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Crucible Furnace: The future

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Introduction

- In Mexico, the estimated consumption of plastics is 66 kg/person/y.
- The most commonly used plastics are polypropylene (PP), polyethylene (PE), and polyethylene terephthalate (PET).
- Mechanical recycling remains the most widely used method for PET recycling
- PET combustion reducing the mass of solids waste by 70 % and can generate 475.73 kJ/kg.
- This energy is used in industrial processes that require heat energy, such as the cement industry and metal smelting.
- Previous research has involved experiments on mechanical recycling, PET combustion in combination with other fuels, plastic mixtures combustion and pyrolysis.
- This article presents the results of numerical simulation of the PET combustion process with energy recovery, applied in a crucible furnace using CFD

Chemical reactions

$$10C_{10}H_8O_4 + 48O_2 \rightarrow 61CO_2 + 4H_2O + 2CH_4 + 10CO + 4C_4H_{10} + 2C_2H_4 + C_7H_8 + 4H_2$$

$$6C_{10}H_8O_4 \rightarrow 8C_6H_6 + 12CO_2$$

$$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$$

$$CO + 0.5O_2 \rightarrow CO_2$$

$$H_2 + 0.5O_2 \rightarrow H_2O$$

$$C_4H_{10} + 0.5O_2 + 0.5H_2O \rightarrow C_4H_9 + H_2O$$

$$4C_4H_9 + O_2 \rightarrow C_3H_6 + C_4H_9O_2 + CH_3 + C_2H_4 + C_2H_5 + C_4H_8 + 0.5H_2$$

$$C_4H_9O_2 \rightarrow C_4H_8O_2H$$

$$C_4H_8O_2H \rightarrow C_4H_8 + O_2 + 0.5H_2$$

Stoichiometry

Reactivos				Productos											
m PET [gr/s]	mol PET	O2 PET	O2 gas	CO2 PET	CO2 gas	H2O PET	H2O gas		O2 total	CO2 Total	H2O total	N2 mol	masa aire [g/s]	aire [kg/s]	execo aire (20%)
1.0	0.0052083	0.0520833	14.028213	0.0520833	8.6108934	0.0208333	10.834639		14.080296	8.6629768	10.855473	52.941915	1932.943103	1.9329431	2.319531724
2.0	0.0104167	0.1041667	14.028213	0.1041667	8.6108934	0.0416667	10.834639		14.13238	8.7150601	10.876306	53.137748	1940.093103	1.9400931	2.328111724
3.0	0.015625	0.15625	14.028213	0.15625	8.6108934	0.0625	10.834639		14.184463	8.7671434	10.897139	53.333582	1947.243103	1.9472431	2.336691724
4.0	0.0208333	0.2083333	14.028213	0.2083333	8.6108934	0.0833333	10.834639		14.236546	8.8192268	10.917973	53.529415	1954.393103	1.9543931	2.345271724
5.0	0.0260417	0.2604167	14.028213	0.2604167	8.6108934	0.1041667	10.834639		14.28863	8.8713101	10.938806	53.725248	1961.543103	1.9615431	2.353851724
6.0	0.03125	0.3125	14.028213	0.3125	8.6108934	0.125	10.834639		14.340713	8.9233934	10.959639	53.921082	1968.693103	1.9686931	2.362431724
7.0	0.0364583	0.3645833	14.028213	0.3645833	8.6108934	0.1458333	10.834639		14.392796	8.9754768	10.980473	54.116915	1975.843103	1.9758431	2.371011724
8.0	0.0416667	0.4166667	14.028213	0.4166667	8.6108934	0.1666667	10.834639		14.44488	9.0275601	11.001306	54.312748	1982.993103	1.9829931	2.379591724
9.0	0.046875	0.46875	14.028213	0.46875	8.6108934	0.1875	10.834639		14.496963	9.0796434	11.022139	54.508582	1990.143103	1.9901431	2.388171724
10.0	0.0520833	0.5208333	14.028213	0.5208333	8.6108934	0.2083333	10.834639		14.549046	9.1317268	11.042973	54.704415	1997.293103	1.9972931	2.396751724
20.0	0.1041667	1.0416667	14.028213	1.0416667	8.6108934	0.4166667	10.834639		15.06988	9.6525601	11.251306	56.662748	2068.793103	2.0687931	2.482551724
30.0	0.15625	1.5625	14.028213	1.5625	8.6108934	0.625	10.834639		15.590713	10.173393	11.459639	58.621082	2140.293103	2.1402931	2.568351724
40.0	0.2083333	2.0833333	14.028213	2.0833333	8.6108934	0.8333333	10.834639		16.111546	10.694227	11.667973	60.579415	2211.793103	2.2117931	2.654151724
50.0	0.2604167	2.6041667	14.028213	2.6041667	8.6108934	1.0416667	10.834639		16.63238	11.21506	11.876306	62.537748	2283.293103	2.2832931	2.739951724
60.0	0.3125	3.125	14.028213	3.125	8.6108934	1.25	10.834639		17.153213	11.735893	12.084639	64.496082	2354.793103	2.3547931	2.825751724
70.0	0.3645833	3.6458333	14.028213	3.6458333	8.6108934	1.4583333	10.834639		17.674046	12.256727	12.292973	66.454415	2426.293103	2.4262931	2.911551724
80.0	0.4166667	4.1666667	14.028213	4.1666667	8.6108934	1.6666667	10.834639		18.19488	12.77756	12.501306	68.412748	2497.793103	2.4977931	2.997351724
90.0	0.46875	4.6875	14.028213	4.6875	8.6108934	1.875	10.834639		18.715713	13.298393	12.709639	70.371082	2569.293103	2.5692931	3.083151724
100.0	0.5208333	5.2083333	14.028213	5.2083333	8.6108934	2.0833333	10.834639		19.236546	13.819227	12.917973	72.329415	2640.793103	2.6407931	3.168951724

