

# Group Interaction Modelling of PETN

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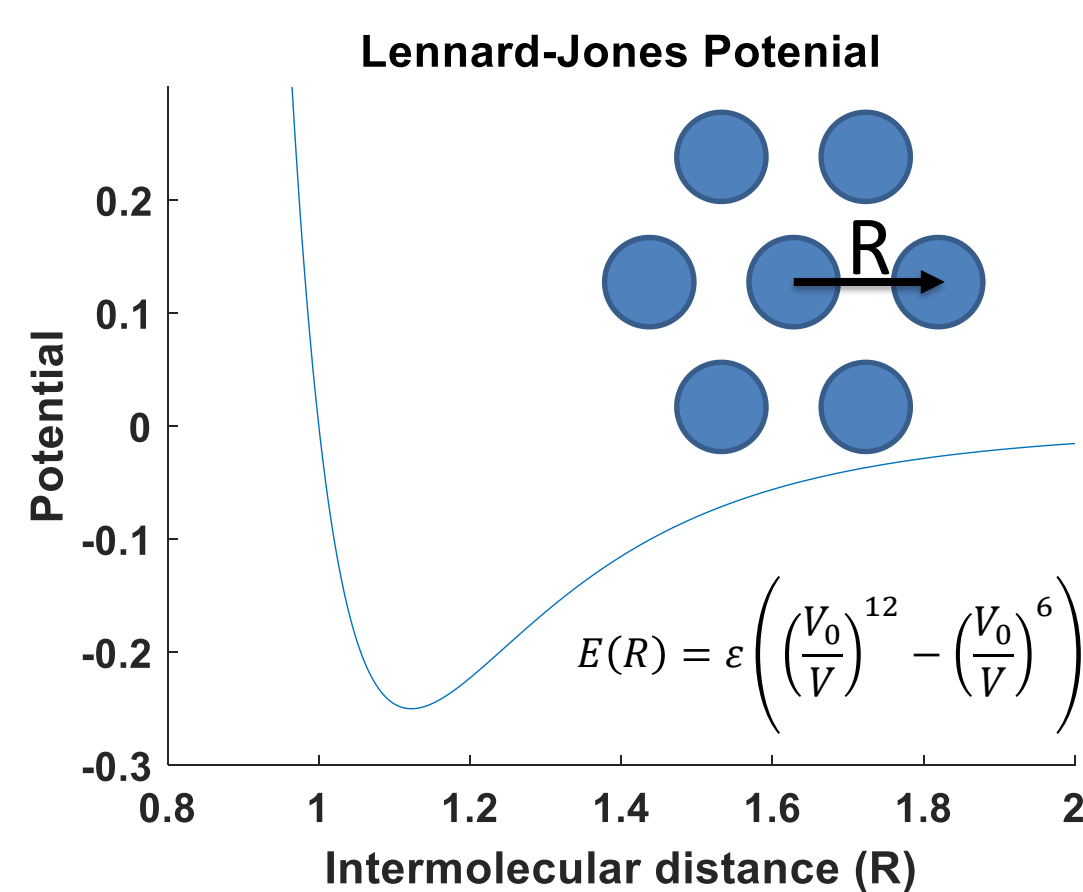
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## Introduction

