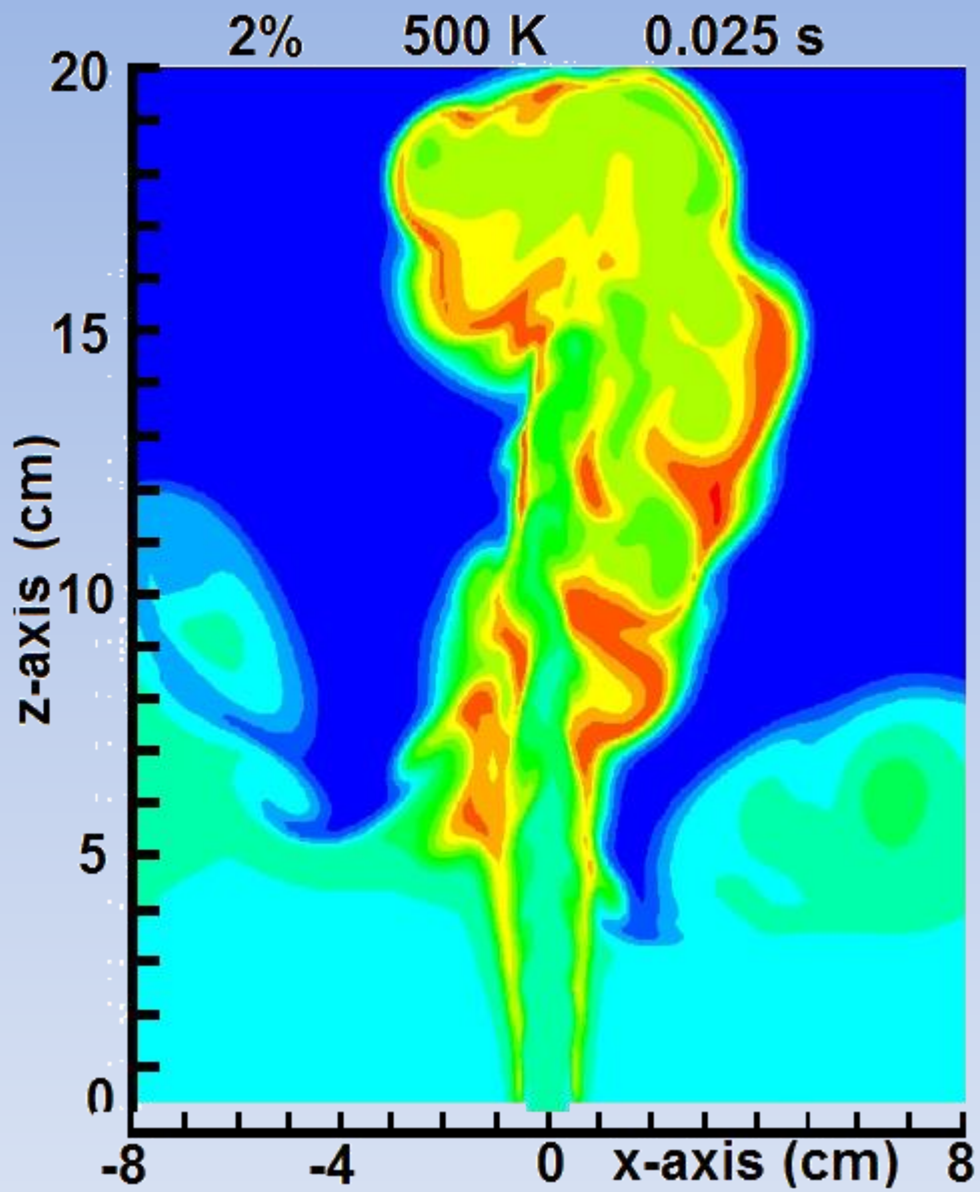

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