Mesh model and boundary conditions

CAD Model and mesh

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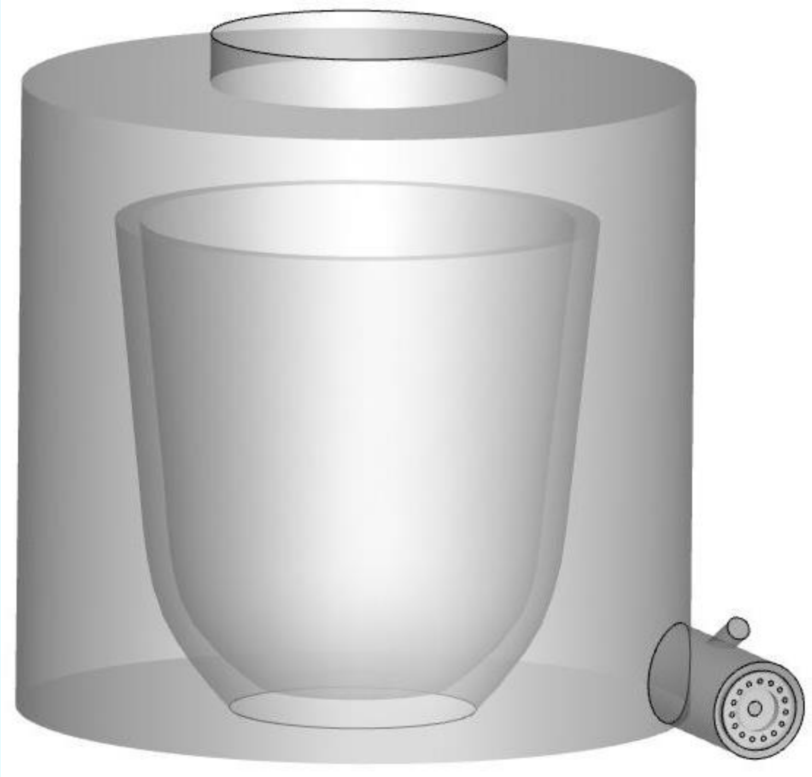

