2-бөлім **Раздел 2** **Section 2**

Механика **Механика** **Mechanics**

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SIMULATION OF CARBON DIOXIDE ADSORPTION ONTO CONSOLIDATED ACTIVATED CARBON IN 2D AXISYMMETRIC SYSTEM

The research work is devoted to the kinetics of adsorption. Needless to say that physical adsorption is of great interest in heat industry according to the number of research papers published in the area annually. The working pair of carbon dioxide and consolidated tablet of AC was considered. The mathematical model built for a cylindrical coordinate system, so the computational domain is a rectangle corresponding to the radial section of the tablet. The rate of adsorption implemented using the LDF (linear driving force) model. The temperature map was constructed for analyzing the behavior of the temperature field. Curves of instantaneous uptake and simulated average temperature are obtained. Simulation results are compared with experimental data and shows good agreement. The study also presents findings of a grid sensitivity analysis. The developed solver is the subject to further expansion to consider more quantities, such as change in porosity, volatile gas concentration, etc.
Key words: activated carbon, adsorption, axisymmetric, carbon dioxide, numerical modeling.

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Нығыздалған белсендірілген көмірге көмірқышқыл газының адсорбциясын 2D осьтік симметриялық жүйеде модельдеу

Зерттеу жұмысы адсорбция кинетикасына арналған. Жыл сайын аталған бағытта жарияланатын ғылыми еңбектердің санына қарасақ, физикалық адсорбцияның жылу өнеркәсібінде үлкен қызығушылық тудыратынын айтудың қажеті жоқ. Көмірқышқыл газы және нығыздалған белсендірілген көмір таблеткасының жұмысшы жұбы қарастырылды. Математикалық модель цилиндрлік координаттар жүйесі үшін құрылды, сондықтан есептеу облысы таблетканың радиалды қимасына сәйкес келетін тік бұрышты төртбұрыш болып табылады. Адсорбция жылдамдығы LDF (сызықтық қозғаушы күш) моделін қолдану арқылы жүзеге асырылды. Жұмыста температура өрісінің өзгеру қарқыны талданды, лездік жұтылу және модельденген орташа температура қисықтары тұрғызылды. Модельдеу нәтижелері эксперименттік деректермен салыстырылды және жақсы сәйкес келетіні анықталды. Зерттеу жұмысы сонымен қатар есептеу нәтижелерінің тордың өлшеміне тәуелділігіне талдау нәтижелерін ұсынады. Әзірленген есептегіш құралды адсорбциялық жұтылу кезіндегі кеуектілік өзгерісі, ұшқыш газ концентрациясы және тағы басқа өзекті шамаларды ескеретіндей етіп ұлғайту күтіледі.
Түйін сөздер: белсендірілген көмір, адсорбция, осьтік симметрия, көмірқышқыл газы, сандық модельдеу.

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Симуляция адсорбции диоксида углерода на консолидированный активированный уголь в 2D осесимметричной системе

Научно-исследовательская работа посвящена кинетике адсорбции. Излишне говорить, что физическая адсорбция представляет большой интерес в теплоэнергетике, судя по количеству научных работ, публикуемых ежегодно в этой области. Рассмотрена рабочая пара углекислого газа и консолидированной таблетки активированного угля. Математическая модель построена для цилиндрической системы координат, поэтому расчетная область представляет собой прямоугольник, соответствующий радиальному сечению таблетки. Скорость адсорбции реализована с использованием модели LDF (линейная движущая сила). Проведен анализ поведения поля температуры. Получены кривые мгновенного поглощения и моделируемой средней температуры. Результаты моделирования согласуются с результатами экспериментального исследования. В работе также представлены результаты анализа чувствительности сетки. Разработанный решатель подлежит дальнейшему расширению для учета большего количества величин, таких как изменение пористости, концентрации летучего газа и т.д.
Ключевые слова: активированный уголь, адсорбция, осевая симметрия, углекислый газ, численное моделирование.

1 Introduction

The process of adsorption has a wide range of applications, it is used in cooling/heating systems, gas separation, gas purification, water filtration, carbon capture, etc. Here is an overview of some recent research findings on adsorption and its use in refrigeration systems. Automotive adsorption-based air conditioning systems are a promising alternative to traditional systems from an environmental and energy saving perspective. Such systems can operate using exhaust heat from an engine. An example of a designed and tested adsorption chiller prototype can be found in Verde et al. [1]. The adsorption system working on a two-bed silica gel was able to produce 2.1 kW cooling capacity.