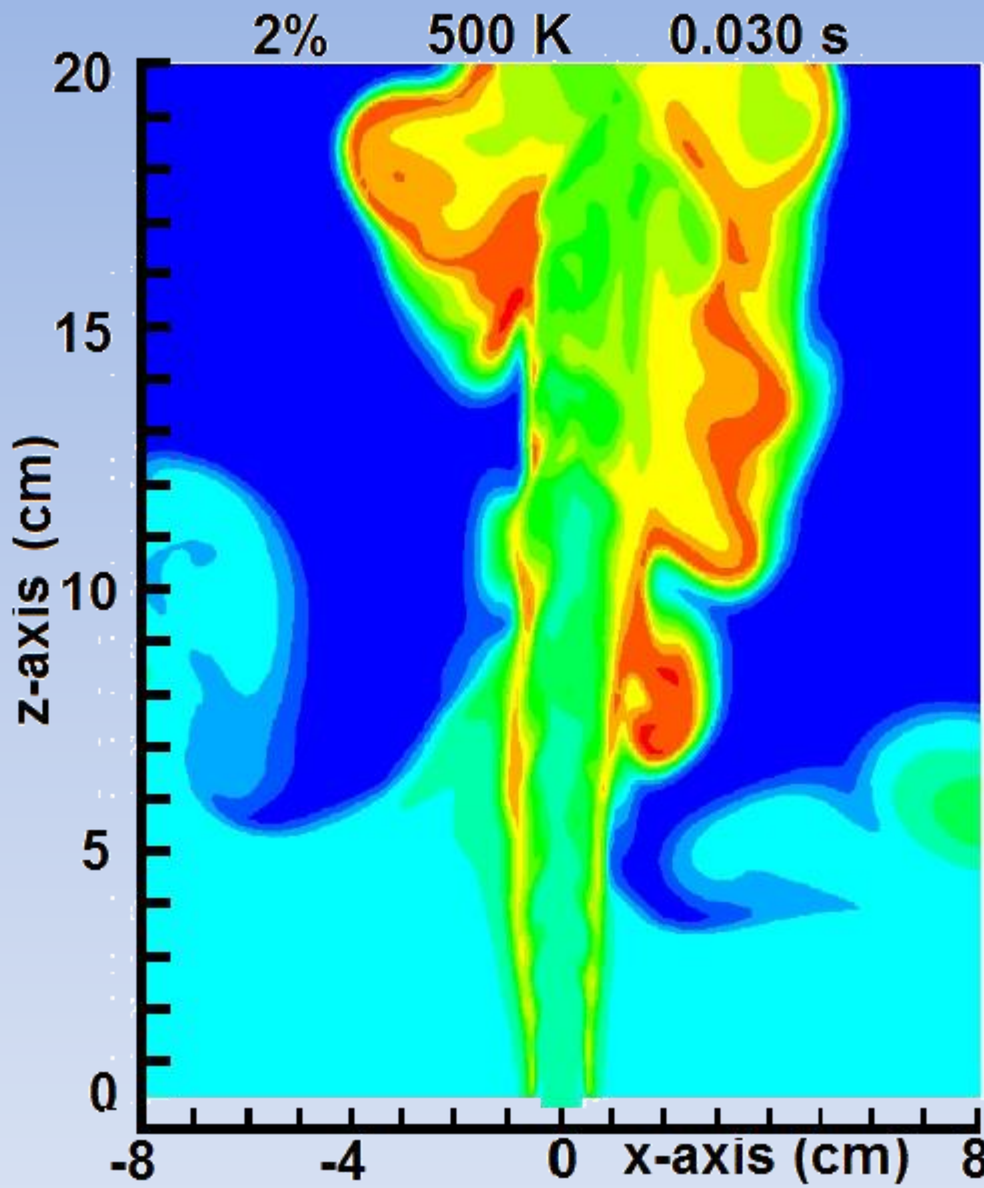

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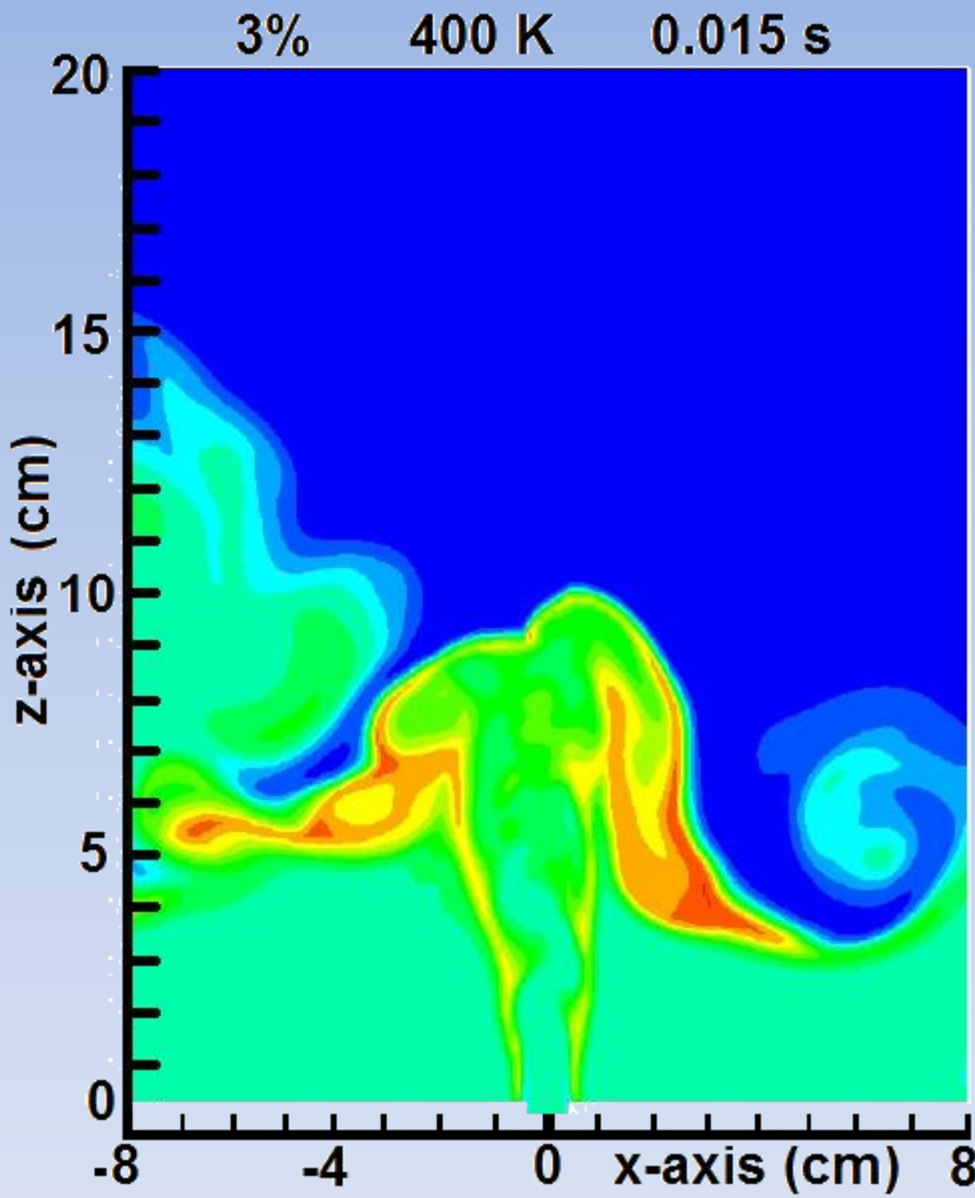