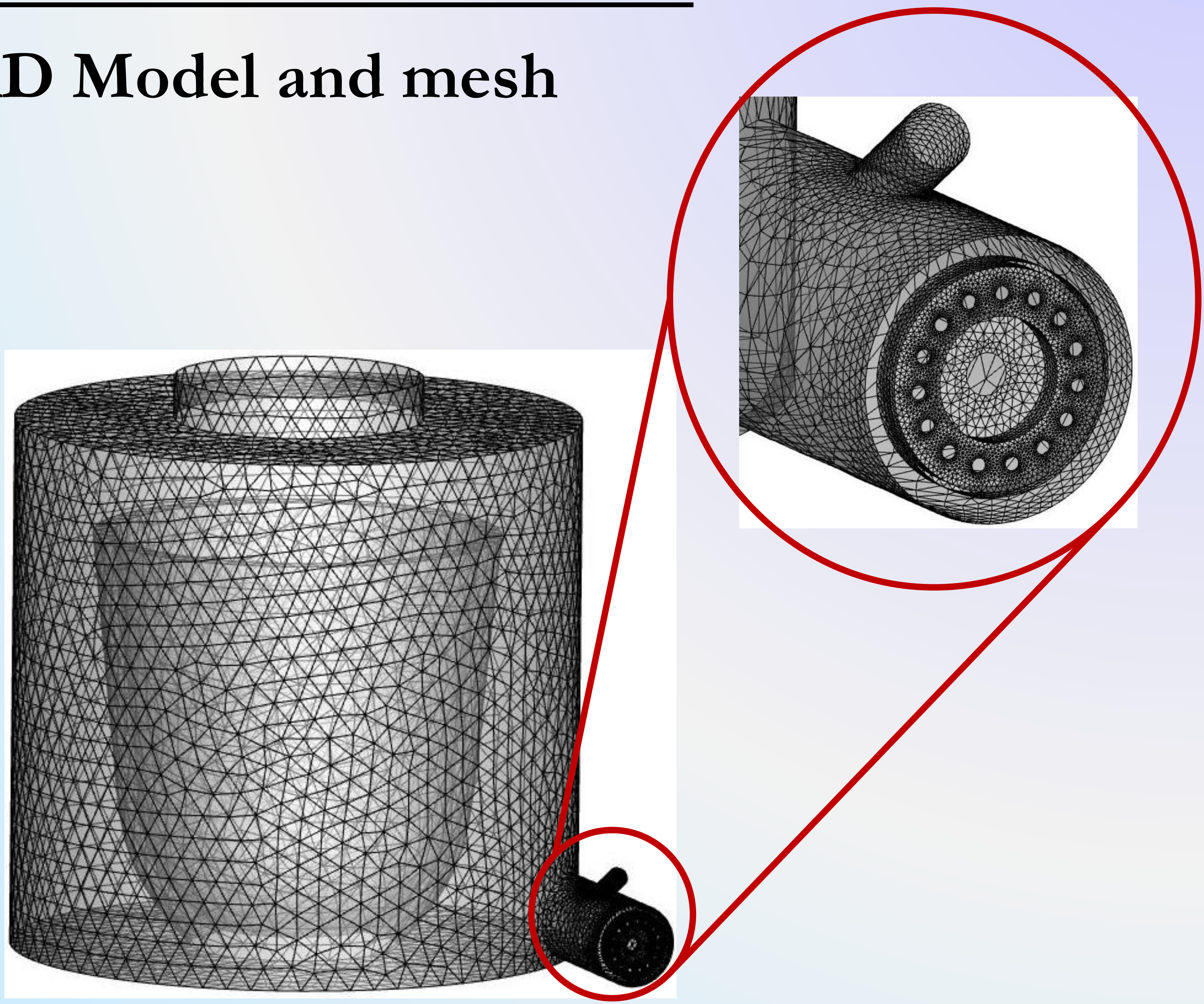

Numerical Model: Initial condition

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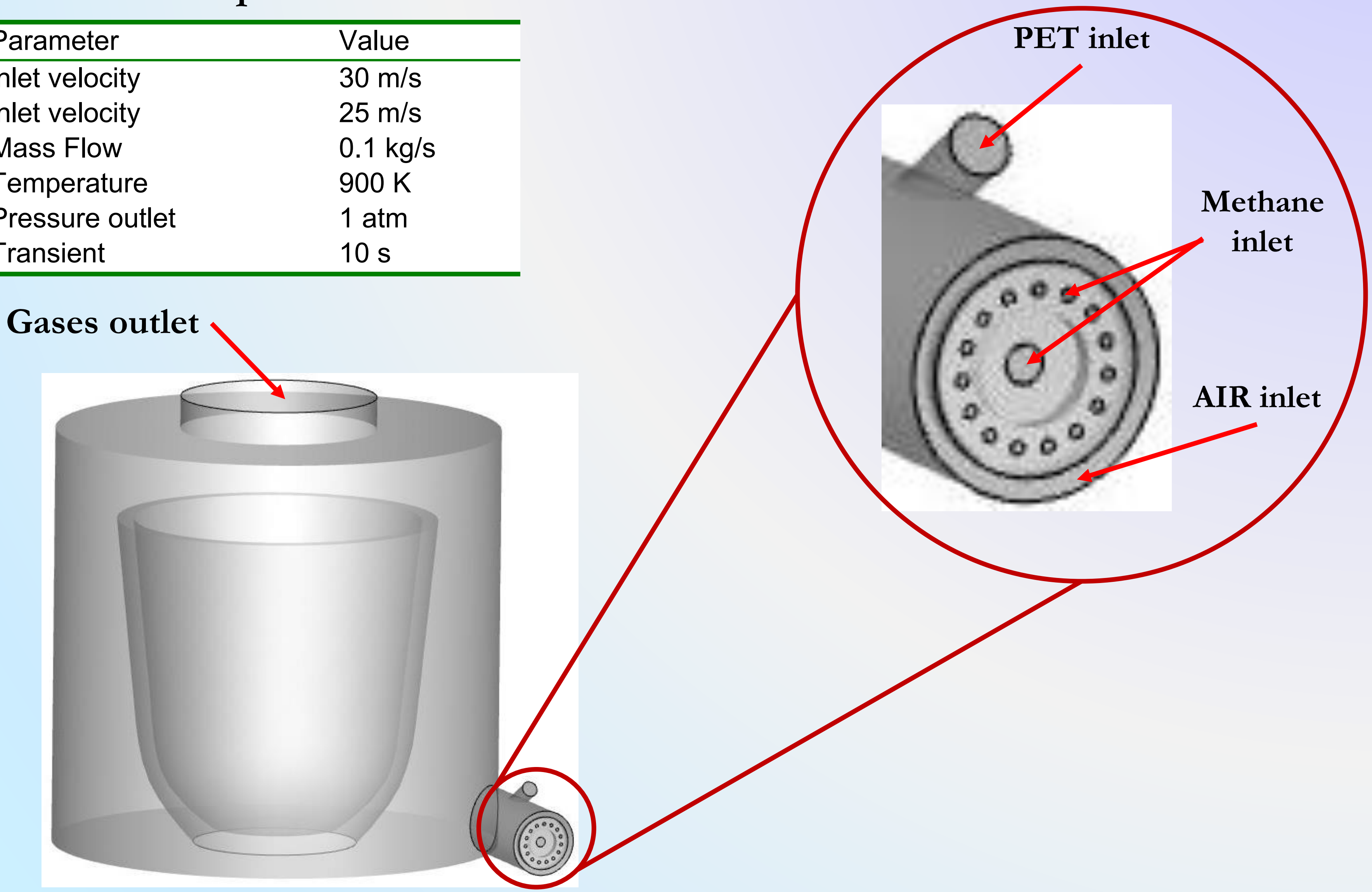
Simulation data of combustion process

