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Simulation of Methane Adsorption in Adsorbed Natural Gas (ANG) Storage System

by

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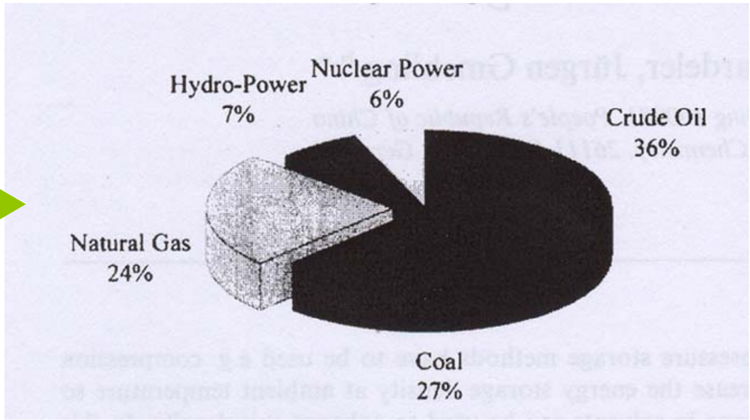
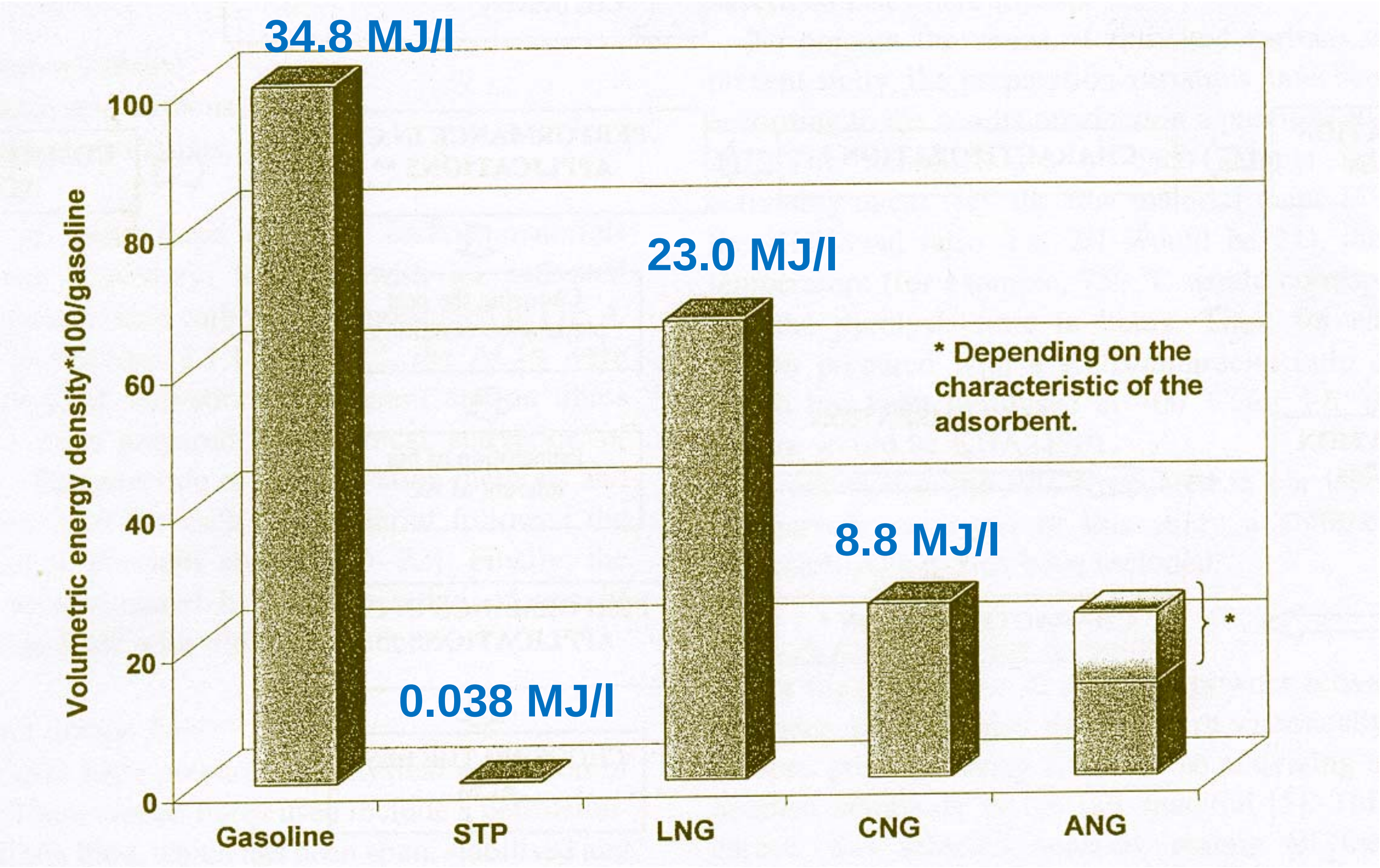
Motivation for storage of Natural Gas