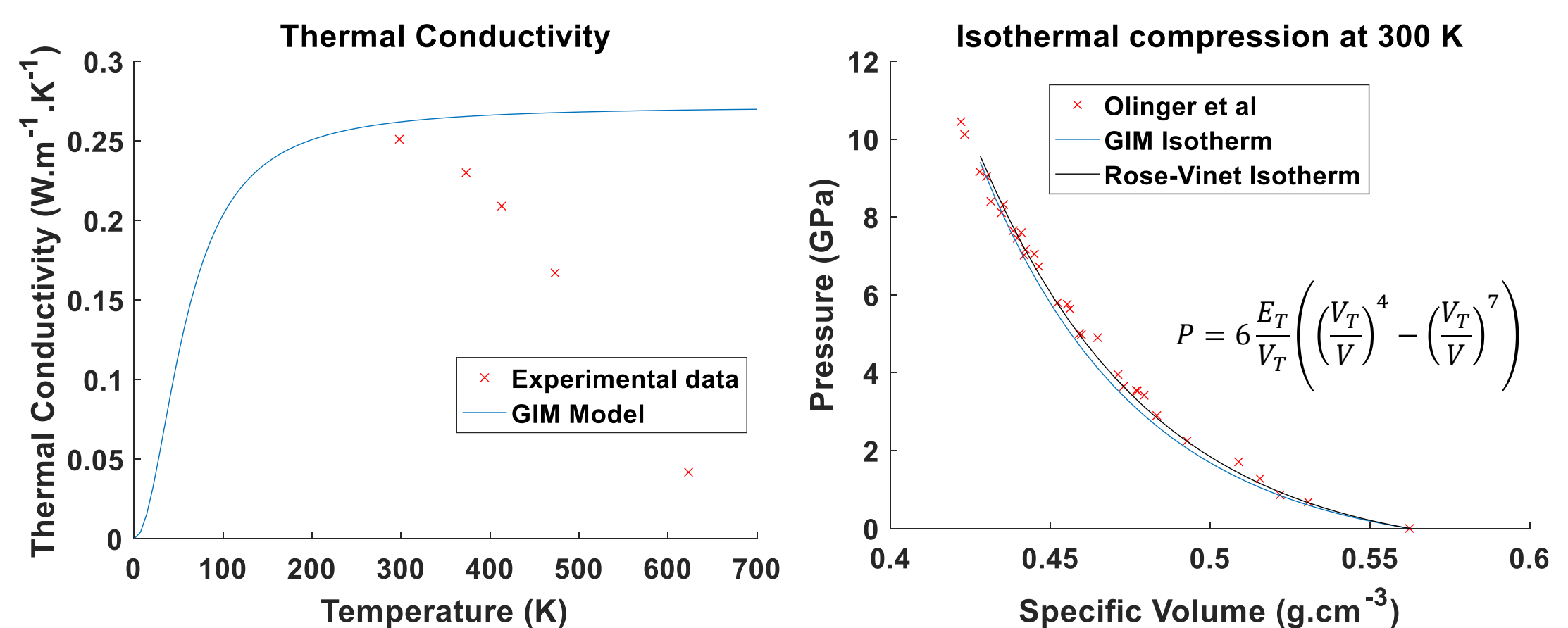
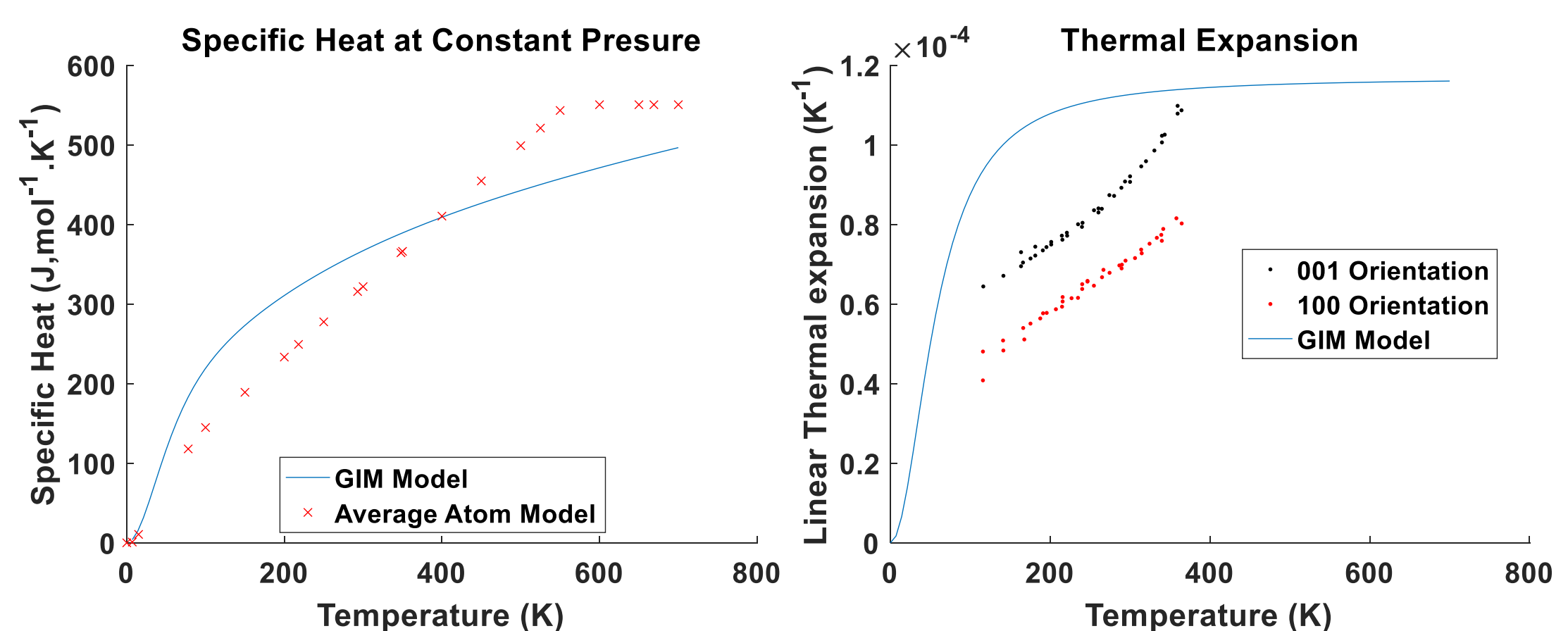
Group Interaction Modelling (GIM) is a simple model developed to predict the properties of polymers based upon the interaction of a potential function between two adjacent molecules, and a thermodynamic energy balance relating the various energy contributions to an ensemble of molecular units. GIM has seen some successful application to predicting the properties of explosives, but has not previously been applied to PETN; as a result the required GIM parameters to model PETN have not been measured or derived. Here we use single point measurements of a number of PETN properties to fit the GIM parameters, and then validate this fitting process by predicting the temperature dependent response of PETN, and comparing these results to experimental data from the literature.