Boundary condition type	Parameter	Value
Air inlet	inlet velocity	30 m/s
Methane gas inlet	inlet velocity	25 m/s
PET inlet	Mass Flow	0.1 kg/s
Furnace and crucible wall	Temperature	900 K
Gases outlet	Pressure outlet	1 atm
Time	Transient	10 s



Numerical Model: Equations

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=0$$ Mass conservation equation

$$\frac{\partial(\rho u)}{\partial t}+div(\rho u u)=-grad\ p+div(\tau)+F$$ Momentum equation

$$\frac{\partial}{\partial t}(\rho\kappa)+\frac{\partial}{\partial x_j}(\rho\kappa u_j)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{(\Pr_t)_\kappa}\right)\frac{\partial\kappa}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_\kappa$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_j}(\rho\varepsilon u_j)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{(\Pr_t)_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right]+\rho C_1 V\varepsilon-\rho C_2\frac{\varepsilon^2}{\kappa+\sqrt{\nu\varepsilon}}+C_{1\varepsilon}\frac{\varepsilon}{\kappa}C_{3\varepsilon}G_b+S_\varepsilon$$

Modelo K-ε Realizable

$$\frac{\partial(\rho E)}{\partial t}+div(\rho E u)=0$$ Energy conservation equation

Numerical Model: discretization schemes

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The spatial discretization schemes

Variable	Discrete scheme
Pressure-velocity coupling	Coupled
Pressure	PRESTO
Density	Quick
Momentum	Second order upwind
Species	Second order upwind
Energy	Second order upwind