Ben-Mansour et al. [2] presented a review on the application of the adsorption process on CO_2 separation from typical power plant exhaust gases. The work discusses the candidate materials for post-combustion carbon capture, the experimental investigations that have been carried out, and numerical models developed to simulate the gas separation. Authors indicate gaps in experimental investigations and in simulation studies considering one dimensional flow. More research work is needed that doesn't not ignore the radial or 3D thermal and adsorption behaviors.

The established patterns in equilibrium adsorption curves in adsorption theory are of an empirical nature. A new approach to constructing equilibrium uptake equations was proposed by the following authors. Yin et al. [3] introduced a new model correlating and predicting adsorption equilibrium concentrations using machine learning method. Sellaoui et al. [4] established theoretical expressions to fit the adsorption isotherms of ibuprofen on activated carbon using grand canonical ensemble. Unlike conventional isotherms models (Langmuir, Freundlich, etc.) the expressions involve physicochemical parameters and are thermodynamically consistent. Sghaier et al. [5] used statistical physics formalism with the grand canonical ensemble to construct isotherm equations. The study performed by applying four expressions and the best isotherm equation fitting experimental data was found. Also

the authors used the statistical physics for expressing and calculating the coefficient of performance (COP) of ethanol/activated carbon systems.

Cai et al. [6] demonstrated silica gel (SG)-water adsorption refrigeration device and compared the performance of three types of composite adsorbents in the refrigeration system. The composites fabricated by mixing SG with MOFs to improve mass transfer characteristics and either with copper chips (CCs) or foamed copper (CFs) of different mass ratio to improve thermal characteristics. Development of new materials by mixing different substances permits limitless possibilities in the field of adsorption application.

Pena and de Lemos [7] numerically investigated unsteady multidimensional heat transfer problem with internal heat generation. The simulation is carried out in a two-dimensional axisymmetric domain and involved reaction and phase transition phenomena. In [8] recent study, we presented results of simulation of CO_2 gas adsorption onto consolidated AC tablet, with the calculation geometry simplified to a one-dimensional case. The mathematical model involved more quantities, such as change in porosity, volatile gas concentration, and accordingly, more equations were solved. The current work investigates the process of CO_2 adsorption by the composite under constant pressure and temperature conditions in 2D axisymmetric system. The energy balance equation and the adsorbed phase balance equations have been solved at a moment, and the solver is subject to further expansion to account for more associated accompanying phenomena.

2 Mathematical model and problem description

The calculation domain is schematically illustrated in Figure 1. The mathematical model built for a cylindrical coordinate system, so the computational domain is a rectangle corresponding to the radial section of the tablet.

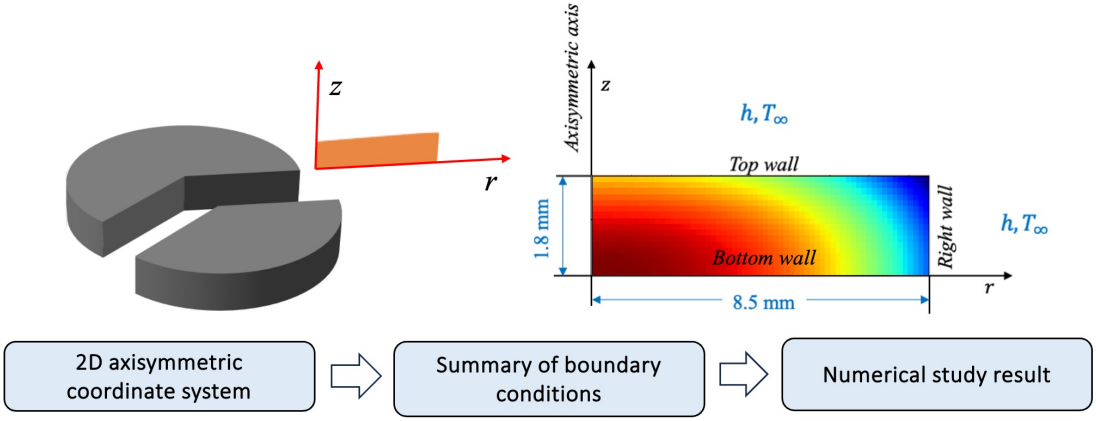

Figure 1: Schematic illustration of calculation domain

The energy conservation equation for the solid adsorbent is as equation (1). The adsorption rate is assumed to follow the Linear Driving Force model, equation (2). The thermal conductivity and capacity of the adsorbent vary with temperature and adsorption rate, since the composition of a unit volumes change with adsorption, also due to the

exothermic nature of the process for the working pair of CO_2/AC. But in the current study they are considered constant due to lack of experimental data.