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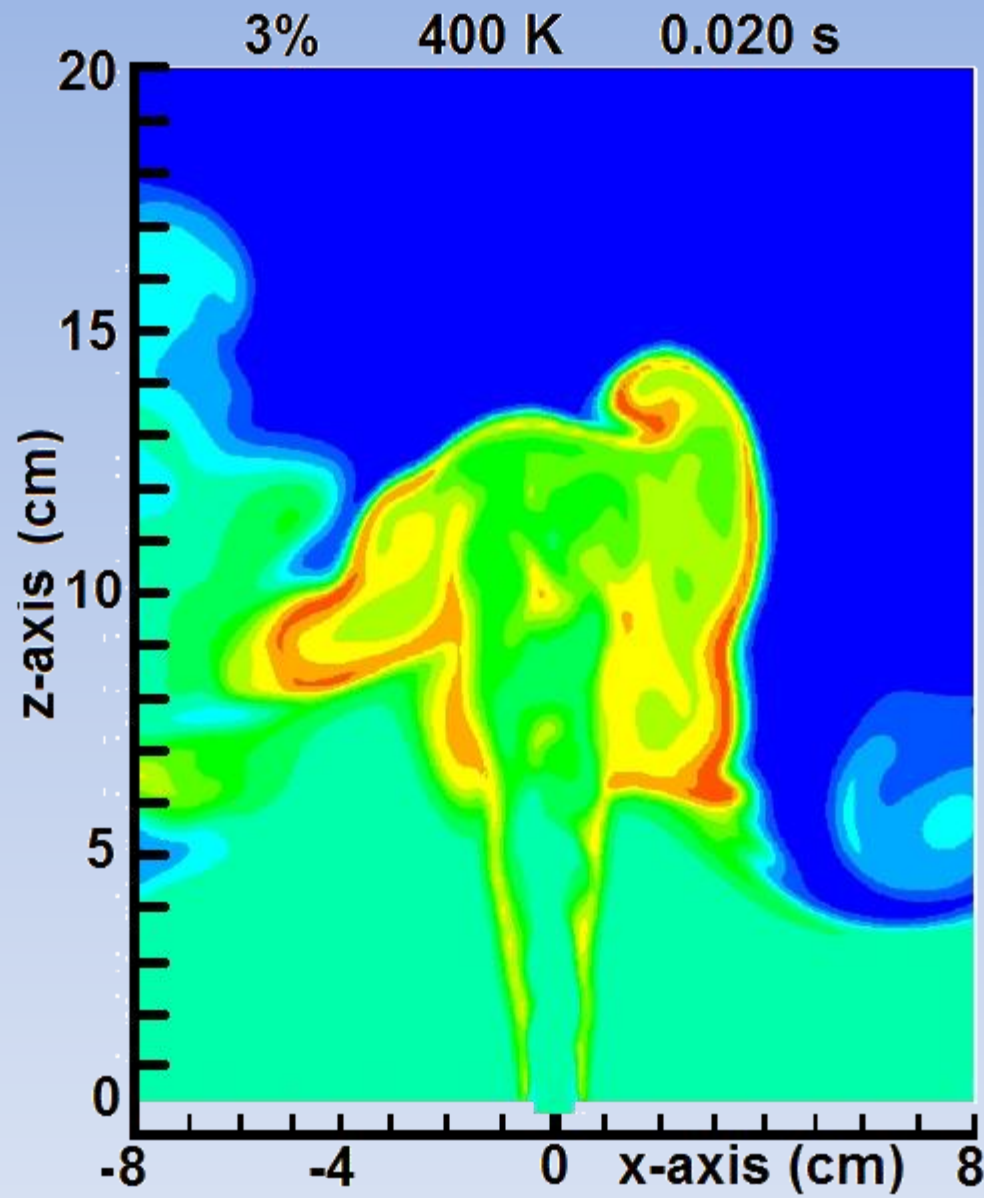