Results. Hydrodynamic behavior

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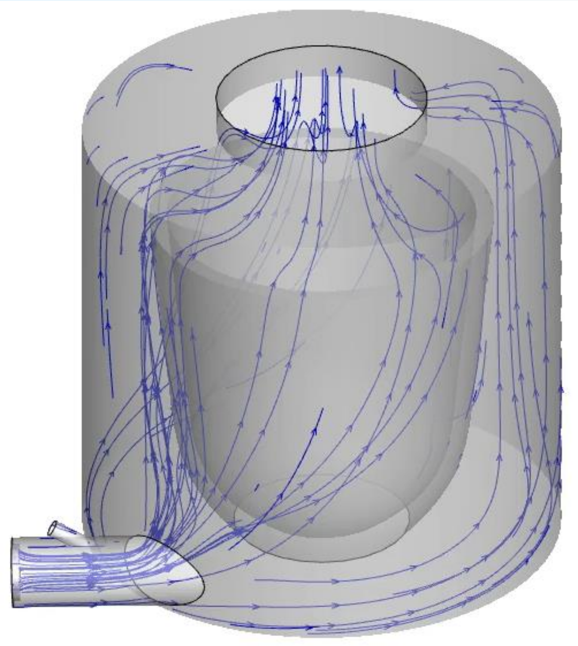
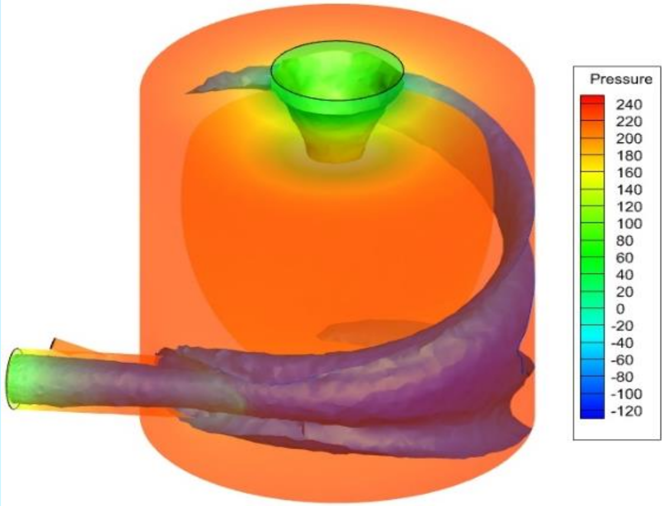
Pathlines of the flow