$$\rho c_{\mathrm{p}} \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(kr \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + \dot{e}_{\mathrm{gen}} \tag{1}$$

$$\frac{\partial q}{\partial t} = k_{\mathrm{LDF}} (T) (q_{\mathrm{eq}} - q) \tag{2}$$

Boundary conditions:

$$-k \frac{\partial T}{\partial z} \bigg|_{\mathrm{z=H}} = h [T - T_{\infty}] \tag{3}$$

$$\frac{\partial T}{\partial z} \bigg|_{\mathrm{z=0}} = 0 \tag{4}$$

$$-k \frac{\partial T}{\partial r} \bigg|_{\mathrm{r=R}} = h [T - T_{\infty}] \tag{5}$$

For the nodes along the longitudinal axis equation (6) is solved.

$$\rho c_{\mathrm{p}} \frac{\partial T}{\partial t} = k \left(2 \cdot \frac{\partial^2 T}{\partial r^2} + \frac{\partial^2 T}{\partial z^2} \right) + \dot{e}_{\mathrm{gen}} \tag{6}$$

Initial conditions, equation (7) and equation (8):

$$q|_{\mathrm{t=0}} = 0 \tag{7}$$

$$T|_{\mathrm{t=0}} = T_{\infty} \tag{8}$$

Problem parameters used for simulation. Dimensions of the tablet used in the simulation: tablet radius 8.5 mm, height 1.8 mm (see Figure 1). The characteristics of the composite consolidated activated carbon taken from previous studies [8,9] and illustrated in Table 1.

The expression for the rate constant of LDF model:

$$k_{\mathrm{LDF}} (T) = k_0 \exp \left(-\frac{E_{\mathrm{a}}}{R\,T} \right) \tag{9}$$

Where R is the gas constant, 8.314 J mol^{-1} K^{-1}. The activation energy and pre-exponential factor are:

$$E_{\mathrm{a}} = -17.34 \,\mathrm{kJ\ mol^{-1}} \tag{10}$$

Table 1: The characteristics of the composite for numerical calculations

Property	**Unit**	**Value**
Heat conductance	$\mathrm{W\,m^{-1}\,K^{-1}}$	0.22
Thermal capacity	$\mathrm{J\,g^{-1}\,K^{-1}}$	0.821
Isosteric heat of adsorption	$\mathrm{kJ\,mol^{-1}}$	19.02
Porosity	-	0.482
Skeletal density	$\mathrm{g\,cm^{-3}}$	0.917
Apparent density	$\mathrm{g\,cm^{-3}}$	0.475
Equilibrium uptake	$\mathrm{g\,g^{-1}}$	0.274

$$k_0 = 1.58 \times 10^{-5}\,\mathrm{s^{-1}} \tag{11}$$

The heat transfer coefficient depends on the difference in temperature between the surface of the heated object and the surrounding temperature T_∞, and on the thermal properties of the medium. The properties of carbon dioxide under given conditions of temperature and pressure are shown in Table 2.

Dimensionless numbers, [10]:

$$Ra = Gr \cdot Pr \tag{12}$$

$$Gr = \frac{\beta \cdot \Delta T \cdot g \cdot L^3}{\nu^2} \tag{13}$$

$$Pr = \frac{\mu_{\mathrm{g}} \cdot c_{\mathrm{p,g}}}{k_{\mathrm{g}}} \tag{14}$$

Table 2: Properties of carbon dioxide at 293.15 °C and 0.535 MPa

Property	**Unit**	**Value**
Pressure	bar	5.35
Temperature	Celsius	20
Density	$\mathrm{kg\,m^{-3}}$	9.96
Specific isobar heat capacity	$\mathrm{kJ\,kg^{-1}\,K^{-1}}$	0.88
Isobar coefficient of thermal expansion	$10^{-3}\,(\mathrm{K^{-1}})$	3.75
Heat conductance	$10^{-3}\,(\mathrm{W\,m^{-1}\,K^{-1}})$	16.44
Dynamic viscosity	$10^{-6}\,(\mathrm{Pa\,s})$	14.72
Kinematic viscosity	$10^{-6}\,(\mathrm{m^2\,s^{-1}})$	1.478