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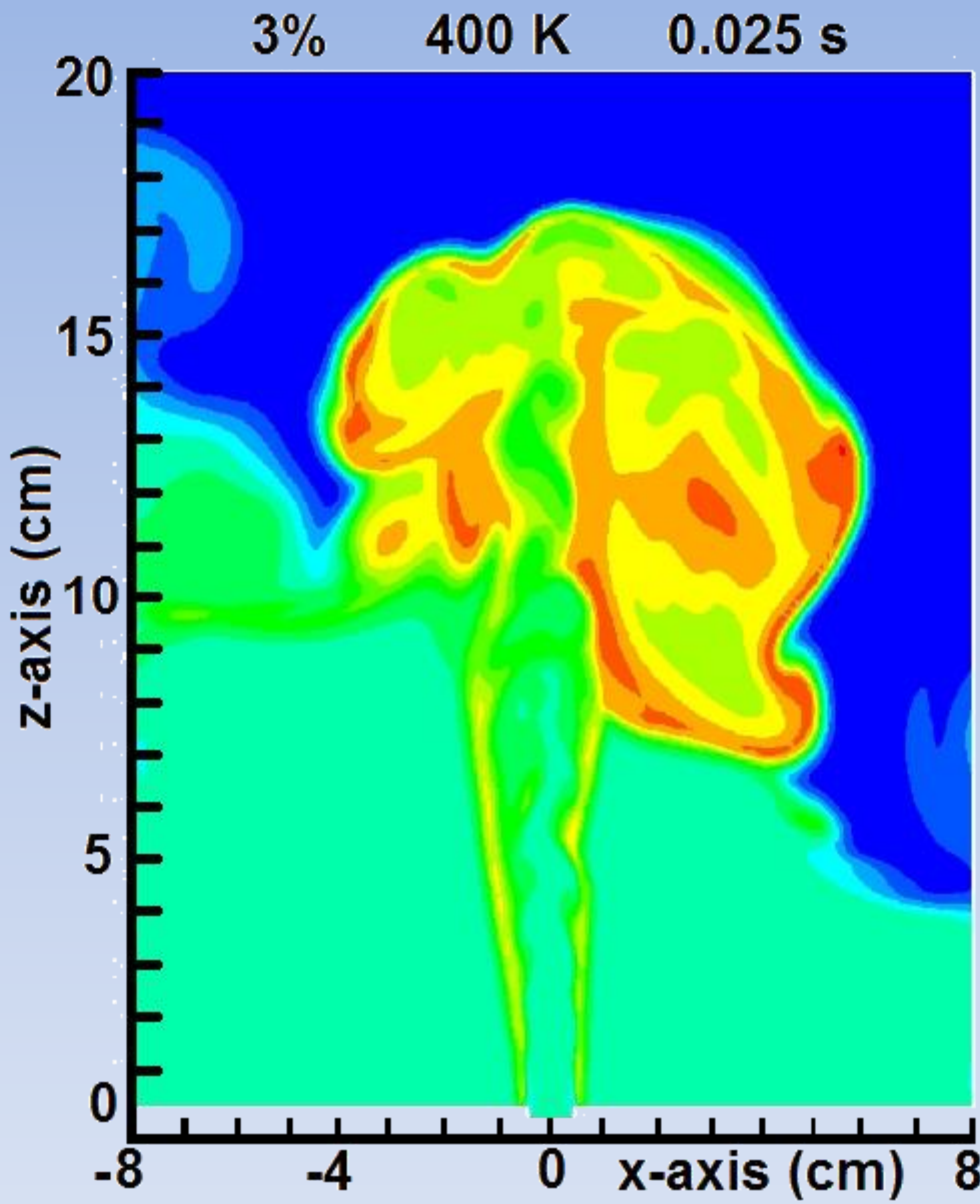

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