Pressure contours in the crucible furnace

Results. Thermal and chemical behavior

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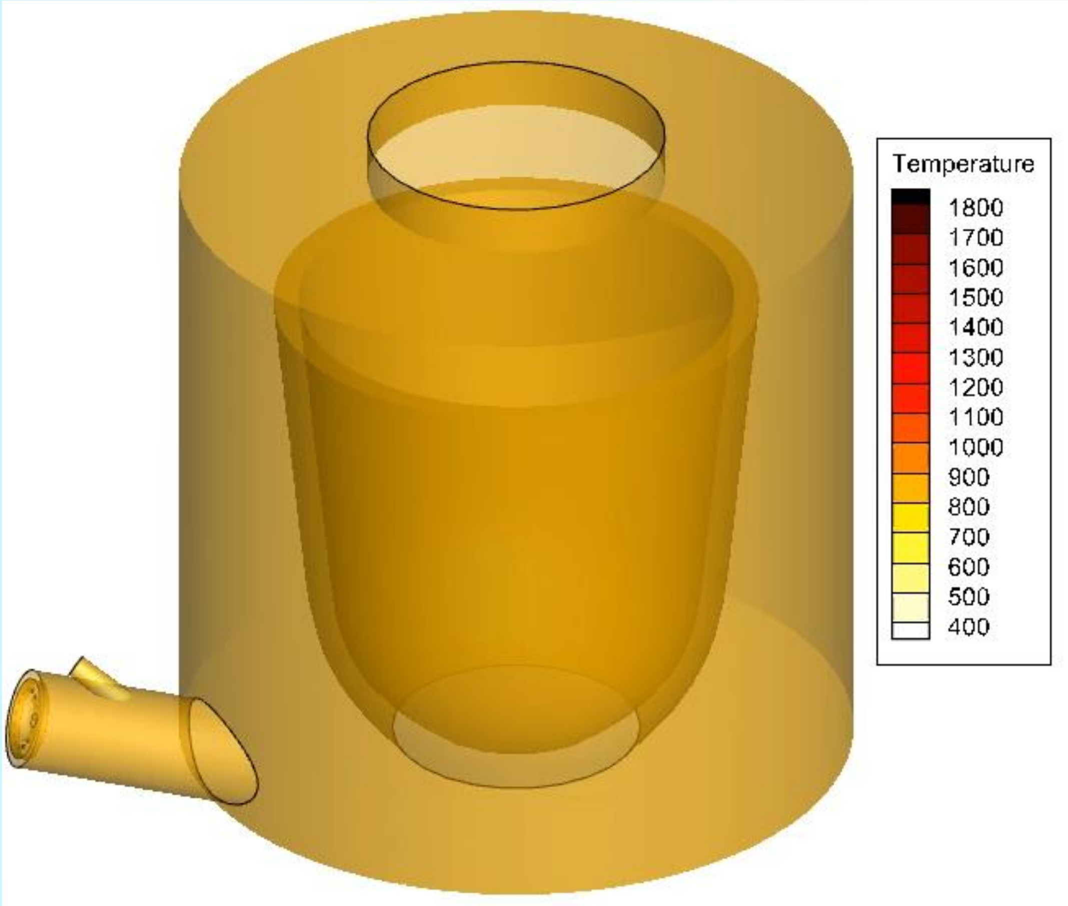
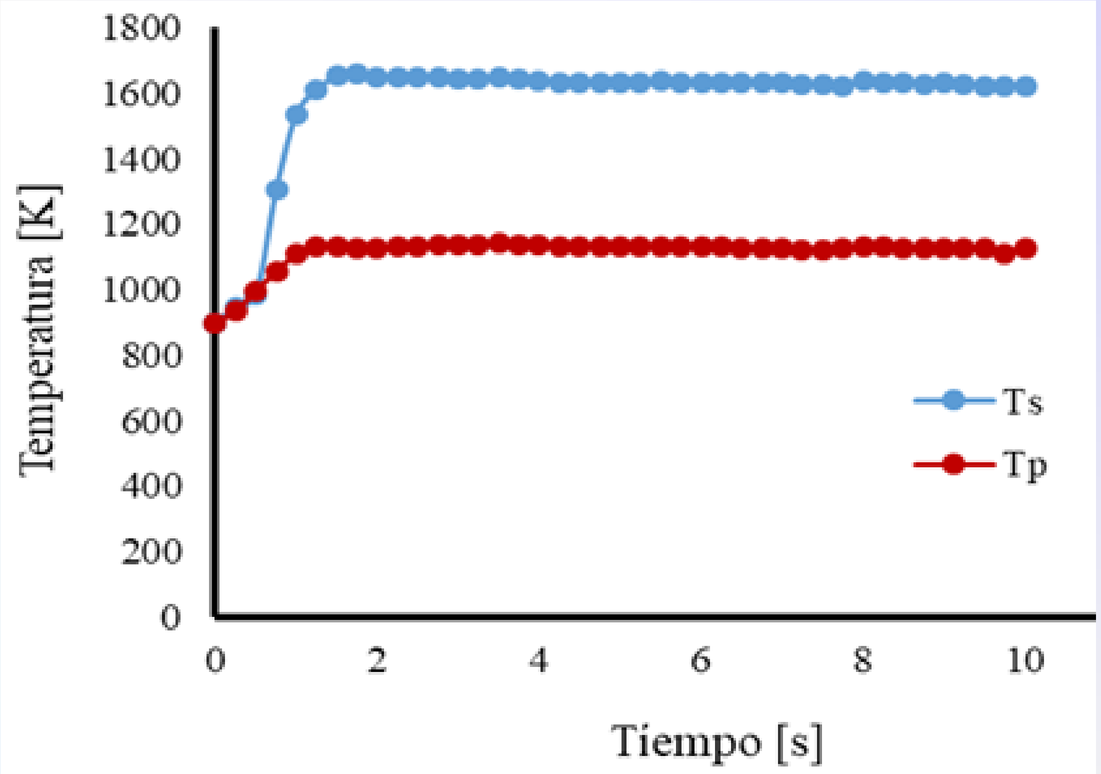