The system of equations has been solved in Python (Version 3.11.5) using the explicit finite difference scheme. Volume average of quantity f found as below:

$$\Theta(f) = \int_0^{\mathrm{H}} \int_0^{\mathrm{R}} (2\pi r \cdot f(r,\ z))\, dr\, dz = \sum_{i=1}^{n} \sum_{j=1}^{m} 2\pi \cdot r_j^* \cdot f\left(r_j^*,\ z_i^*\right) \cdot \Delta r \cdot \Delta z \tag{15}$$

$$T_{\text{ave}} = \frac{\int T\, dV}{V} \tag{16}$$

$$q_{\text{ave}} = \frac{\int q\, dV}{V} \tag{17}$$

3 Results and discussion

The temperature field behaves as expected, the outer boundaries are colder than the core. Figure 2 shows the instantaneous temperature field at the same time instant 18 seconds calculated using 8x32 nodes, 12x48 nodes and 16x64 nodes. The results illustrated upside down due to peculiarity of the visualization library. The proper grid sensitivity analysis was performed to avoid grid size dependent results, Appendix A. The grid refinement allows more accurate calculation and detailed temperature map.

The calculation result of the previous study obtained using non-isothermal pore change model for the 1D case illustrated for comparison [8]. Two temperature profiles are shown in Figure 3, one obtained using 2D axial symmetric geometry in scope of the current study, and the other obtained using abovementioned 1D non-isothermal pore change model. The non-isothermal pore change model counts the effects associated with change in porosity, and mobile gas penetration into the tablet. But due to the 1D geometry the convective heat loss though the side wall cannot be determined. When using a 2D case the cooling occurs faster indicating the heat loss through the sides. The findings are reasonable and consistent with recent results.

According to the experimental measurement the adsorption rate is high during the first 300 seconds and declined rapidly thereafter. It achieves a plateau at around 600 seconds and remains constant, when no further change in adsorption uptake is noticed. Therefore, only the first 600 seconds are of interest as a simulation time. The instantaneous average simulated uptake compared with experimental data.

Figure 4 illustrates the adsorption uptake over time. Black dots indicate the experimental data, the dashed blue line indicates simulation result of the current study. Solid purple line shows the result obtained in previous study using non-isothermal pore change model.

4 Conclusions

Recent review articles point to the need for more experimental and numerical studies that do not ignore the radial or 3D thermal and adsorption behaviours. The present paper shows simulation results obtained for a cylindrical coordinate system, so the computational domain is the radial section of the tablet. Currently the energy balance equation and the adsorbed phase balance equations are solved. The validation of the developed solver is performed via comparison with the results obtained experimentally and using one-dimensional model of recently published study. The developed solver is the subject to further expansion to consider more quantities, such as change in porosity, volatile gas concentration, etc. In-situ measurements of the sample's temperature and thermal properties are challenging