## Theory

GIM assumes a hexagonal geometry in which a molecule is surrounded by six identical molecules interacting via a Lennard-Jones potential. This two-dimensional configuration leads to significant simplifications in the analysis, compared to MD or similar techniques.



## Selected GIM properties versus experimental results



Single Point Values (300 K)

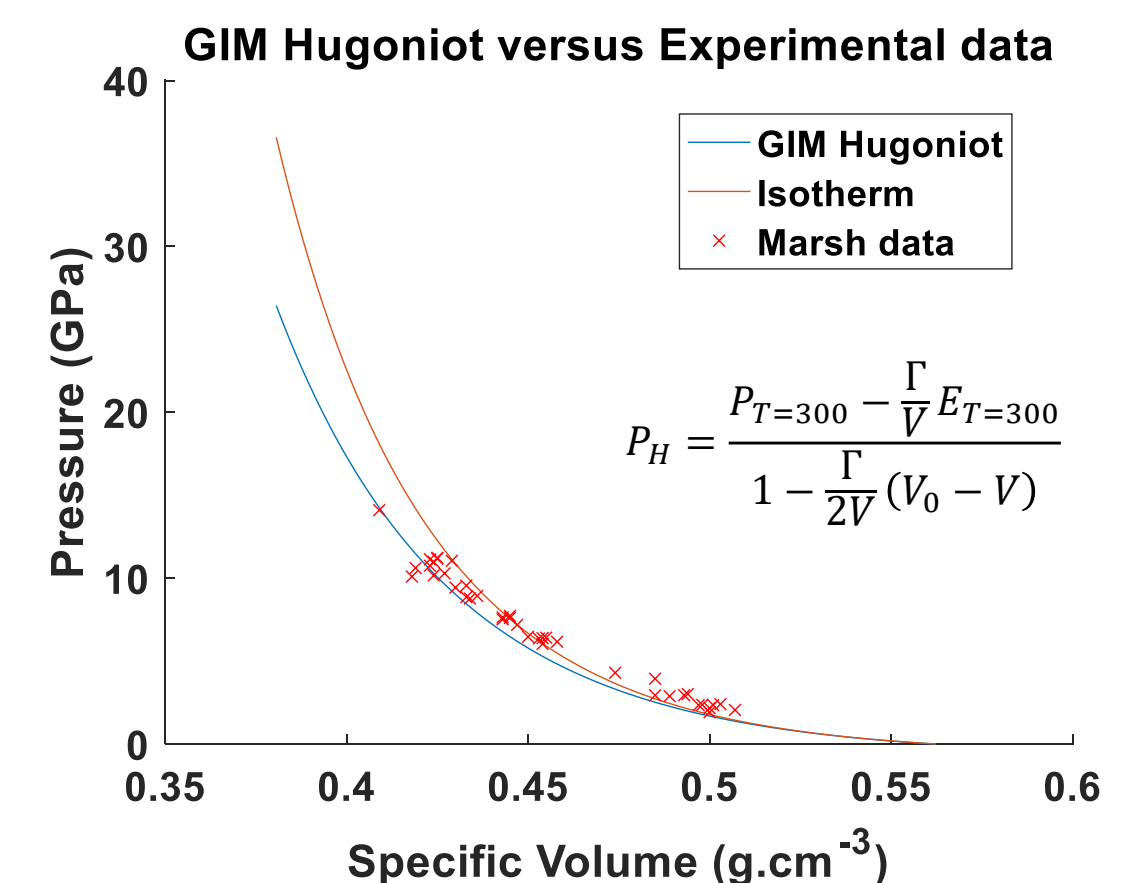
	Experiment	GIM	Ratio
Density (g.cm <sup>-3</sup> )	1.778	1.778	1
T <sub>melt</sub> (K)	416	417	1
B <sub>T</sub> (GPa)	8.3	8.3	1
Gamma	1.05	1.36	0.78