Temperature isosurface in the crucible furnace



Graph of temperature [K] versus time [s]

Results. Thermal and chemical behavior

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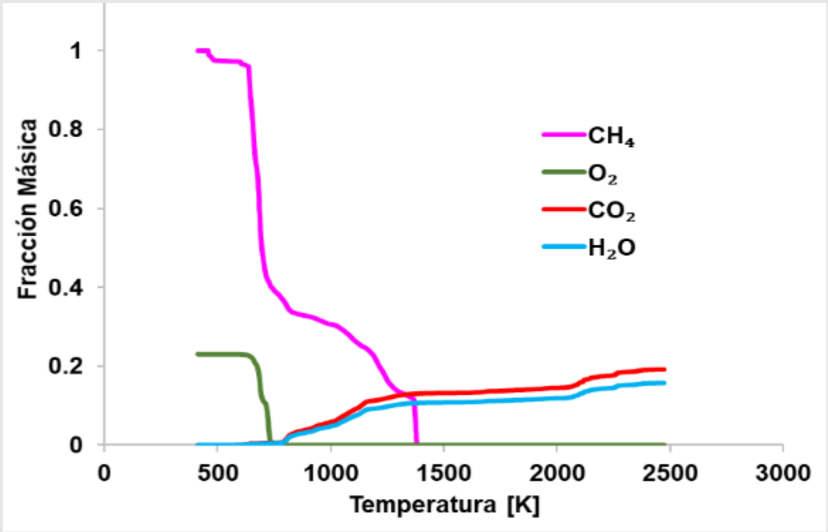
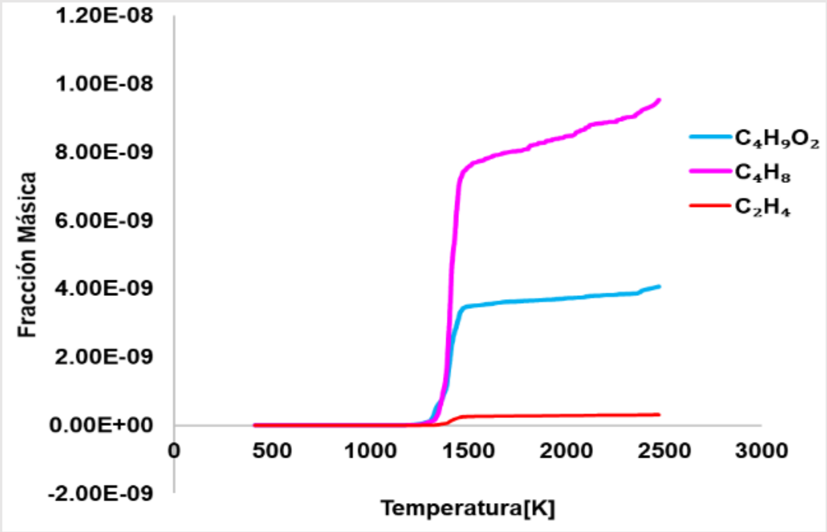
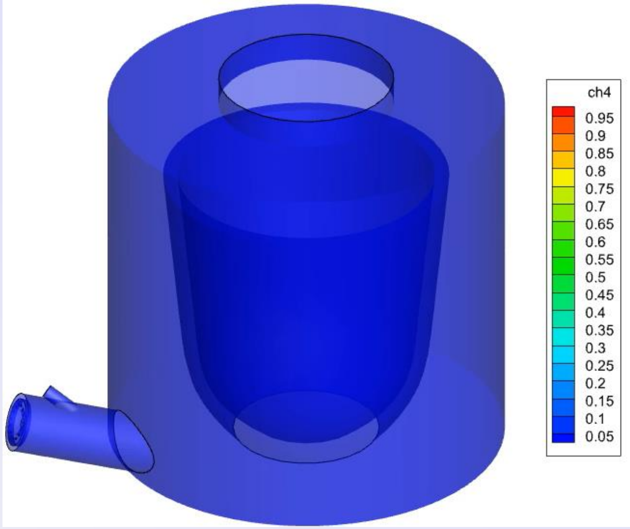
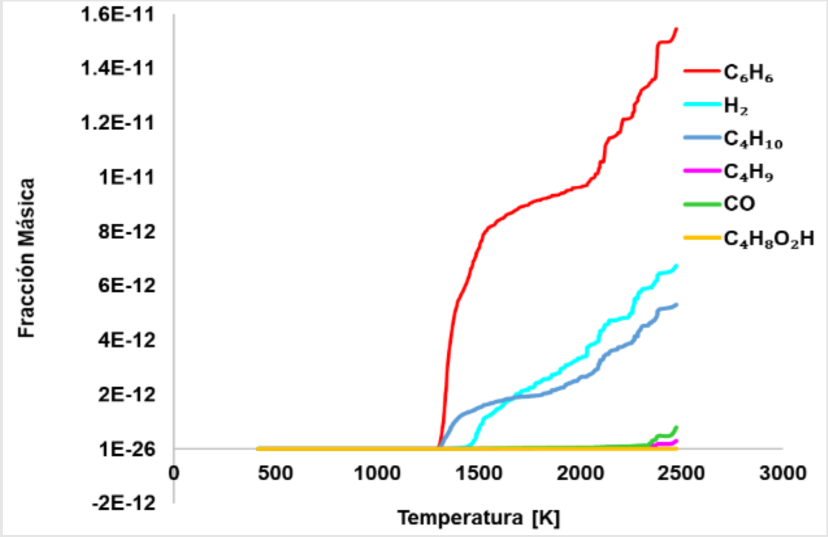
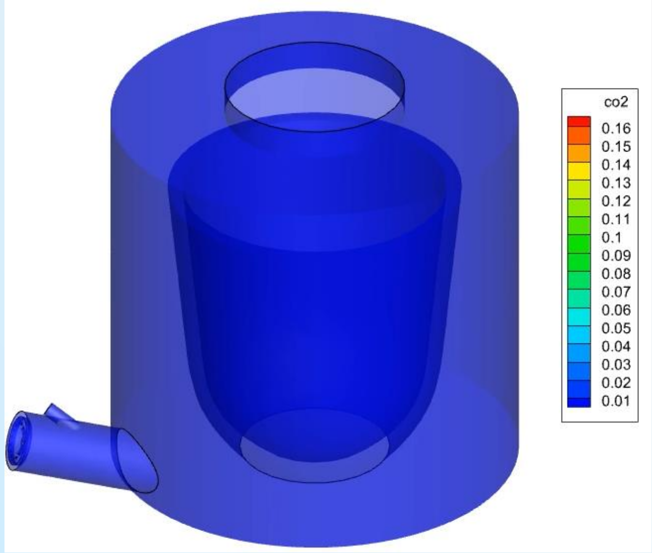
Graph of mass fraction versus temperature [K]