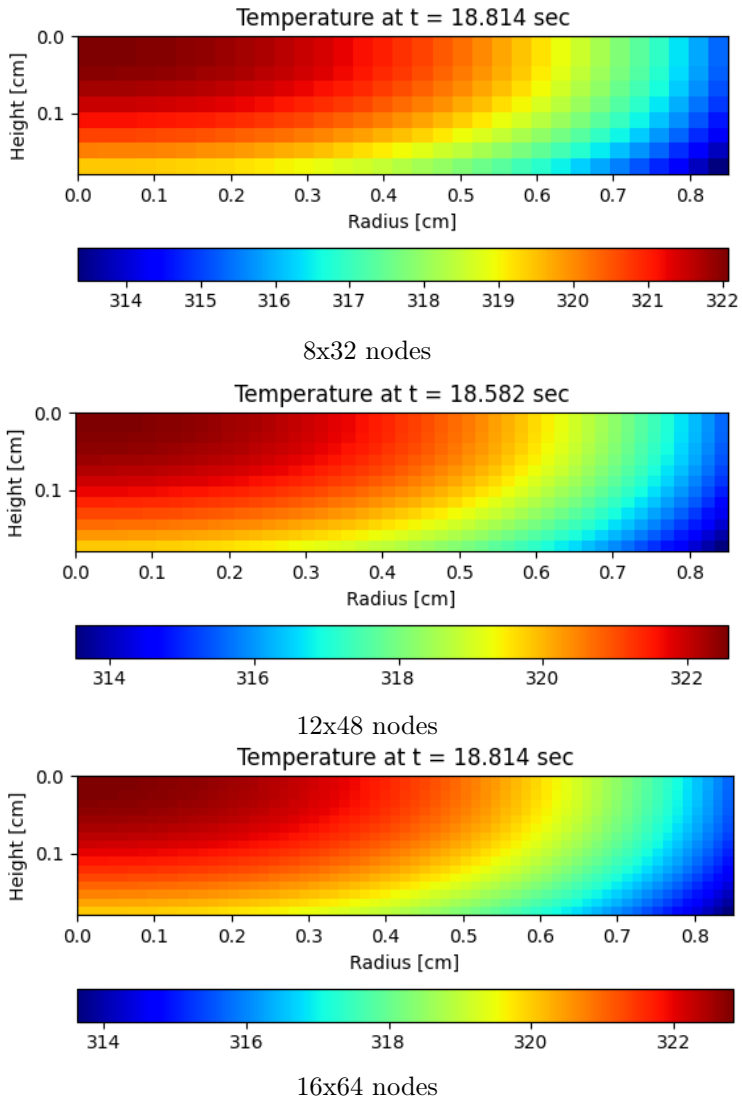

Figure 2: Instantaneous temperature field at 18 seconds calculated using different mesh refinements: (a) 8x32 nodes, (b) 12x48 nodes, (c) 16x64 nodes

experimental investigation work. The validation of the simulated temperature profiles with experimental data is of great interest.

Research highlights

– Gas adsorption onto activated carbon tablet simulated in 2D axisymmetric system.

– Dynamics curves for key parameters were constructed and compared with results of a recent one-dimensional numerical study.

– Adsorption uptake curves were compared with experimental data.

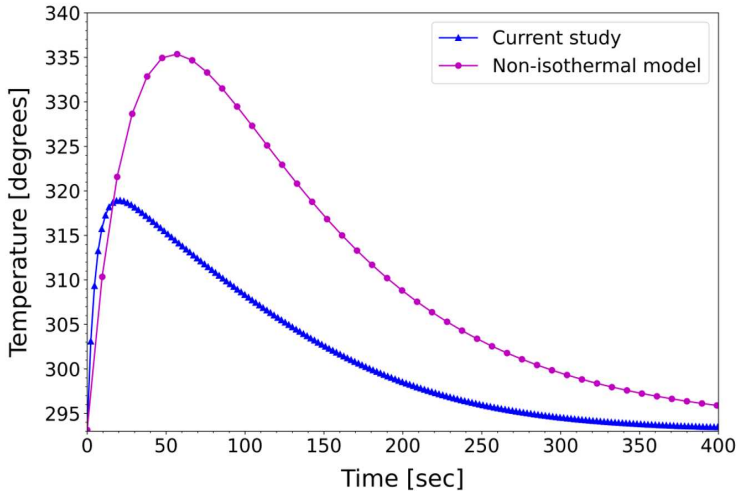

Figure 3: Mean temperature profiles obtained using 2D axial symmetric geometry (blue line), and 1D non-isothermal pore change model (purple line) [8]