World Energy Resources



- **Abundantly available in nature**
- **Potentially attractive fuel for transportation sector due to high octane number (i.e. 130 compared to 90 that of gasoline)**
- **Low cost compared to gasoline, diesel etc.**
- **Environmentally friendly due to very low emission of CO_2 and other air pollutants**

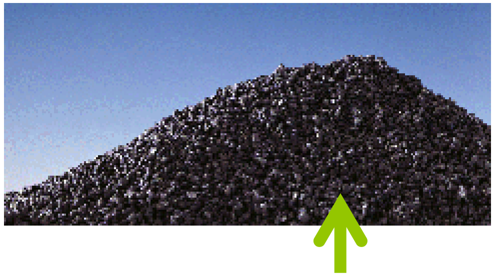
Comparison of energy density of various NG storage systems with Gasoline



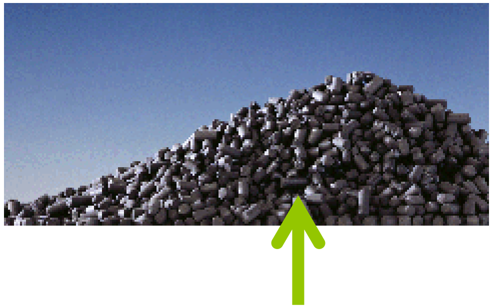
* Depending on the characteristic of the adsorbent.