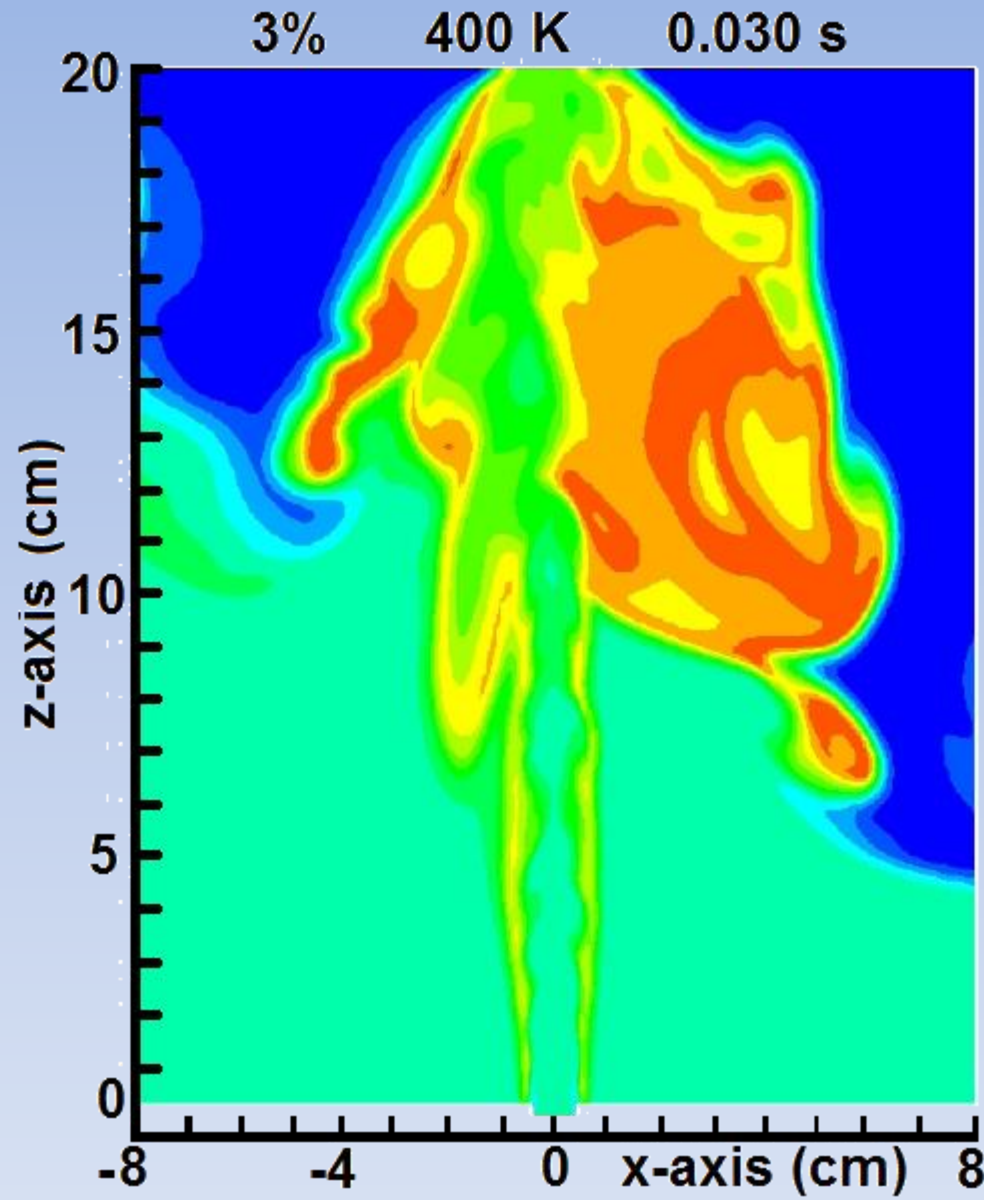

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C.S.M.