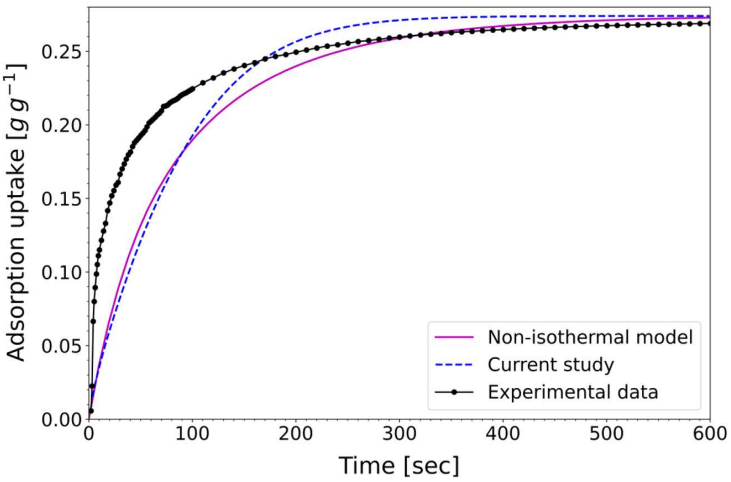

Figure 4: Adsorption uptake obtained using 2D axial symmetric geometry (dashed blue line) and 1D non-isothermal pore change model (solid purple line). Black line corresponds to the experimental data

Declaration of Competing Interest

The author declares that she has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Interim Results

Figure 5 shows the average temperature profiles obtained for 3 different cases: (a) for adaptive $k_{\mathrm{LDF}}(T)$ and $h(T)$, (b) for fixed k_{LDF} and adaptive $h(T)$, and (c) for both fixed k_{LDF} and h. The mean temperature T_{ave} varies over time according to the Figure 6. The calculation results for 4 different grid sizes illustrated. The grid sensitivity analysis shows good convergence of the curves towards the result obtained on the finest grid, Table 3. The grid size cannot be reduced indefinitely. The computational result is reasonable for 12x48 nodes. Further refinements increase the calculation time only, and do not affect much on the temperature profiles.

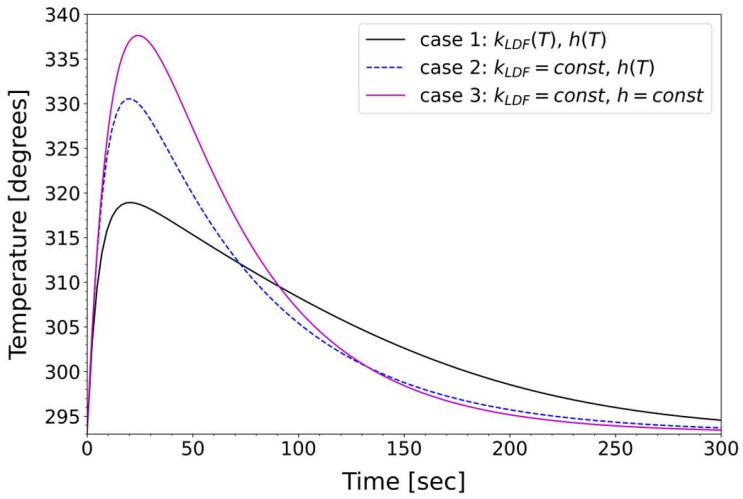

Figure 5: Temperature profile obtained using 3 different cases

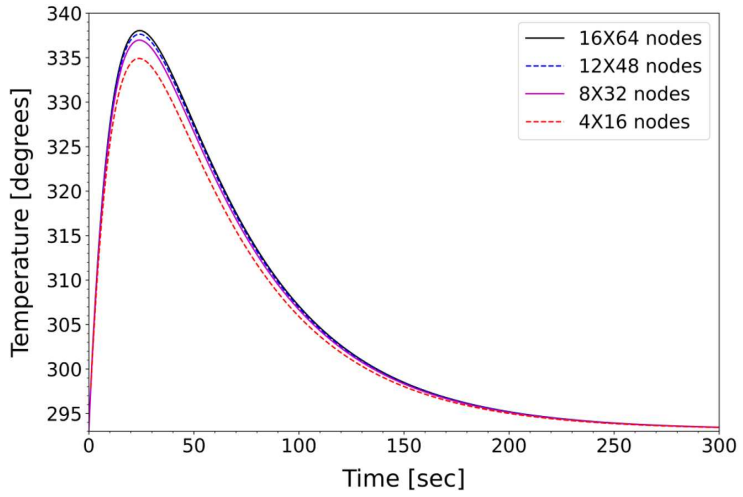

Figure 6: Grid sensitivity analysis. Mean temperature over time.

Table 3: Maximum temperature observed for different grid sizes

Number of nodes	16x64	12x48	8x32	4x16
$T_{\max}$	338.04	337.64	336.97	334.69

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