Lozano-Castelló et al., Fuel, 2002

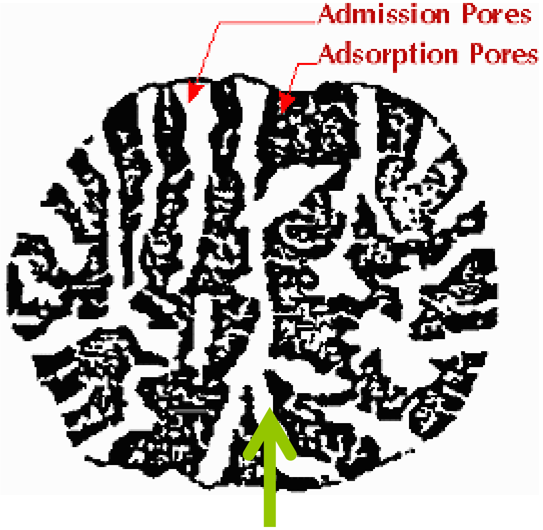
ANG Cylinder & Adsorbents



Granular Activated carbon



Pelleted Activated carbon

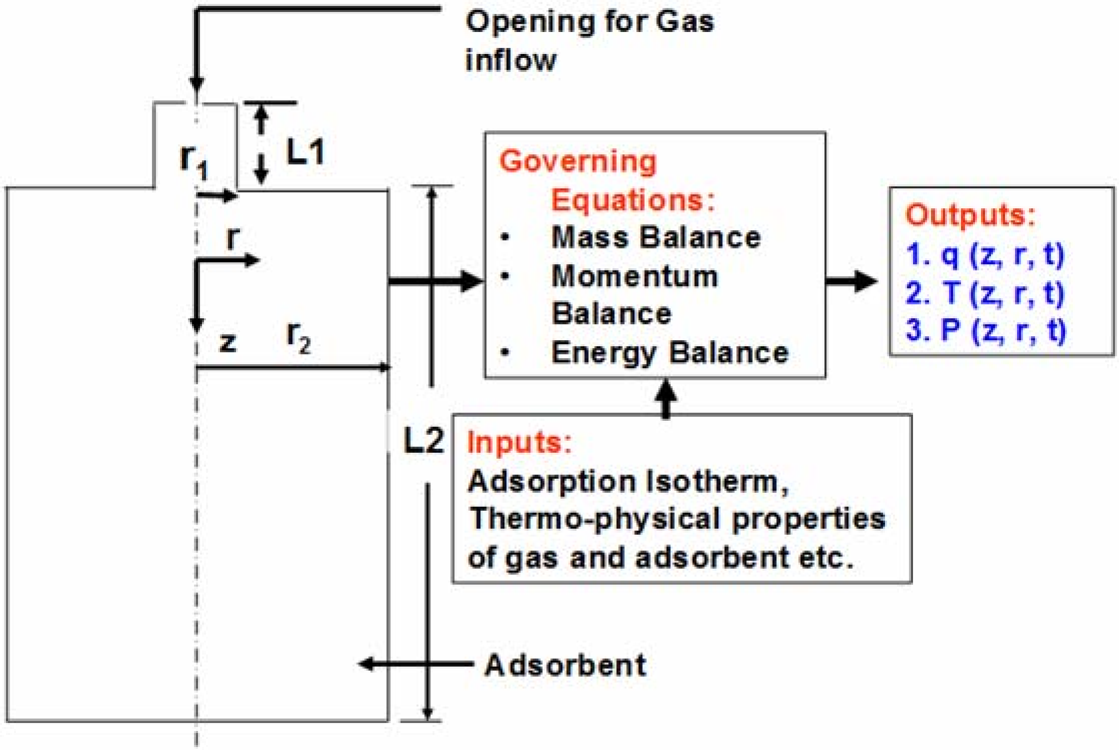


Cross Sectional view of Adsorbent Bed

Thermal effects affecting the performance of ANG Technology

1. If heat of adsorption released during charge is not removed from the storage system, less methane is adsorbed as the bed heats up.
2. If the heat of adsorption is not resupplied during discharge, the bed temperature drops, increasing the residual amount of NG that remains in storage at depletion .

2-D Transport Model for Adsorption of Methane in Packed Bed of Nanoporous Adsorbents



Governing Equations:
- Mass Balance
- Momentum Balance
- Energy Balance

Outputs:
1. q (z, r, t)
2. T (z, r, t)
3. P (z, r, t)

Inputs:
Adsorption Isotherm, Thermo-physical properties of gas and adsorbent etc.

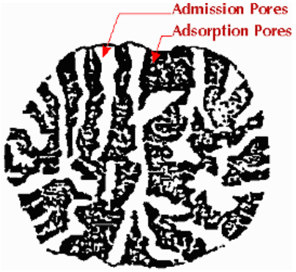
ANG System

Model Formulation

Continuity Equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_t \rho_g + \rho_b q\right) + \nabla\cdot\left(\rho_g \mathbf{u_g}\right) = 0 \qquad \ldots(1)$$

$$\rho_g = \frac{PM_g}{RT} \qquad \ldots(2)$$



q can be obtained by Dubinin-Astakhov Equation (DA).

$$q = \rho_{ads} W_o \exp\left[-\left(\frac{A}{\beta E_o}\right)^n\right] \qquad \ldots(3)$$

$$A = RT\ln\left(\frac{P_s}{P}\right) \qquad \ldots(4)$$

$$P_s = P_{cr}\left(\frac{T}{T_{cr}}\right)^2 \qquad \ldots(5)$$

$$\rho_{ads} = \frac{\overline{\rho}_{ads}}{\exp\left[\alpha_e\left(T - \overline{T}_b\right)\right]} \qquad \ldots(6)$$