## GIM parameters vs EoS relevant properties at 300 K

	van der Waals Volume, $V_W$ (119 cm <sup>3</sup> .mol <sup>-1</sup> )	Energy of Coherence, $E_{Coh}$ (1.3 × 10 <sup>5</sup> J.mol <sup>-1</sup> )	Characteristic Temperature, $\theta_1$ (387 K)	Skeletal Modes (N = 32)	Atomic Group Frequencies ( $\theta_E$ )
Specific Volume, $V$ (1.778 g.cm <sup>-3</sup> )	$V = \frac{1.26V_W}{\sqrt[3]{1 - \sqrt{0.107 + \frac{Nk}{4} \frac{A_N}{E_{Coh}} (T - \frac{\theta_1}{6.7} \tan^{-1}(\frac{6.7T}{\theta_1})}}}}$				
Specific heat at constant pressure, $C_p$ (341 J.mol <sup>-1</sup> .K <sup>-1</sup> )	$C_p = NR \frac{(\frac{6.7T}{\theta_1})^2}{1 + (\frac{6.7T}{\theta_1})^2} + 17.2 \frac{N^2}{E_{Coh}} \frac{(\frac{6.7T}{\theta_1})^2}{1 + (\frac{6.7T}{\theta_1})^2} + R \sum_{N_E} \frac{(\frac{\theta_E}{T})^2 e^{\frac{\theta_E}{T}}}{(e^{\frac{\theta_E}{T}} - 1)^2}$				
Bulk Modulus, $B_T$ (8.3 × 10 <sup>9</sup> Pa)	$B_T = 1.7 \times 10^6 \frac{E_{Coh}}{V_W} \left( \frac{2(\frac{V_0}{V})^6 - (\frac{V_0}{V})^{12}}{(\frac{V_0}{V})^2 - 1} \right)$				
Volumetric Thermal Expansion, $\alpha$ (1.4 × 10 <sup>-4</sup> K <sup>-1</sup> )	$\alpha = 1.38 \frac{N}{E_{Coh}} \frac{(\frac{6.7T}{\theta_1})^2}{1 + (\frac{6.7T}{\theta_1})^2}$				
Thermal Conductivity, $\lambda$ (0.488 W.m <sup>-1</sup> .K <sup>-1</sup> )	$\lambda_n = 5.4 \times 10^{-11} N \sqrt{\frac{B}{ML}} \frac{(\frac{6.7T}{\theta_1})^2}{1 + (\frac{6.7T}{\theta_1})^2}$				
Melting Temperature, $T_M$ (416 K)	$T_{Melt} = 0.224\theta_1 + 0.084 \frac{E_{Coh}}{N}$				

## A GIM based Equation of State

Porter and Gould published a relationship for an isotherm based on GIM parameters. In addition to this it is possible to derive a relationship for the Grüneisen gamma using GIM. Combining these two allows a Grüneisen type equation of state ( $P = P_{Ref} + \Gamma/V (E_{Ref} - E)$ ) to be produced



## Conclusions

Single state GIM fitting of PETN has produced a mixture of successes and failures. The majority of parameters are well matched at 300 K. The 300 K isotherm is extremely well fit, the specific heat reasonably well fit, the thermal expansion is correct to an order of magnitude, and the thermal conductivity has the wrong functional form.

It is possible to produce a Grüneisen equation of state using GIM, and the results appear to be acceptable when used to predict the shock Hugoniot of single crystal PETN.

## Key References

- [1] Porter, D., Group Interaction Modelling of Polymer Properties, 1995
- [2] Porter, D. and Gould, P., J. Phys. IV France 134 (2006) 373–378