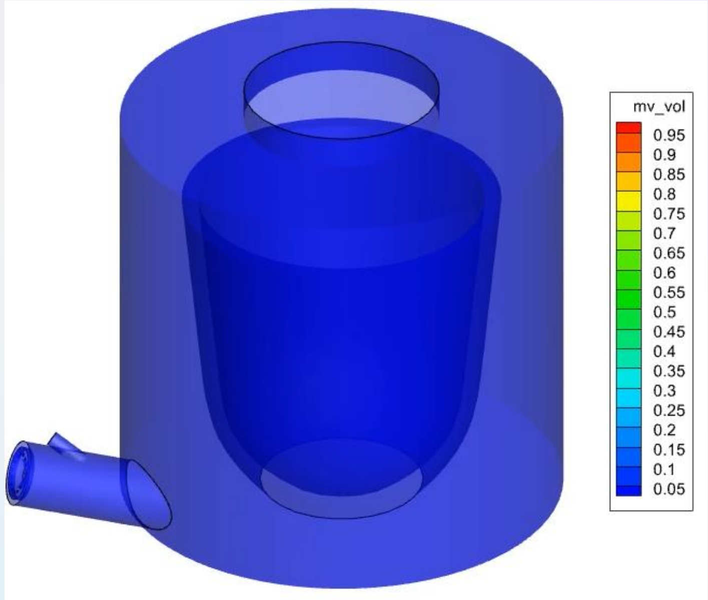












Results. Thermal and chemical behavior

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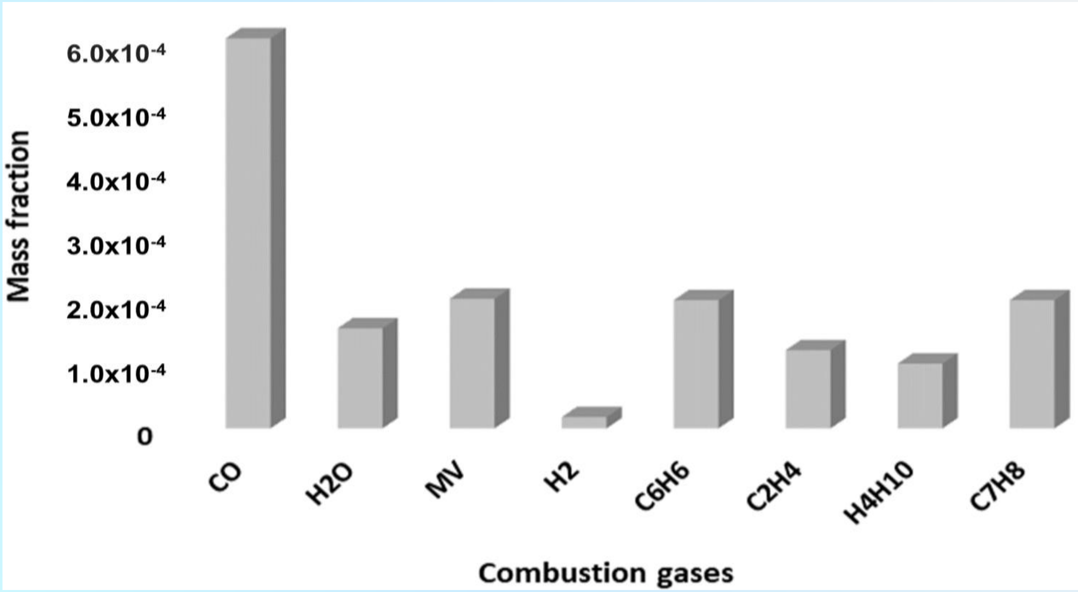

Comparative graph of mass fraction species

Amounts of components in the furnace outlet

Species	ppm
MV	57
CO_2	685
H_2O	31
H_2	3
CO	121
C_6H_6	53
C_4H_{10}	20
C_7H_8	40

Conclusions

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- CFD analysis of PET combustion process applied for energy.
- K-epsilon standard model which is useful to simulate swirl flows.
- The pressure was discretized using the PRESTO method.
- The maximum temperature reached was 1,600 Ks.
- The gas outlet temperature was measured at 1600 K, and the average temperature inside the combustion chamber was 1100 K.
- Combustion gas emissions were lower than those permitted by the Mexican Official Standard NOM-085-SEMARNAT-2011.

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