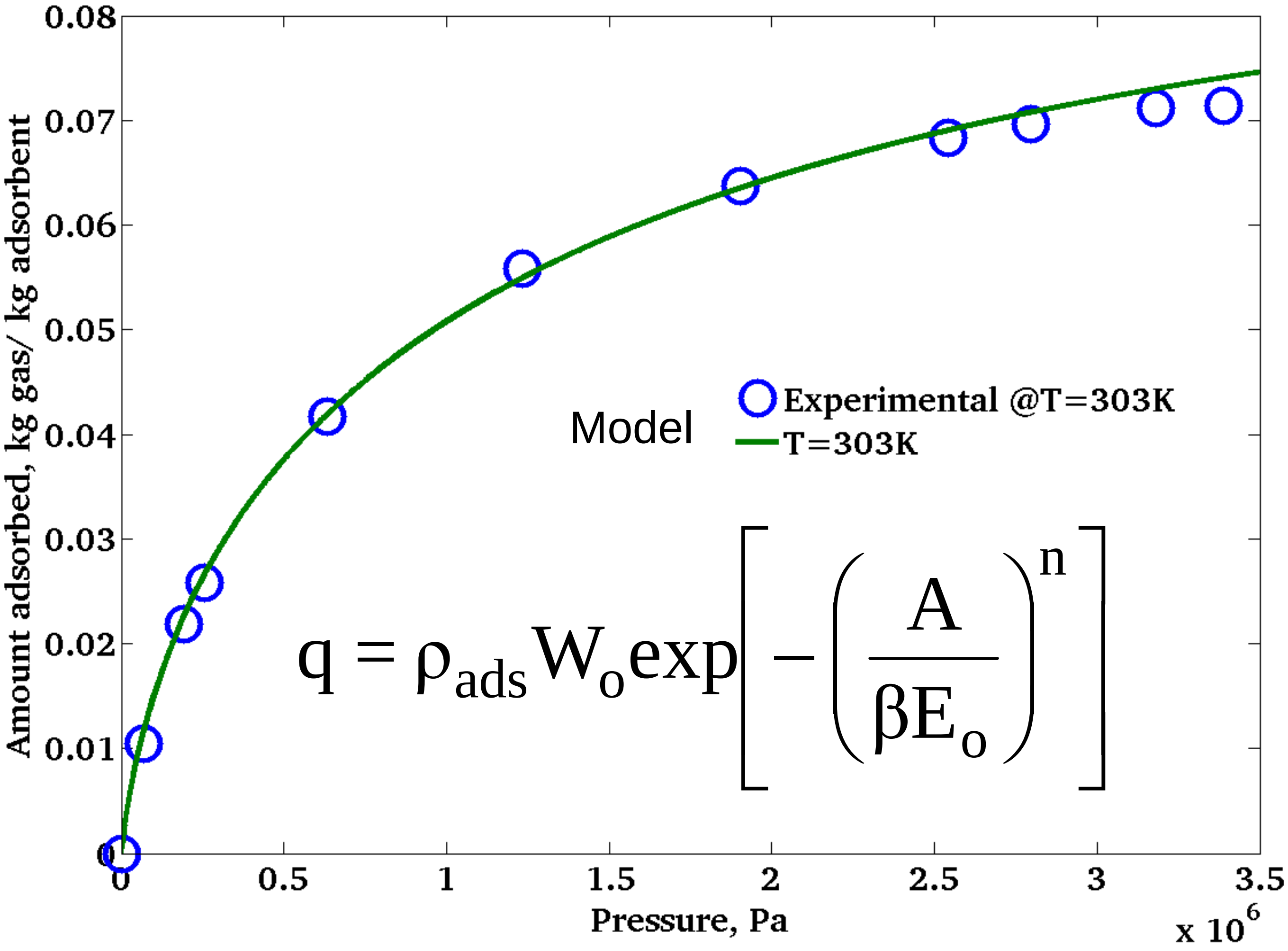
Momentum Equation:

$$\frac{\rho_g}{\varepsilon_t}\frac{\partial \mathbf{u_g}}{\partial t}+\frac{\rho_g}{\varepsilon_t^2}\left(\mathbf{u_g}\cdot\nabla\right)\mathbf{u_g}=-\nabla P+\mu_g\nabla^2\mathbf{u_g}-\frac{\mu_g}{K}\mathbf{u_g} \quad \ldots(7)$$

Energy Equation:

$$\rho C_p\frac{\partial T}{\partial t}+C_{pg}\nabla\cdot\left(T\rho_g\mathbf{u_g}\right)=\nabla\cdot\left(\lambda_{eff}\nabla T\right)+\rho_b\left|\Delta H\right|\frac{\partial q}{\partial t}$$