LABORIS GLORIA LUDI

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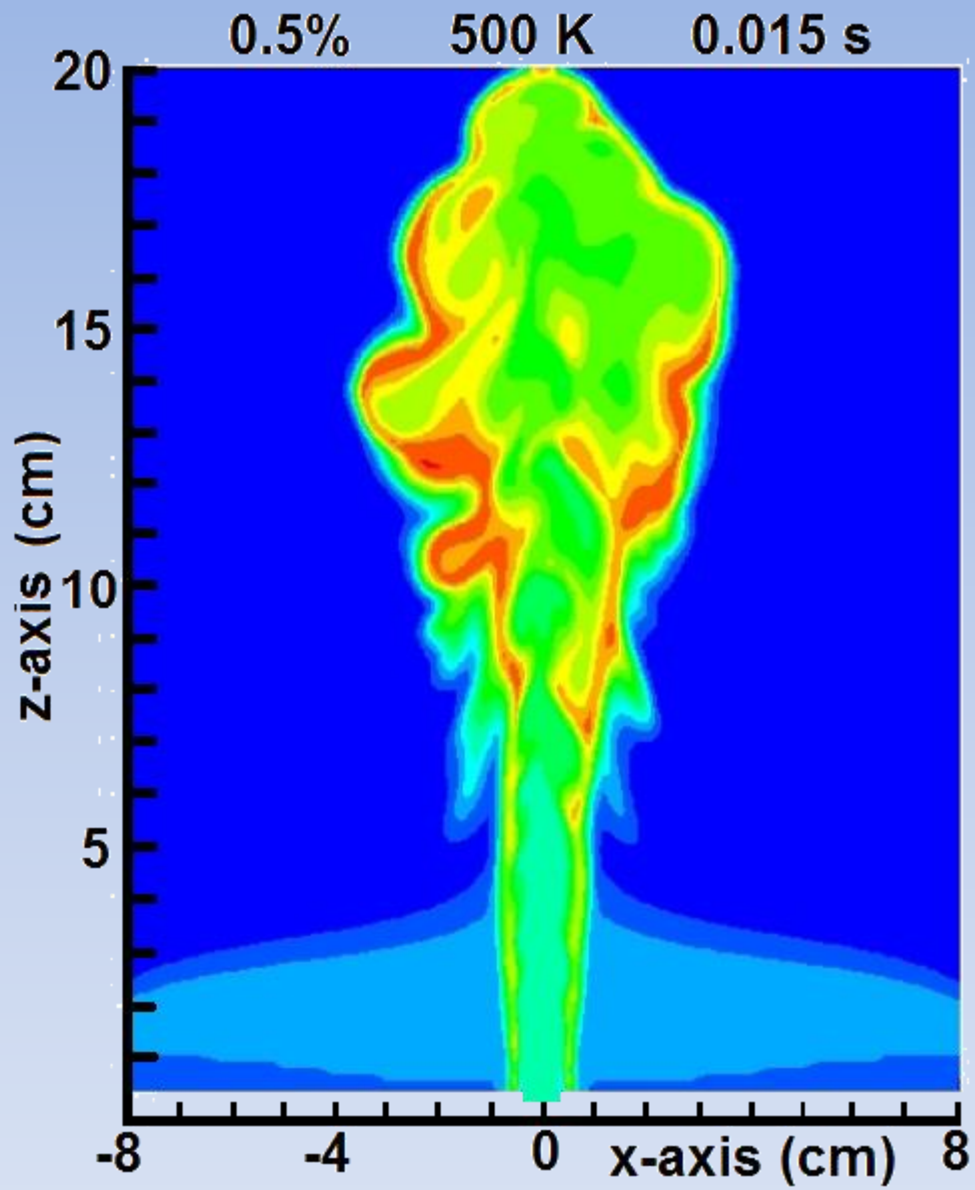

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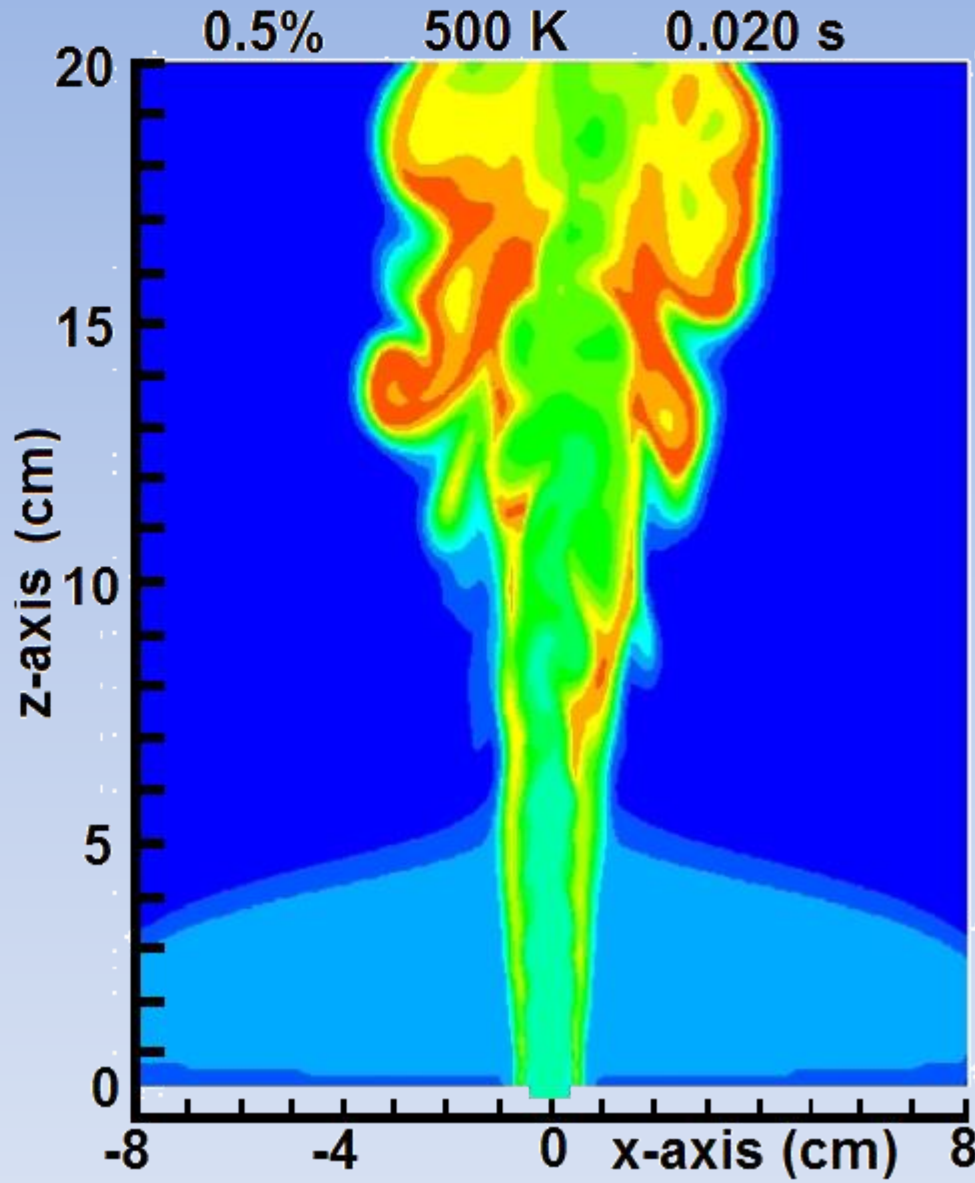