$$+\varepsilon_t R\rho_g\frac{\partial T}{\partial t} \quad \ldots(8)$$



Model

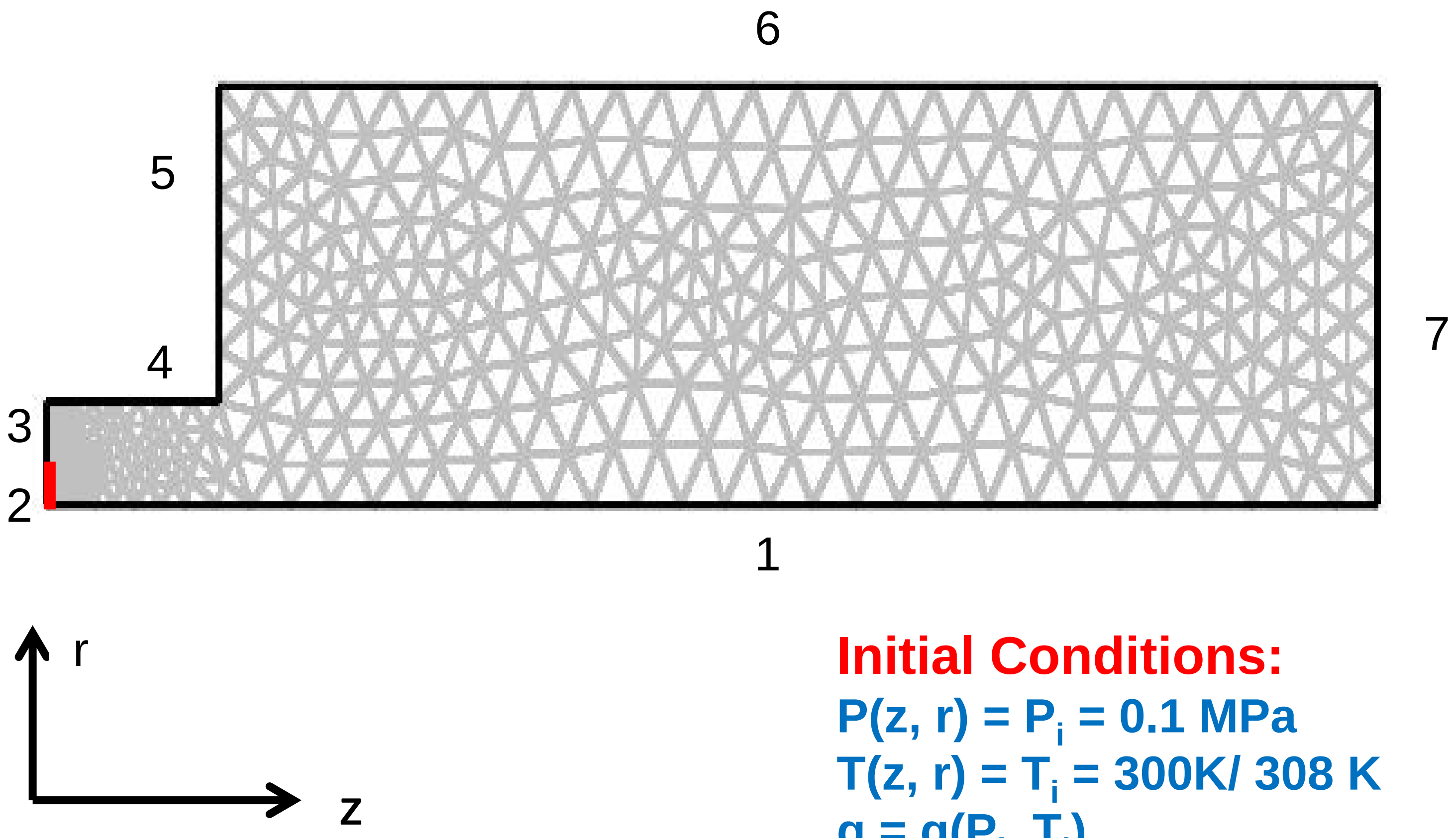
$$q = \rho_{ads} W_o \exp\left[-\left(\frac{A}{\beta E_o} \right)^n \right]$$

Simulation Details

Numerical Technique: **Finite Element Method** for solving Coupled Partial differential equations like Navier Soke, Energy and DA equaions

Sofware used: COMSOL MULTIPHYSICS 3.5a with Module "Chemical Engineeing",
solver PARDISO
2D- Axi-symmteric geometry with triangular mesh

Convergence Precision: 1.0E-06



Initial Conditions:

$P(z, r) = P_i = 0.1$ MPa

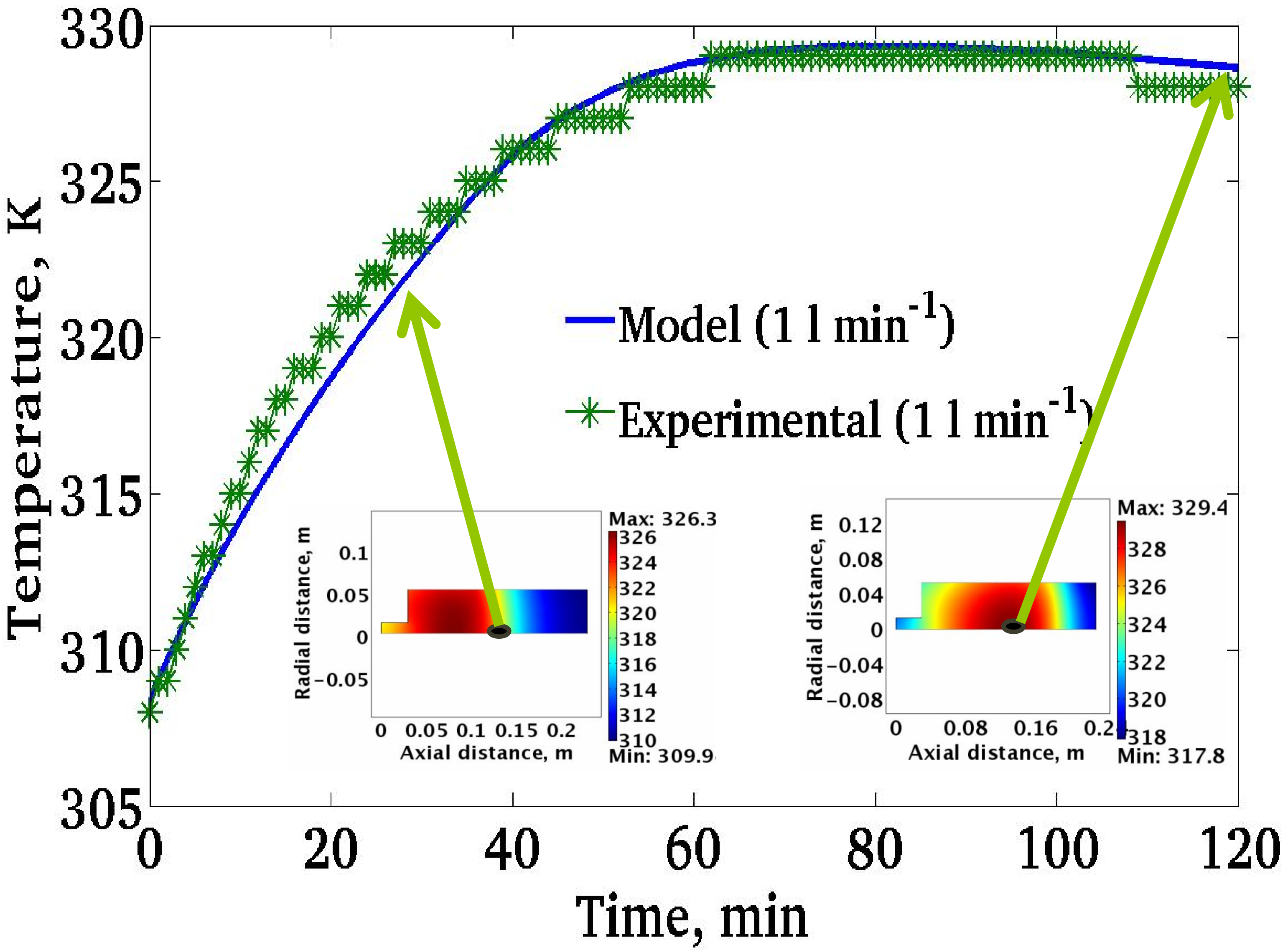
$T(z, r) = T_i = 300K/\ 308$ K

$q = q(P_i, T_i)$

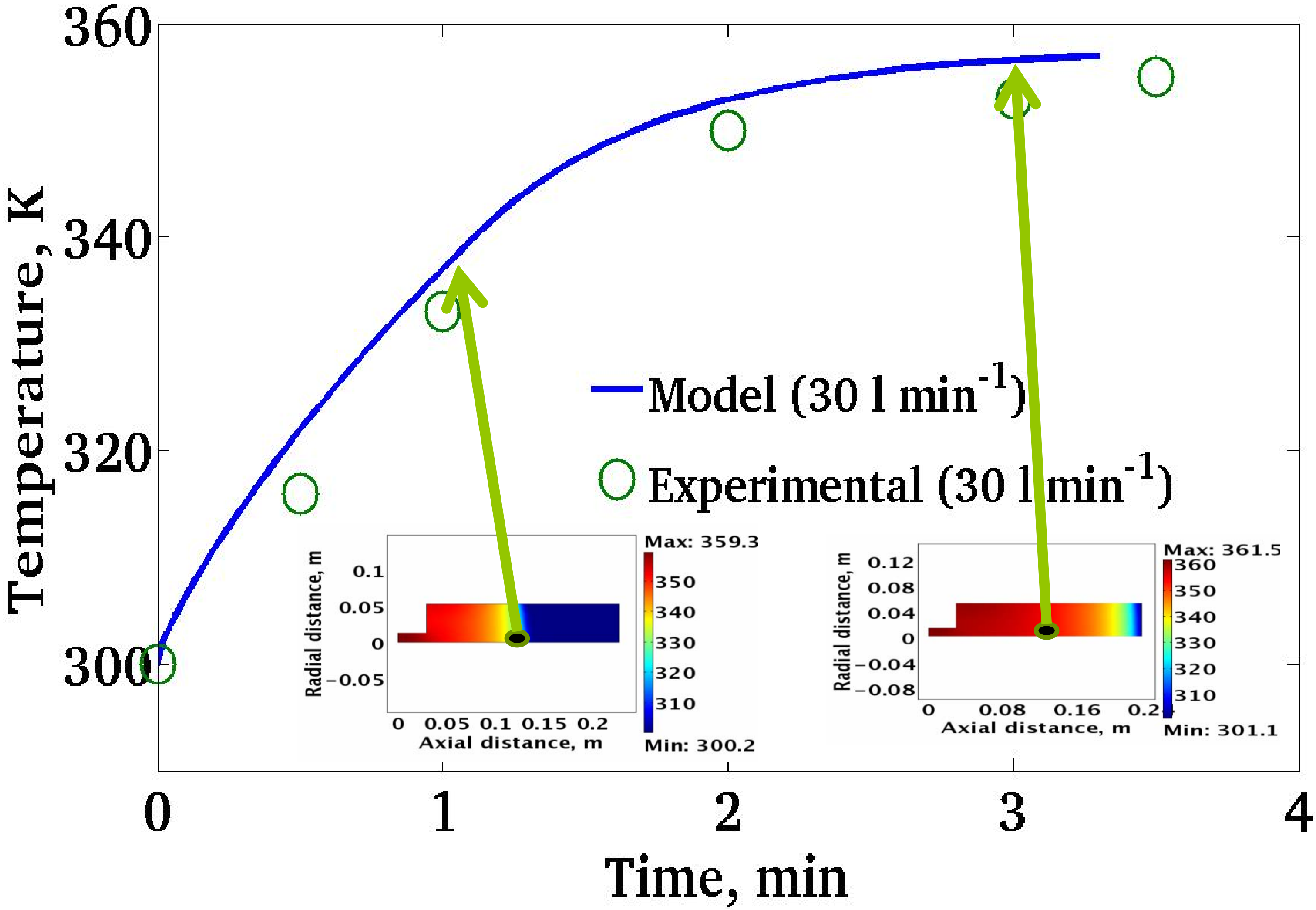
For boundaries at 3,4,5,6 and 7, wall with no slip boundary condition for flow equations and convective heat flux boundary condition for energy equation are used

At boundary 2, Heat flux inlet boundary condition for energy eqn and Velocity inlet for flow equation

symmetry boundary condition at boundary 1



Temperature Profile during charging @ 1.0 l /min



Temperature Profile during charging @ 30.0 *l* /min

Adsorption data at controlled flow rates

Q (*l* min^{-1})	**ΔT_{max}**	**V_f (*l*)**	$\frac{V_f}{V_{bed}}$ **(V/V)**	**t_f (min)**
1.0	21	120.0	65.9	120.0
30.0	58	99.0	54.4	3.3

Conclusion

- At high charging rates (30.0 / min^{-1}), although filling time is about 3.3 min (within practically feasible range), the reduction of storage capacity is about 17.5% compared to that of low charging rates (1.0 / min^{-1}).
- The large temperature increase of about 58^{0} compared to that of low charging rates (1.0 / min^{-1}) makes the system inefficient.
- The longer filling time of 2.0 hours with charging rate of 1.0 / min^{-1} also makes the system impractical.
- The model that has been reported in this work can be used to optimize the condition for gas storage applications.

Thank You