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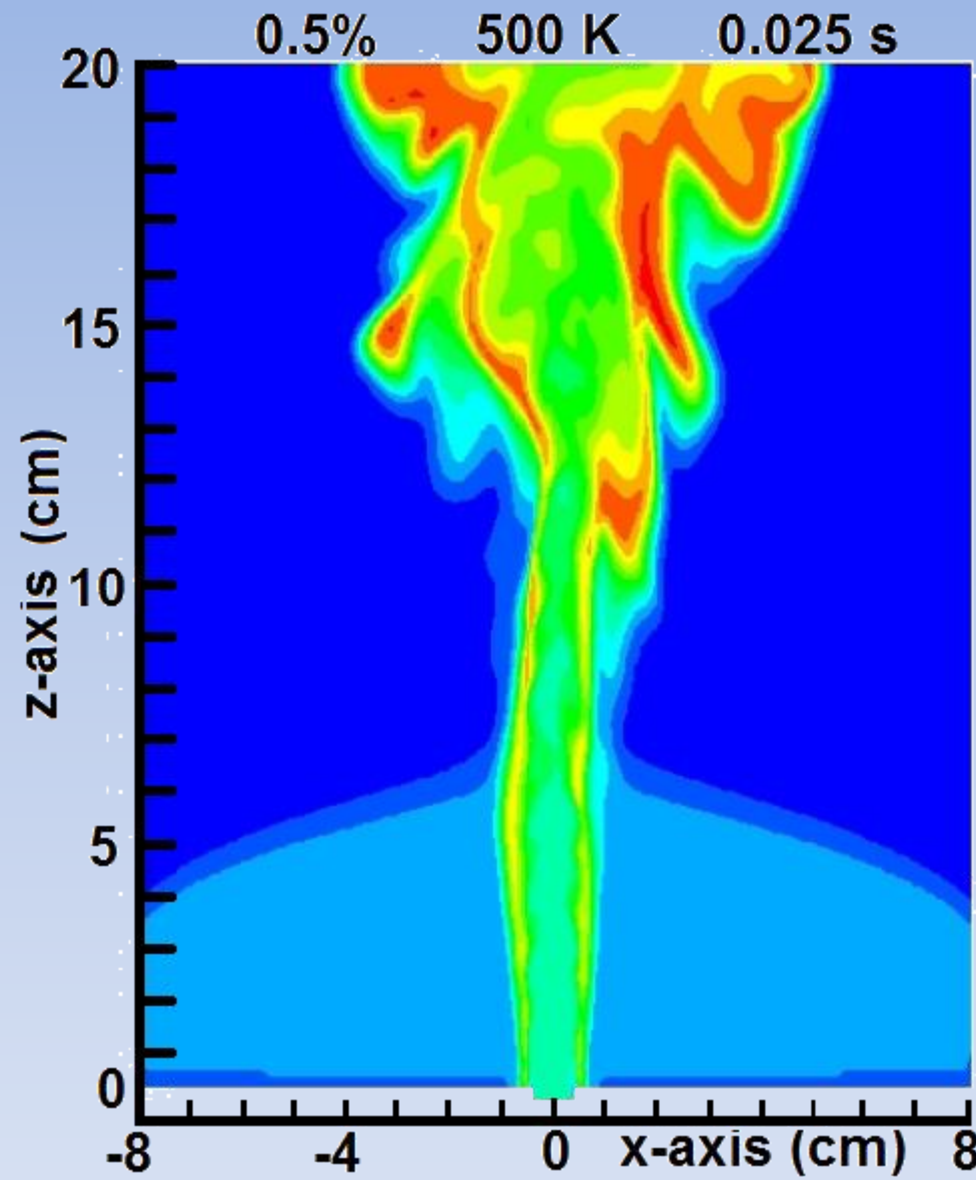

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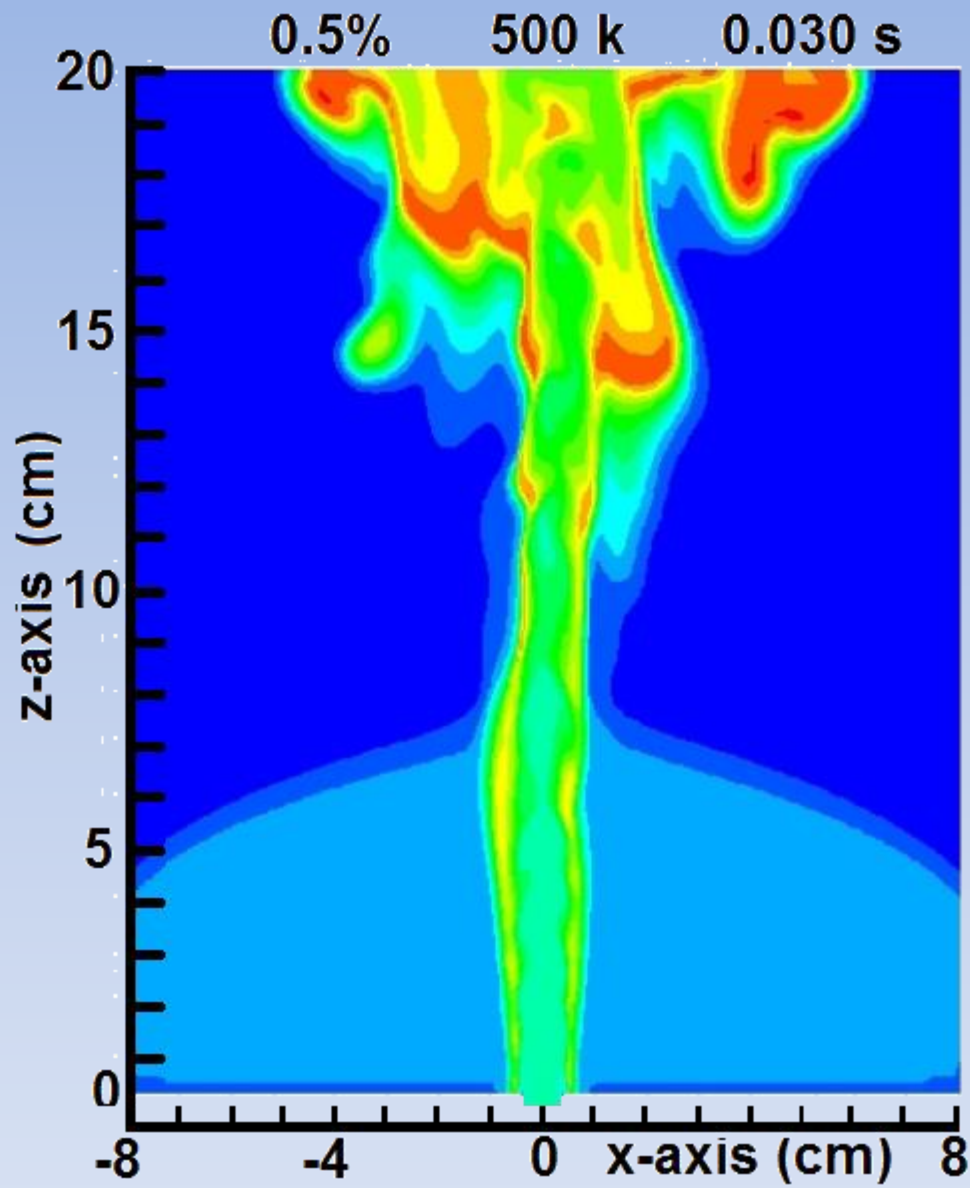

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The key result is the 0.5% VAM concentration Sufficient to justify the argument that the

VamTurBurner© design is viable.

Thank you

Questions